

Chemical Process Dynamics and Controls

Book II

(Chapters 10-14)

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Chapter 10. Dynamical Systems Analysis

Section 1. Finding fixed points in ODEs and Boolean models

Title: Finding Fixed Points in ODEs and Boolean Models

Note:  [Video lecture](#) available for this section!

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Date Presented: October 24, 2006, Revised: October 22, 2007

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

1.1 Introduction

Engineers can gain a better understanding of real world scenarios by using various modeling techniques to explain a system's behavior. Two of these techniques are ODE modeling and Boolean modeling. An important feature of an accurate ODE model is its fixed point solutions. A fixed point indicates where a steady state condition or equilibrium is reached. After locating these fixed points in a system, the stability of each fixed point can be determined (see subsequent Wikis). This stability information enables engineers to ascertain how the system is functioning and its responses to future conditions. It also gives information on how the process should be controlled and helps them to choose the type of control that will work best in achieving this.

1.2 Concept Behind Finding Fixed Point

A fixed point is a special system condition where the measured variables or outputs do not change with time. In chemical engineering, we call this a steady state. Fixed points can be either stable or unstable. If disturbances are introduced to a system at steady state, two different results may occur:

1. the system goes back to those original conditions (stable point)
2. the system deviates from those conditions rapidly (unstable point)

Subsequent wiki articles will discuss these different types of fixed points in more detail. The focus of this article will be simply finding fixed points, not classifying them. We will discuss several methods of finding fixed points, depending on the type of model employed.

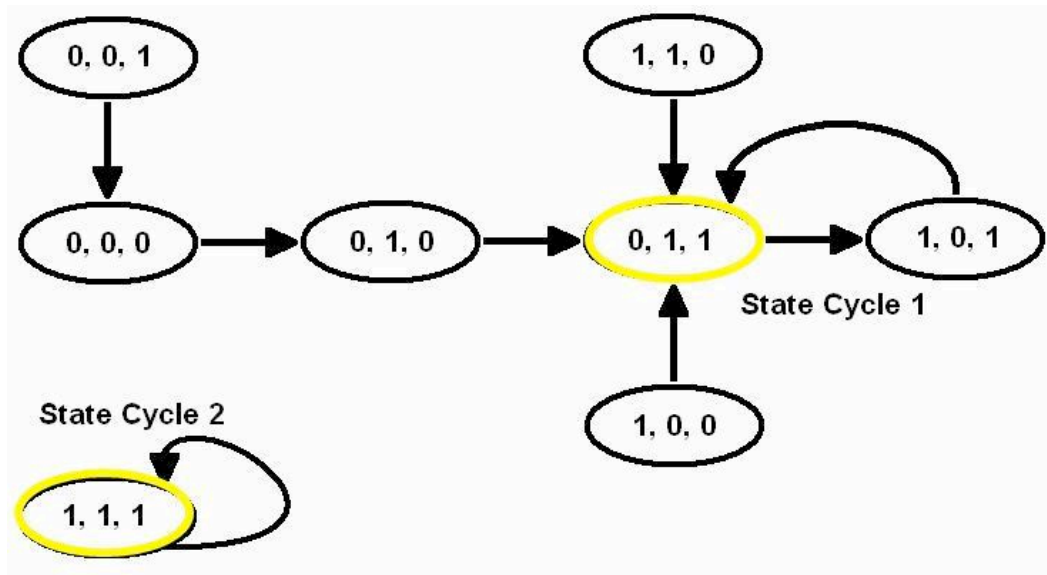
1.2.1 ODE Model

When a process or system is modeled by an ODE or a set of ODEs, the fixed points can be found using various mathematical techniques, from basic hand calculations to advanced mathematical computer programs. Independent of the method used, the basic principle remains the same: **The ODE or set of ODEs are set to zero and the independent variables are solved for.** At the points where the differential equations equal zero there is no change occurring. Thus, the solutions found by setting the ODEs equal to zero represent the numerical values of independent variables (i.e. temperature, pressure, concentration) at steady state conditions. If a single ODE or set of ODEs becomes too complicated to be solved by hand, a mathematical program such as Mathematica can be used to find fixed points. The latter part of this article focuses on how to use Mathematica to find fixed points of complicated systems of ODEs.

Note that in some cases there may not be an analytical method to find a fixed point. This case commonly occurs when the solution to a fixed point involves a high degree polynomial or another mathematical function that does not have an analytical inverse. In these cases, we can still find fixed points numerically if we have the parameters.

1.2.2 Boolean Model

A Boolean Model, as explained in “Boolean Models,” consists of a series of variables with two states: True (1) or False (0). A fixed point in a Boolean model is a condition or set of conditions to which the modeled system converges. This is more clearly seen by drawing state transition diagrams.



State Transition Diagram from [BooleanModels](#)

From the state transition diagram above, we can see that there are two fixed points in this system: 0,1,1 and 1,1,1. Starting in any state on the diagram and following the arrows, one of these two states will be reached eventually, indicating that the system tends to achieve either of these sets of operating conditions. If slight disturbances are introduced to the system while it is operating at one of these sets of conditions, it will return to 0,1,1 or 1,1,1. Also noted in the state transition diagram are state cycles. The difference between a state cycle and a fixed point is that a state cycle refers to the entire set of Boolean functions and transition points leading to the steady-state conditions, whereas a fixed point merely refers to the one point in a state cycle where steady-state conditions are reached (such points are indicated by a yellow circle in the diagram).

1.3 Finding Fixed Points: Four Possible Cases

There are four possible scenarios when finding the fixed points of an ODE or system of ODEs:

- 1.) One fixed point
- 2.) Multiple fixed points
- 3.) Infinite fixed points
- 4.) No fixed points

1.3.1 One Fixed Point

The first type of ODE has only one fixed point. An example of such an ODE is found in the Modeling of a Distillation Column [\[1\]](#). An ODE is used to model the energy balance in the nth stage of the distillation column:

$$\frac{dT_n}{dt} = \frac{1}{M_W} [L_{n-1}x_{n-1} - Wx_W] [T_{n-1} - T_n] + \frac{q_r}{M_W c_p}$$

Which can also be written as:

$$\frac{dT_n}{dt} = \frac{1}{M_W} [L_{n-1}x_{n-1} - Wx_W] [T_{n-1}] + \frac{q_r}{M_W c_p} + \frac{1}{M_W} [L_{n-1}x_{n-1} - Wx_W] T_n$$

If initial conditions i.e. $T_{n-1}, L_{n-1}, x_{n-1}$ are known, the equation above reduces to:

$$\frac{dT_n}{dt} = a + bT_n$$

Where a and b are constants since all the variables are now known.

$$a = \frac{1}{M_W} [L_{n-1}x_{n-1} - Wx_W] [T_{n-1}] + \frac{q_r}{M_W c_p}$$

$$b = \frac{-1}{M_W} [L_{n-1}x_{n-1} - Wx_W]$$

By analyzing the equation $\frac{dT_n}{dt} = 0 = a + bT_n$, we can immediately

deduce that at steady state $T_n = -\frac{a}{b}$. Clearly, there is only one fixed point in this system, only one temperature of the distillation column which will be at steady-state conditions. We can use Mathematica to solve for the fixed point of this system and check our results. In Mathematica, the `Solve[]` function can be used to solve complicated equations and systems of complicated equations. There are some simple formatting rules that should be followed while using Mathematica:

1. Type your equation and let the differential be called an arbitrary variable (e.g. `T[t]`)
2. Type `Solve[T[t]==0,T]` and hit Shift+Enter
3. This produces an output contained inside curly brackets

Please read the [Solving ODEs with Mathematica](#) section for more information on syntax and functions.

A sample of how the format in Mathematica looks like is shown below:

```
In[36]:= T[t] = a + b * T
         Solve[T[t] == 0, T]

Out[36]= a + b T

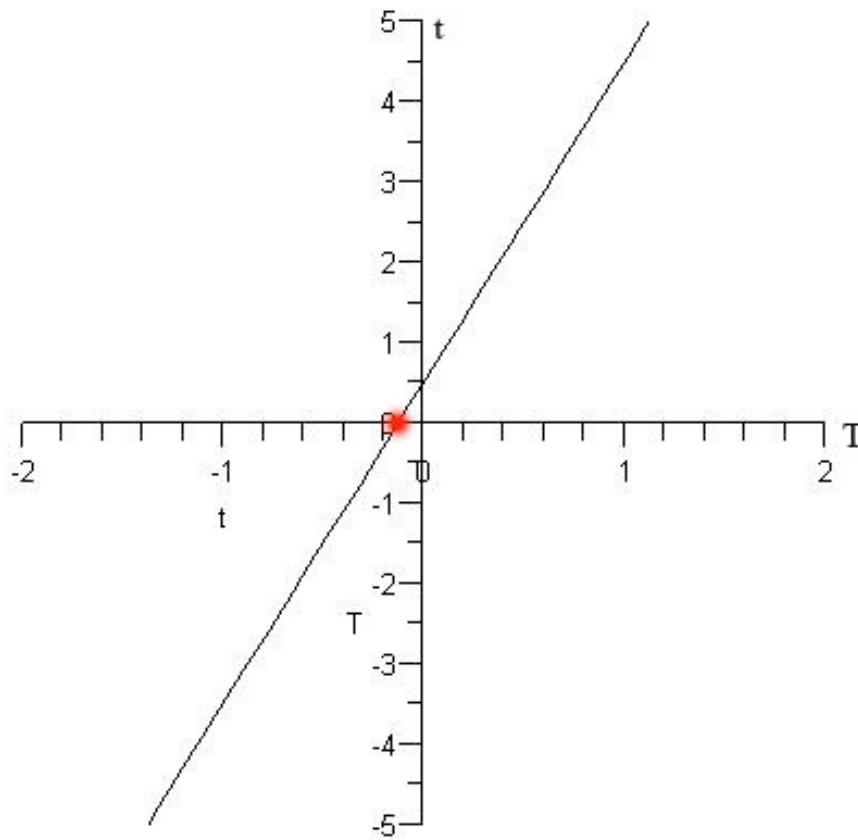
Out[37]= {{T -> -a/b}}
```

Maple can be used to visualize a single fixed point. Wherever the plot intersects the x-axis represents a fixed point, because the ODE is equal to zero at that point.

The following Maple syntax was used to plot the ODE: `plot(0.5+4t, t=-2..2,T=0..5,color=black);`

The constant $a = 0.5$ and the constant $b = 4$ in the above example.

The resulting graph is below, the red point indicates at what T a fixed point occurs:



Solving a single fixed point for an ODE and a controller in Mathematica

1. Identify what type of controller it is (P, I , PI, or PID etc.)
2. Identify your ODE equations (Is the controller a function of the ODE?)

Example: Solve for the fixed points given the three differential equations and the two controllers (u1 and u2).

$$\begin{aligned} \frac{dH}{dt} &= (1/A)(F_{in} - F_{out}) \\ \frac{dF_{in}}{dt} &= K_{(v1)}(u_1) \\ \frac{dF_{out}}{dt} &= K_{(v2)}(u_2)H \end{aligned}$$

Where H is the level in the tank, F_{in} is the flow in, F_{out} the flow out, and u_1 and u_2 are the signals to the valves v_1 and v_2 . K_{v1} and K_{v2} are valve gains (assumed to be linear in this case, although this does not have to be). Note that the exit flow also depends on the depth of fluid in the tank.

You next parameterize your model from experimental data to find values for the constants:

$A=2.5$ meters squared

$K_{v1}=0.046$ meters cubed/(minute mA)

$K_{v2}=0.017$ meters squared/(minute mA)

Next you want to add:

- A full PID controller to regulate F_{out} via FC1 connected to v_2 .
- A P-only controller to regulate H via LC1 connected to v_1 .

For this system you want to maintain the tank level at 3 meters and the exit flow (F_{set}) at 0.4 m³ /minute. The following Mathematica code should look as follows:

```

u1 = offset1 + Kc1 * (3 - H[t]);
u2 = offset2 + Kc2 * (0.4 - Fout[t]) + (1 / tauI) * X[t] + tauD * (-Fout'[t]);
eqns = {X'[t] == 0.4 - Fout[t], H'[t] == (1 / A) * (Fin[t] - Fout[t]), Fin'[t] == Kv1 * u1,
  Fout'[t] == Kv2 * u2 * H[t], H[0] == 0, Fin[0] == 0, Fout[0] == 0, X[0] == 0};
param = {Kv1 -> 0.046, Kv2 -> 0.017, A -> 2.5};
sol = Solve[eqns /. param /. {H'[t] -> 0, Fin'[t] -> 0, Fout'[t] -> 0, X'[t] -> 0},
  {H[t], Fin[t], Fout[t], X[t]}]
{{Fin[t] -> 0.4, X[t] -> ((-3. Kc1 - 1. offset1) offset2 tauI) / (3. Kc1 - offset1), Fout[t] -> 0.4, H[t] -> (3. Kc1 + offset1) / Kc1}}

```

1.3.2 Multiple Fixed Points

Multiple fixed points for an ODE or system of ODEs indicate that several steady states exist for a process, which is a fairly common situation in reactor kinetics and other applications. When multiple fixed points exist, the optimal steady-state conditions are chosen based on the fixed point's stability and the desired operating conditions of the system.

The following is an example of a system of ODEs with multiple fixed points:

$$\frac{dC_A}{dt} = 14C_A - 2C_A^2 - C_A C_B$$

$$\frac{dC_B}{dt} = 16C_B - 2C_B^2 - C_A C_B$$

The above system of ODEs can be entered into Mathematica with the following syntax:

```

Multiple_Fixed_Point.nb *
In[9]:= CA'[t] = 14 CA - 2 CA^2 - CA * CB
        CB'[t] = 16 CB - 2 CB^2 - CA * CB
        Solve[{CA'[t] == 0, CB'[t] == 0}, {CA, CB}]

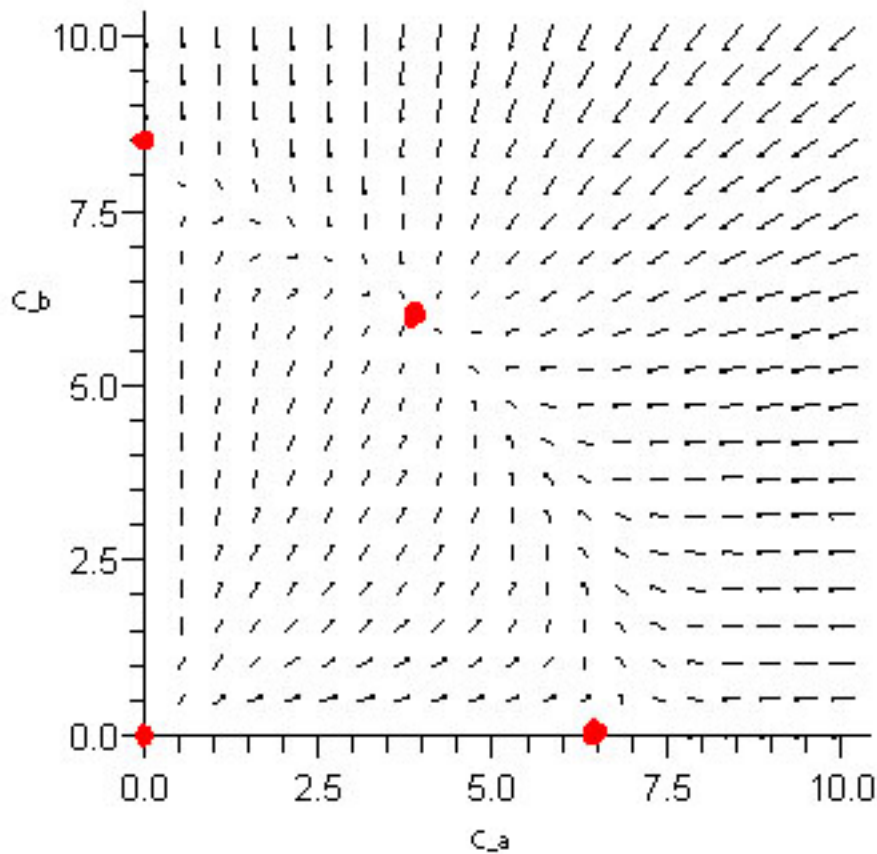
Out[9]= 14 CA - 2 CA^2 - CA CB
Out[10]= 16 CB - CA CB - 2 CB^2
Out[11]= {{CA -> 0, CB -> 0}, {CA -> 0, CB -> 8},
          {CA -> 4, CB -> 6}, {CA -> 7, CB -> 0}}
  
```

This system in particular has four fixed points. Maple can be used to visualize the fixed points by using the following syntax:

with(plots):

*fieldplot([14*x-2*x^2-x*y,16*y-2*y^2-x*y],x=0..10,y=0..10,fieldstrength=log);*

The first line initializes the plotting package within Maple that allows for plotting vector fields. The second line uses the command “fieldplot” and inputs the two ODEs that make up the system. The scales of the x and y-axis are set to range from 0 to 10. The fieldstrength command is mainly used for visual purposes, so that the direction of the arrows becomes more apparent. Below is the resulting plot:



The red dots indicate the fixed points of the system. On the plot, these points are where all the surrounding arrows converge or diverge. Converging arrows indicate a stable fixed point, in this example the point at (4,6) is a stable fixed point. Diverging arrows indicate an unstable fixed point, in this example (0,0), (0,8) and (7,0) are unstable fixed points.

1.3.3 Infinite Fixed Points

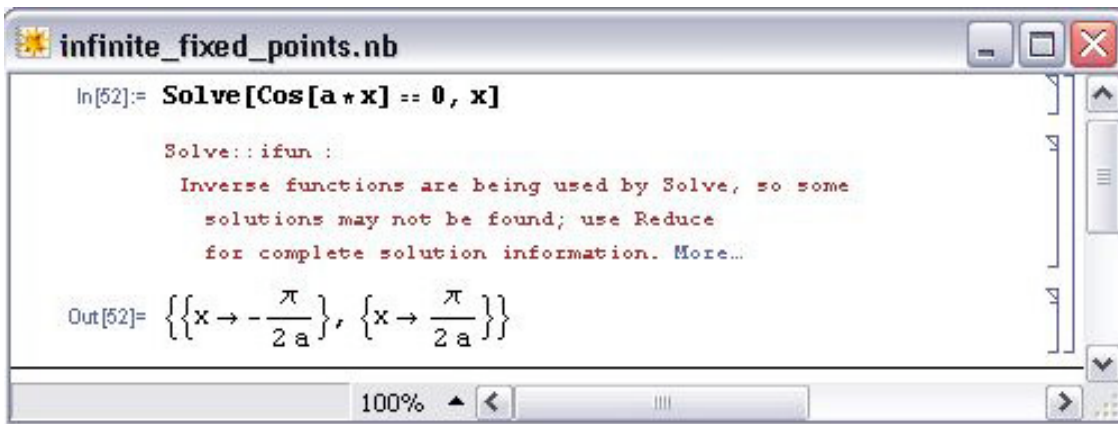
An example of an ODE with infinite fixed points is an oscillating ODE such as:

$$\frac{dy}{dx} = \cos(ax)$$

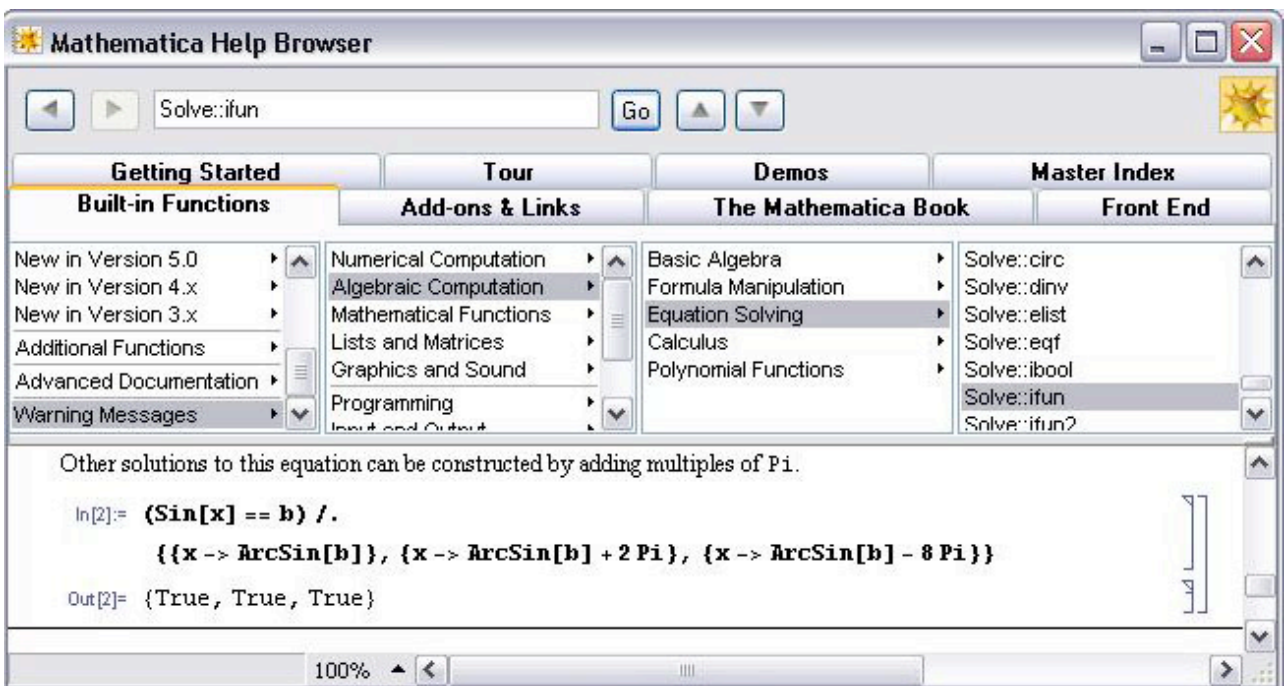
where a is a constant.

Using Mathematica to solve for the fixed points by setting

$$\frac{dy}{dx} = 0 = \cos(ax)$$



If you click the "More" link on Mathematica it will basically state that there are other solutions possible according to the Help section shown below:

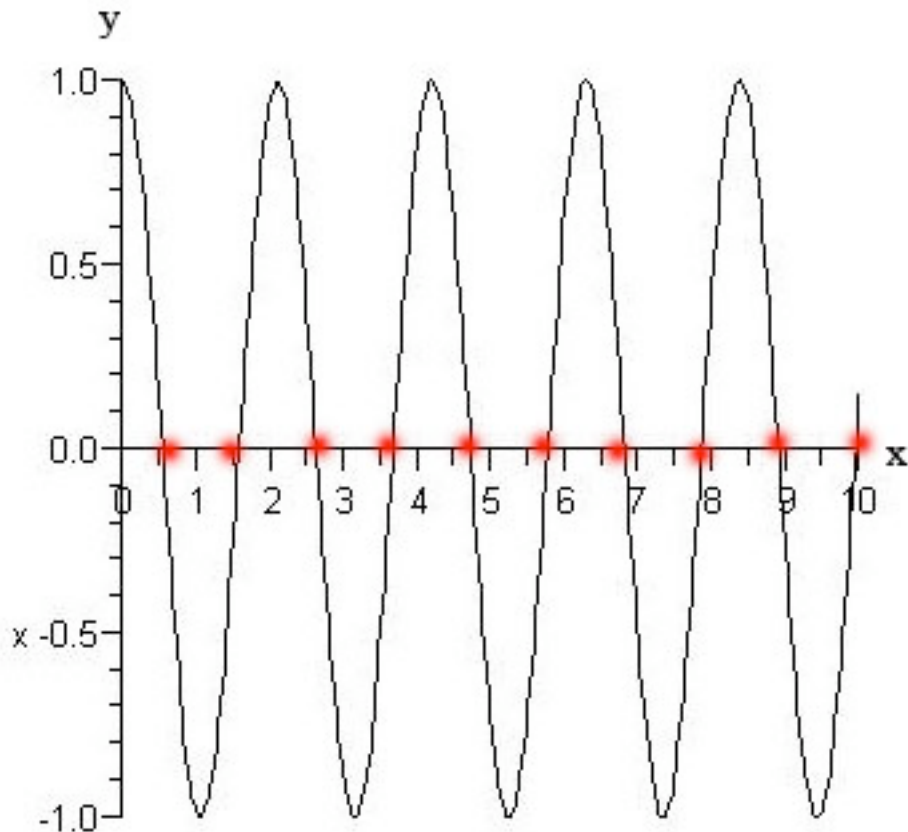


The Maple syntax used to graph the solved differential equation is:

```
plot(cos(3t),t=0..10,T=-1..1,color=black);
```

The constant $a = 3$ in this case.

The infinite fixed points can be seen in the graph below, where anytime the function crosses the x axis, we have a fixed point:



1.3.4 No Fixed Points

The fourth type of ODE does not contain fixed points. This occurs when a certain variable (such as temperature or pressure) has no effect on a system regardless of how it changes. Generally, systems with this sort of behavior should be avoided because they are difficult to control as they are always changing.

This can be modeled by vertical or horizontal lines due to the fact that no fixed points are found by setting the line equal to zero. An ODE is used to model a line held constant at a:

$$\frac{dT}{dt} = a$$

Where, a can be any constant except 0.

Intuitively, trying to find a fixed point in this system is not possible, because a constant such as 3 can never equal zero. Solving this ODE is not possible even by analyzing the system. Therefore, when inputting this into Mathematica, it yields $\{\}$. The notation $\{\}$ means that there are no fixed points within the system. The image below is how Mathematica solves the ODE.

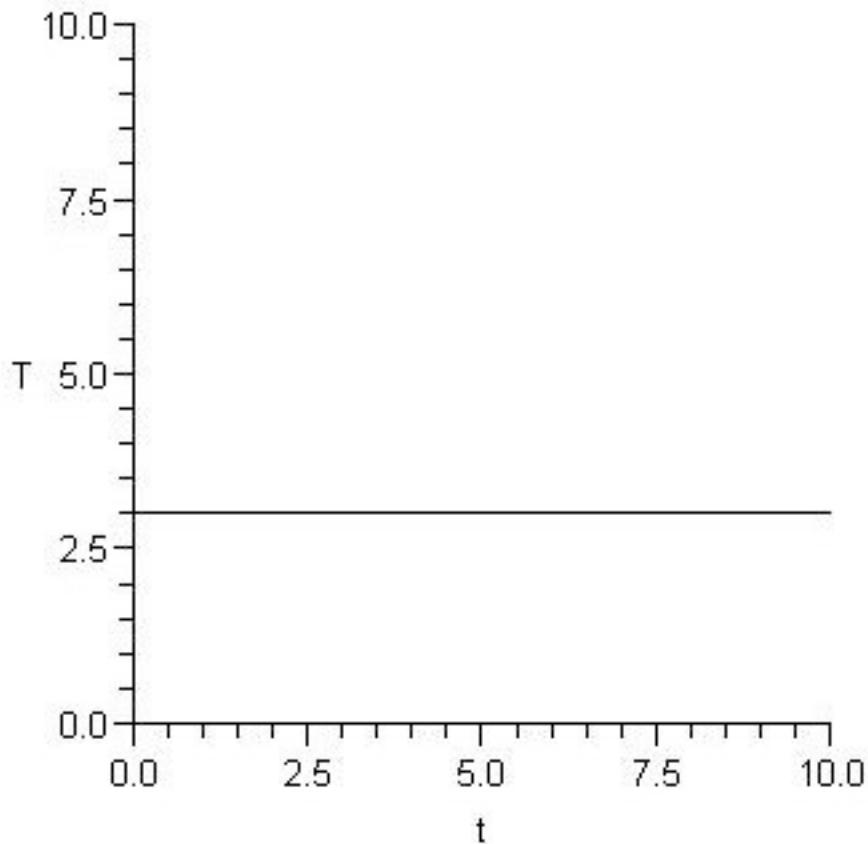


By using Maple (version 10), one can visually see a lack of fixed points by using the following syntax:

```
plot(3, t = 0..10, T = 0..10, color = black);
```

The constant $a = 3$ in the above case.

This image shows that the line is horizontal and never crosses the x axis, indicating a lack of fixed points.



1.4 Summary

A fixed point is a system condition where the measured variables or outputs do not change with time. These points can be stable or unstable; refer to [Using Eigenvalues to evaluate stability](#) for an introduction to a common method for determining stability of fixed points.

There are four possible cases when determining fixed points for a system described by ODEs:

- One fixed point
- Multiple fixed points
- Infinite fixed points
- No fixed points

There are methods described above for using Mathematica or Maple to solve for the fixed points in each case. Fixed points can also be determined for a Boolean model.

Knowing the fixed points of a system is very important when designing a control architecture for the system. These are the operating conditions that the system will exhibit

at steady-state. Controllers can have influence on the fixed points, so a thorough analysis of fixed points using equations describing the system and the controllers should be conducted before implementation of the control scheme.

1.5 Worked out Example 1: Manipulating a System of Equations

Recall the example system of ODEs used in the Multiple Fixed Points Section:

$$\begin{aligned}\frac{dC_A}{dt} &= 14C_A - 2C_A^2 - mC_AC_B \\ \frac{dC_B}{dt} &= 16C_B - 2C_B^2 - nC_AC_B\end{aligned}$$

Find how the fixed points change when $m = 2$ and $n = 3$.

SOLUTION

```

Example 1.nb *
In[12]:= CA'[t] = 14 CA - 2 CA^2 - 2 CA * CB
          CB'[t] = 16 CB - 2 CB^2 - 3 CA * CB
          Solve[{CA'[t] == 0, CB'[t] == 0}, {CA, CB}]

Out[12]= 14 CA - 2 CA^2 - 2 CA CB

Out[13]= 16 CB - 3 CA CB - 2 CB^2

Out[14]= {{CA -> 0, CB -> 0}, {CA -> 0, CB -> 8},
          {CA -> 2, CB -> 5}, {CA -> 7, CB -> 0}}
  
```

1.6 Worked out Example 2: System of ODEs

You are asked to estimate the fixed point(s) of a heat exchanger in your plant. The fixed points correspond to the temperatures of your tube-side (hot) and shell-side (cold) fluids respectively, $T_{1,out}$ and $T_{s,out}$. Neglect heat loss to the surrounding area i.e.

$$hA(T_s - T_\infty) = 0$$

Given the two main ODEs used to model a heat exchanger, use Mathematica to solve for the fixed points of the system in terms of the known variables.

$$m c_p \frac{dT_{t,out}}{dt} = \rho c_p F_{t,in} T_{t,in} - \rho c_p F_{t,out} T_{t,out} - \frac{kA}{\Delta z} (T_{t,out} - T_{s,out})$$

(equation 1)

$$m c_p \frac{dT_{s,out}}{dt} = \rho c_p F_{s,in} T_{s,in} - \rho c_p F_{s,out} T_{s,out} - \frac{kA}{\Delta z} (T_{s,out} - T_{t,out}) - hA(T_s - T_\infty)$$

(equation 2)

The values for m , c_p , Q , $F_{t,in}$, $F_{t,out}$, k , A , δz , and $T_{t,in}$, $F_{s,in}$, $F_{s,out}$, $T_{s,in}$ are given and fixed.

Please refer to the Wiki article on [HeatExchangeModel](#) for detailed explanation on the meaning of the variables and the derivation of the ODEs above.

Hint: Lump up all known variables under one general variable

SOLUTION

Simplify the 2 equations to the ODEs below:

$$\frac{dT_{t,out}}{dt} = a - bT_{t,out} - c(T_{t,out} - T_{s,out})$$

(equation 1a)

$$\frac{dT_{s,out}}{dt} = d - eT_{s,out} - f(T_{s,out} - T_{t,out})$$

(equation 2a)

where

$$a = \frac{\rho F_{t,in} T_{t,in}}{m}, \quad b = \frac{-\rho F_{t,out}}{m}, \quad c = \frac{kA}{\Delta z m c_p} \text{ and}$$

$$d = \frac{\rho F_{s,in} T_{s,in}}{m}, \quad e = \frac{\rho F_{s,out}}{m}, \quad f = \frac{kA}{\Delta z m c_p}$$

Type these equation into Mathematica using the appropriate syntax and use the Solve[] function to find the fixed points.

```

example2.nb
In[3]:= DTt[t] = a - b*Tt[t] - c*(Tt[t] - Ts[t])
        DTs[t] = d - e*Ts[t] - f*(Ts[t] - Tt[t])
        Solve[{DTt[t] == 0, DTs[t] == 0}, {Tt[t], Ts[t]}]

Out[3]= a - bTt[t] - c(-Ts[t] + Tt[t])

Out[4]= d - eTs[t] - f(Ts[t] - Tt[t])

Out[5]= {{Tt[t] -> -(-cd - ae - af)/(be + ce + bf), Ts[t] -> -(-bd - cd - af)/(be + ce + bf)}}

```

We have found our fixed point. Just plug in the variables as defined earlier for a, b, c, d, e, f and you will obtain the temperatures in terms of the useful parameters.

1.7 Multiple Choice Question 1

The solutions found by setting the ODE equal to zero represent:

- a) independent variables not at steady state conditions
- b) dependent variables not at steady state conditions
- c) independent variables at steady state conditions
- d) dependent variables at steady state conditions

Answer: C

1.8 Multiple Choice Question 2

How many fixed points are there when the following equation is solved by Mathematica?

$$\frac{dT}{dt} = 8t - 4t^2 - t^3$$

- a) none
- b) 1
- c) 2

d) 3

Answer: D

1.9 Sage's Corner

Stability of Fixed Points


<http://video.google.com/googleplayer.swf?docId=-5690380917022362654>

[slides for this talk](#)

1.10 References

- Edwards H., Penney D.(2003), *Differential Equations: Computing and Modeling*, Third Edition. Prentice-Hall. [ISBN 0130673374](#)
- Strogatz, Steven H.(2001), *Nonlinear Dynamic and Chaos: With Applications to Physics, Biology, Chemistry, and Engineering*, 1st Edition. Addison-Wesley. [ISBN 0738204536](#)

Section 2. Linearizing ODEs

Note:  [Video lecture](#) available for this section!

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Date Presented: October 24, 2006; Revised: October 22, 2007

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

2.1 Introduction

Chemical engineering processes often operate in nonlinear and unsteady manners (i.e. not always at steady state), and are generally governed by nonlinear ordinary differential equations (ODEs). The ODE is a relation that contains functions of only one independent variable and derivatives with respect to that variable. Many studies have been devoted to developing solutions to these equations, and in cases where the ODE is linear it can be solved easily using an analytical method. However, if the ODE is nonlinear and not all of the operating parameters are available, it is frequently difficult or impossible to solve equations directly. Even when all the parameters are known, powerful computational and mathematical tools are needed to completely solve the ODEs in order to model the process. In order to simplify this modeling procedure and obtain approximate functions to describe the process, engineers often linearize the ODEs and employ matrix math to solve the linearized equations.

A linear equation is an equation in which each term is either a constant or the product of a constant times the first power of a variable. These equations are called "linear" because they represent straight lines in Cartesian coordinates. A common form of a linear equation in the two variables x and y is $y = mx + b$. This is opposed to a nonlinear equation, such as $m = e^x + x^2 + 2x + 5$. Even though $2x + 5$ is a linear portion of the equation, e^x and x^2 are not. Any nonlinear terms in an equation makes the whole system nonlinear.

Non-linear system of equations:

$$\frac{dA}{dt} = 3A^2 + 2B + C - 7D^3$$

$$\frac{dB}{dt} = A + C^2 + 2D$$

$$\frac{dC}{dt} = A + 4B^2 - C^2$$

$$\frac{dD}{dt} = 2C - D$$

After linearization (around the steady state point $\{-0.47, -0.35, 0.11, 0.23\}$):

$$\begin{pmatrix} A' \\ B' \\ C' \\ D' \end{pmatrix} = \begin{pmatrix} -2.83 & 2 & 1 & 0 \\ 1 & 0 & 0.23 & 0 \\ 1 & -2.78 & -0.23 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} + \begin{pmatrix} k_1 \\ k_2 \\ k_3 \\ k_4 \end{pmatrix}$$

Note that each equation is comprised solely of first order variables.

Even though it is unlikely that the chemical engineering process to be modeled operates in a linear manner, all systems can be approximated as linear at a point. This is preferred as linear systems are much easier to work with than nonlinear equations. Although linearization is not an exact solution to ODEs, it does allow engineers to observe the behavior of a process. For example, linearized ODEs are often used to indicate exactly how far from steady state a given process deviates over specified operating ranges. This wiki page discusses how to solve a linearized ODE by hand and by using Mathematica, and proceeds to work out several examples of linearized ODEs commonly seen in chemical engineering practice.

2.2 Applications to Chemical Engineering

As mentioned above, linearizing ODEs allows engineers to understand the behavior of their system at a given point. This is very important because many ODEs are impossible to solve analytically. It will also lead to determining the local stability of that point. Most of the time a system will be linearized around steady state, but this is not always the case. You may be interested in understanding the behavior of your system at its operating point or equilibrium state (not necessarily steady state). The linearization approach can be used for any type of nonlinear system; however, as a chemical engineer, linearizing will

usually involve ODEs. Chemical engineers use ODEs in applications such as CSTRs, heat exchangers, or biological cell growth.

It is also important to understand the advantages and disadvantages of linearizing a system of ODEs:

2.2.1 Advantages

- Provides a simpler, more convenient way to solve the ODEs
- The behavior of a process can be observed
- Any type or order of ODE can be used

2.2.2 Disadvantages

- The solution is only an exact solution at the chosen point; otherwise it is an approximation and becomes less accurate away from the point
- Although linearizing is a quicker alternative, it takes time to initially learn the process (ex: using Mathematica)

Another use for linearization of the equations that govern chemical processes is to determine the stability and characteristics of the steady states. Systems of linearized ODEs can be used to do this, and the methods of doing so can be found in [Fixed Points, Eigenvectors and Eigenvalues](#), and [Using eigenvalues and eigenvectors to find stability and solve ODEs](#)

2.3 General Procedure for Linearization

Linearization is the process in which a nonlinear system is converted into a simpler linear system. This is performed due to the fact that linear systems are typically easier to work with than nonlinear systems. For this course, the linearization process can be performed using Mathematica. The specific instructions on how to do this can be found below.

1. Choose a relevant point for linear approximation, two options available are:

- Steady state- points where system does not change
- Current location- given where you are now

2. Calculate the Jacobian matrix at that point. The Jacobian is essentially a Taylor series expansion.

3. Solve to find unknown constants using algebraic methods.

2.4 Linearization by Hand

In order to linearize an ordinary differential equation (ODE), the following procedure can be employed. A simple differential equation is used to demonstrate how to implement

this procedure, but it should be noted that any type or order of ODE can be linearized using this procedure.

1. Use a Taylor series expansion (truncating after the linear terms) to approximate the right-hand side of the ODE.

$$\frac{dx}{dt} = f(x) = 3x^2$$

Let's say we start with the following ODE: $\frac{dx}{dt} = f(x) = 3x^2$. This ODE describes the behavior of some variable, x , with respect to time.

A Taylor series is a series expansion of a function about a point. If $x = a$, an expansion of a real function is given by:

$$f(x) = \sum_{n=0}^{\infty} \frac{f^n(a)}{n!} (x - a)^n$$

$$f(x) = f(a) + f'(a)(x-a) + \frac{f^2(a)}{2!}(x-a)^2 + \frac{f^3(a)}{3!}(x-a)^3 + \dots + \frac{f^n(a)}{n!}(x-a)^n + \dots$$

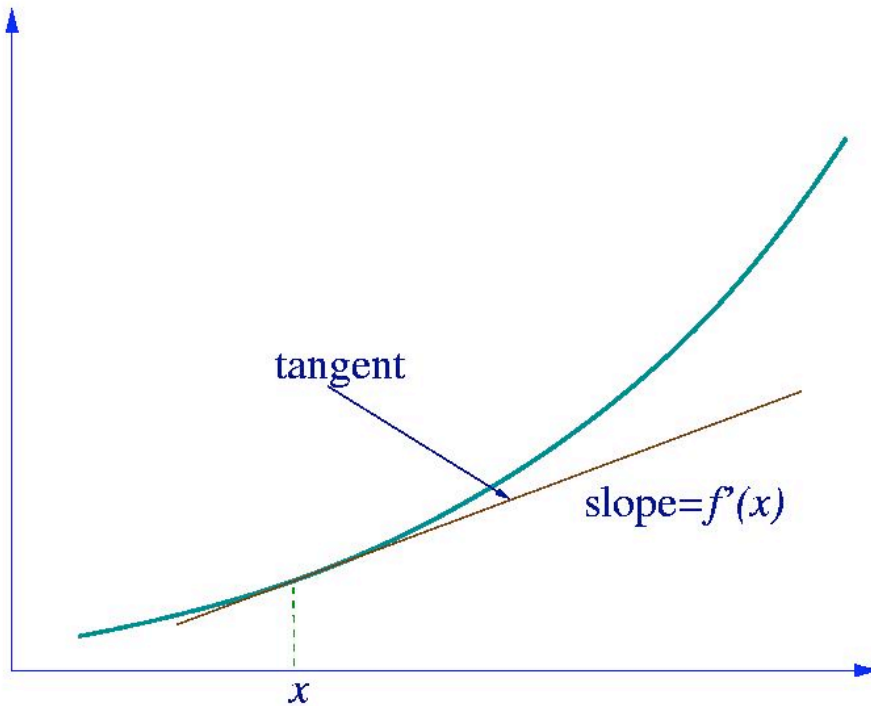
When $x=0$, the function is also known as Maclaurin series. Taylor's theorem states that any function satisfying certain conditions can be expressed as a Taylor series.

For simplicity's sake, only the first two terms (the zero- and first-order) terms of this series are used in Taylor approximations for linearizing ODEs. Additionally, this truncation (ie. "chopping" off the $n=2$ and higher terms from the polynomial shown above) assures that the Taylor Series is a linear polynomial. If more terms are used, the polynomial would have $(x - a)^2$ and higher order terms and become a nonlinear equation. The variable 'a' in the Taylor series is the point chosen to linearize the function around. Because it is desired that most processes run at steady state, this point will be the steady state point. So, our differential equation can be approximated as:

$$\frac{dx}{dt} = f(x) \approx f(a) + f'(a)(x - a) = f(a) + 6a(x - a)$$

Since a is our steady state point, $f(a)$ should always be equal to zero, and this simplifies our expression further down to:

$$\frac{dx}{dt} = f(x) \approx f'(a)(x - a) = 6a(x - a)$$



The graph shown above shows the approximation of $f(x)$ at $(x, f(x))$. As mentioned previously, linearization is only an approximation for any given function near a continuous point. When working with a system of ODEs, the Jacobian is written as a matrix. It is the matrix of constants needed to describe a system's linearity. The Jacobian may be thought of as how much a system is distorted to take on a linear identity. A jacobian matrix will always be a square (#rows = #columns) and it shows how each equation varies with each variable. The Jacobian matrix is defined as:

$$J(x_1, \dots, x_n) = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \dots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_n}{\partial x_1} & \dots & \frac{\partial y_n}{\partial x_n} \end{bmatrix}$$

And is used as such:

Nonlinear system

$$\frac{dx}{dt} = 2x^3 + \cos(5y) - 12 \arctan(z - 3)$$

$$\frac{dy}{dt} = 7y^3 + \sin(5x)$$

$$\frac{dz}{dt} = 1.3 \log(x + y)$$

Linearized system

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} J_1 & J_2 & J_3 \\ J_4 & J_5 & J_6 \\ J_7 & J_8 & J_9 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}$$

Jacobian matrix

Example

Lets say you have the following set of equations and you want to find its jacobian matrix around the point A=3,B=2.

$$\frac{dA}{dt} = 3A - A^2 - AB$$
$$\frac{dB}{dt} = 6B - AB - 2B^2$$

We find the jacobian by taking the derivative of each equation with respect to each variable.

$$\frac{d(3A - A^2 - AB)}{dA} = 3 - 2A - B, \quad \frac{d(3A - A^2 - AB)}{dB} = -A$$
$$\frac{d(6B - AB - 2B^2)}{dA} = -B, \quad \frac{d(6B - AB - 2B^2)}{dB} = 6 - A - 4B$$

These are the equations in the matrix. The values of the variables from whatever point we are linearizing are then put into these equations and calculated out to get the Jacobian.

$$Jac = \begin{bmatrix} 3 - 2A - B & -A \\ -B & 6 - A - 4B \end{bmatrix} \quad A = 4, B = 2$$

$$Jac = \begin{bmatrix} -7 & -4 \\ -2 & -6 \end{bmatrix}$$

2. Change the approximation by linearizing around a steady state point in order to describe how the process deviates from steady state.

The following substitution can be made:

$$\frac{dx}{dt} = \frac{d(x - a)}{dt}$$

$$\frac{d(x - a)}{dt} \approx 6a(x - a)$$

This substitution is allowed because 'a' is a constant, and the derivative of a constant is zero.

Substituting (x-a) for x signifies that our differential equation now shows how our function, x, deviates away from the steady state value, a, with respect to time. This deviation, (x-a), is commonly expressed as x'. It should also be noted that the quantity '6a' is a constant, and thus will be further recognized as 'A'.

Our final linearized equation becomes:

$$\frac{dx'}{dt} \approx Ax'$$

The once nonlinear ODE, $\frac{dx}{dt} = f(x) = 3x^2$, has now been simplified into a linear differential equation.

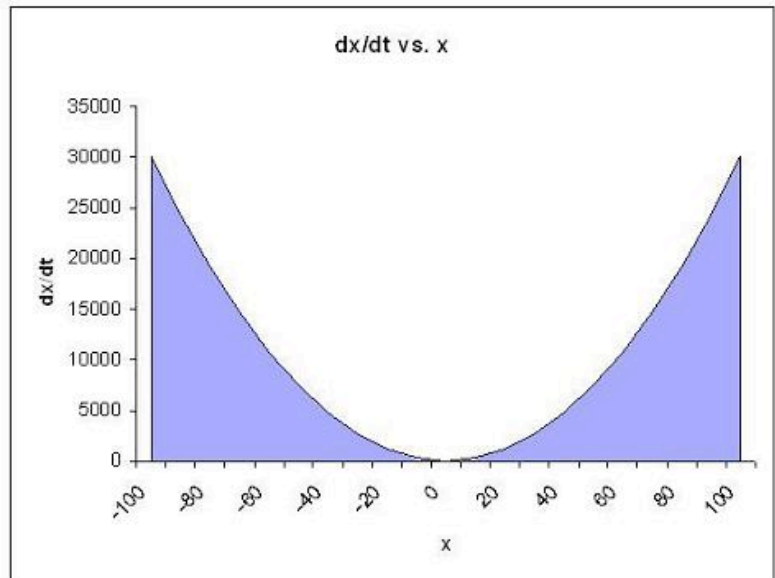
The procedure of linearization typically occurs around the steady state point or points of a specified process. Engineers anticipate a certain change in output for the particular steady state point, and may proceed to linearize around it to complete their approximation.

Please follow the graphic below for further detail. Note that a steady state point occurs when $dx / dt = 0$

Linearization for a Steady- State Point:

ODE: $dx/dt = 3x^2$

x	dx/dt	Linearization	Error
-100	30000	0	30000
-90	24300	0	24300
-80	19200	0	19200
-70	14700	0	14700
-60	10800	0	10800
-50	7500	0	7500
-40	4800	0	4800
-30	2700	0	2700
-20	1200	0	1200
-10	300	0	300
0	0	0	0
10	300	0	300
20	1200	0	1200
30	2700	0	2700
40	4800	0	4800
50	7500	0	7500
60	10800	0	10800
70	14700	0	14700
80	19200	0	19200
90	24300	0	24300
100	30000	0	30000



To Find the Steady- State Point: $d/dx [dx/dt] = d/dx [3x^2] = 6x = 0 @ x = 0$ & $dx/dt = 0$

To Linearize: $d(x-a)/dt = 6*a*(x-a) + C$ $C =$ Corrective Constant $a =$ point chosen on x axis to linearize around

$d(x-a)/dt = 6*a*(x-a) + C$

$dx/dt = 0 = 6*0*(x-0) + C$ Therefore, $C = 0$

$dx/dt = 0$

The area shaded in light blue indicates the error associated with this particular linearization. Extensive deviation from the steady- state point produces significant error.

As can be seen, moving farther away from the steady state point results in significantly larger deviation, and thus error (actual-linearization).

Occasionally, for very unique operating conditions, plant management may decide to momentarily run a process outside of strict steady state conditions (perhaps a unique start-up procedure, shut-down recovery, etc.). To reinforce the concept of linearization around an unsteady state point (arbitrarily chosen in this example), please consider the following visual representation. Note that $a=50$ and $C=7500$ in the first plot.

Differential Equation: $dx/dt = f(x) = 3x^2$

C is held constant at 7,500 for the first plot.

x	dx/dt	Linearization
-100	30000	-37500
-90	24300	-34500
-80	19200	-31500
-70	14700	-28500
-60	10800	-25500
-50	7500	-22500
-40	4800	-19500
-30	2700	-16500
-20	1200	-13500
-10	300	-10500
0	0	-7500
10	300	-4500
20	1200	-1500
30	2700	1500
40	4800	4500
50	7500	7500
60	10800	10500
70	14700	13500
80	19200	16500
90	24300	19500
100	30000	22500

Using the linearization:

$$d(x-a)/dt = 6*a(x-a) + C$$

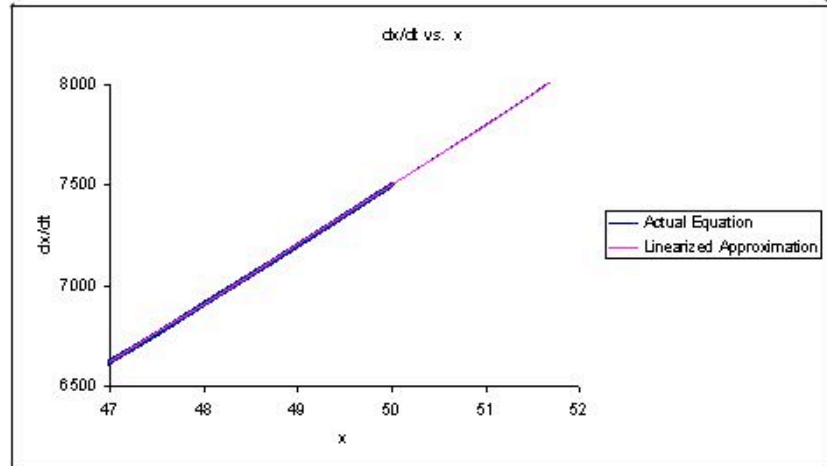
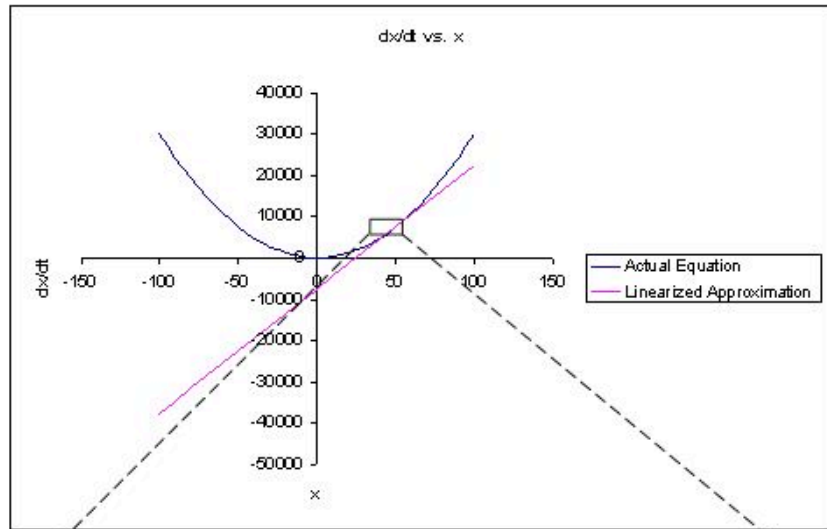
$$d(x-50)/dt = 6*50(x-50) + C$$

$$d(x-50)/dt = 300(x-50) + 15,000$$

x	d(x-50)/dt
47	6627
48	6912
49	7203
50	7500
51	7803
52	8112

$$6*50(x-50) + C = 3*(x)^2$$

x	C
47	7527
48	7512
49	7503
50	7500
51	7503
52	7512



The second plot is a magnification of a small section of the first plot. As one can readily notice, both the linear approximation and the actual graph overlap almost exactly over this small range. This illustrates how this particular linearization could be used to approximate this region of the function and can describe its behavior quite accurately. This approximating technique using the linearization of ODE can be performed around different points (different values of a) using the same method in order to model the behavior of the rest of the dx/dt vs x function. Note: frequent recalculation of the integration constant, C , permits for increased accuracy in approximation.

2.5 Example of a Simple Linearization Process in Use

Provided a circumstance in which developing a rigorous analytical solution is unfeasible due to time, access to computing resources, or mathematical ability, the linearization process offers a convenient and swift alternative.

An appropriate introduction to linearization application is featured in section 5.3 of the Bequette reading and has been described below.

The following model describes the behavior of tank height as a function of time (t), faced with a steady- state incoming liquid flowrate. dh/dt represents the change in height of the fluid contained within the tank as a function of time, h indicates the height (or level) or the fluid contained within the tank, F represents the magnitude of incoming flow. The following model describes the tank level/height fluctuation as function of both the current height (h) and flow (F). Fluid enters the tank as flow per area of the inlet(F/A), and leaves as a function of a corrective proportional term, β , also per area of the outlet, multiplied by the square root of the current height.

Instead of fluid leaving through this term, we may also consider it a form of feedback control, which subsequently reduces the amount of inlet fluid instead (depends on the application, the final result is identical). Therefore:

$$\frac{dh}{dt} = f(h, F) = \frac{F}{A} - \frac{\beta}{A} * \sqrt{h}$$

Important note about the relevance of the provided variables:

F_s indicates the initial flow rate for the described system and is important in calculating the intercept and subsequently the calculative corrective term for the linearization (if the linearization is not performed at steady-state, as in this example). h_s describes the tank height for the specified flow rate, F_s . Upon plugging in the value of h_s into the linearized formula, you will notice that $f(h, F_s) = 0$, the point on the plot where both the linearization and the characteristic equation coincide (i.e. are tangent).

h remains a variable for the derivation so that students may notice that it is a dependant variable (dependent upon the flowrate). Bequette must (and does) provide both the values for F_s, h_s so that a linearization may proceed (otherwise we will simply have an equation describing the slope with no characteristic point to pass through).

System Parameters (F_s is an example flow rate at steady state, this information is used to determine the intercept of the linearized formula):

$$A = 1ft^2; h_s = 5ft; \beta = \frac{1}{\sqrt{5}} \frac{ft^{2.5}}{min}; F_s = \frac{1ft^3}{min}$$

Rewriting the system with the input variables:

$$\frac{dh}{dt} = f(h, F_s) = 1 + \frac{1}{\sqrt{5}} * \sqrt{h}$$

To linearize around a certain point, simply evaluate the derivative of the desired function and add in a corrective constant, C, represented by the value of the function at the initial (specified) condition.

$$f(h, F_s)_{approx.} = f(h, F_s) + \frac{\partial f}{\partial h} \Big|_{h, F_s} (h - h_s)$$

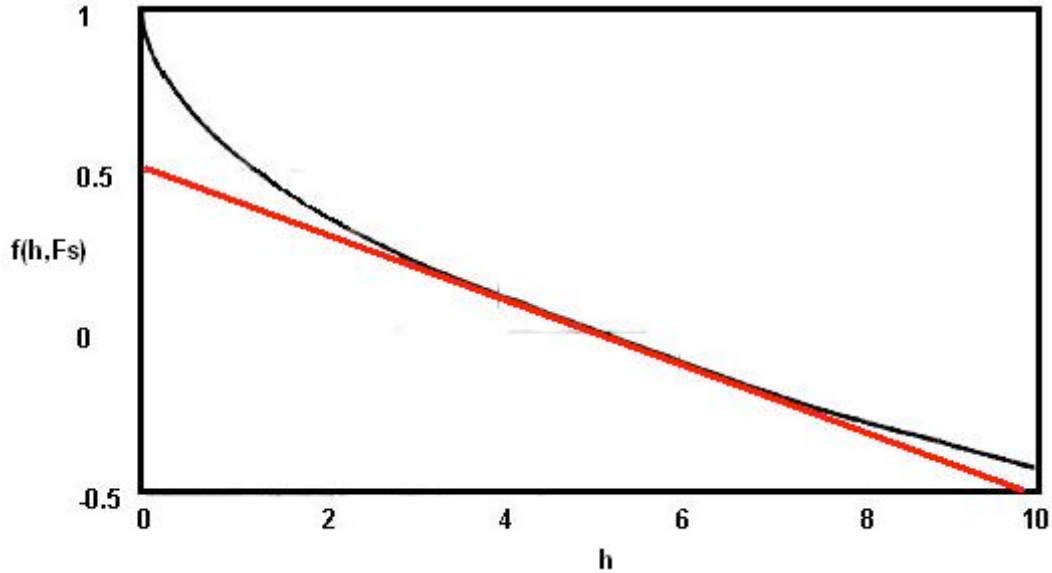
$$f(h, F_s)_{approx.} = 0 + \frac{-1}{2\sqrt{5}\sqrt{h_s}} \Big|_{h, F_s} (h - h_s)$$

Selecting, h=5 to linearize around, we present an adapted version of the text example (linearization is in red):

$$f(h, 1)_{approx.} = 0 + \frac{-1}{2\sqrt{5}\sqrt{5}} \Big|_{h, F_s} (h - 5)$$

$$f(5, 1)_{approx.} = 0 + \frac{-1}{2\sqrt{5}\sqrt{5}} \Big|_{h, F_s} (5 - 5) = 0$$

$$**f(h,1)_{approx.} = - 0.1 * (h - 5)**$$



The physical significance of this example:

The model describes a situation where a tank maintains the steady state set point, a level (height) of 5 feet, by regulating the input (and/or output) flow rate(s). A height above the preferred level of 5 ft. results in a negative height change per time; conversely, a height below the preferred level of 5 ft. results in a positive height change per time, so as to always approach the steady state level.

Also, please note that the linearized system responds relatively slower than the characteristic equation system (non-linear) when tank level falls below 5 ft. and faster than the characteristic equation system when the tank level is above 5 ft.

Please read on below to learn a step-by-step technique on how to complete this method for most equations.

2.6 Linearization using Mathematica

Most ODEs are not as simple as the example worked out above. For those that can be solved analytically, the 'by-hand' method from the previous section can be used, although the math becomes tricky and tedious when one is dealing with systems of ODEs. For those that cannot be solved analytically and can only be approximated numerically, it is sometimes impossible to do the numerical analysis by hand. For these ODEs, powerful computational tools such as Mathematica can be used to perform linearization.

The following Mathematica file contains a worked out example (CSTR w/ heat exchange). This example contains multiple ODEs and multiple types of variables. When dealing with ODEs, there are three main type of variables: state, input, and output. State variables describes the system at any given time (ie. C_a , C_b , T , etc.). Input variables are simply inputs into the system. Output variables are those that are not directly related to

the inputs, but are dependent on the state variables (ie. k, the reaction constant). You will discover in the CSTR example that it is necessary to linearize state variables and output variables separately.

Before proceeding to the Mathematica file we will first present some of the Mathematica commands that will be necessary to linearize the CSTR example.

Note that you need to press shift+enter (shift+return on Mac) after a command to evaluate the expression.

Example:

```
In[1]= ((0.04587*54.32497+4.59058433734947^7)/48700043)^131.94564
```

```
Out[1]= 0.000411241
```

Another thing to note is the use of assignment and equality operators.

= is called **immediate assignment operator** and **:=** is called **delayed assignment operator**. When immediate assignment operator is used, the right hand side of the operator is evaluated every time an assignment is made. However, when delayed assignment operator is used, the right hand side is evaluated only when the value of the expression on the left hand side is requested.

```
lhs=rhs      rhs is intended to be the "final value" of
lhs (e.g., f[x_]=1-x^2)      lhs:=rhs      rhs gives a
"command" or "program" to be executed whenever you ask for
the value of lhs (e.g., f[x_] := Expand[1-x^2])
```

```
p := x^3 - 6 x^2 + 11 x - 6
```

This input, which produces no output, assigns the polynomial expression to the variable p. The assignment is done because this polynomial may be used again later, so the assignment saves retyping it. The **equality operator ==**, which is used here to form the equation we are asking Mathematica to solve:

```
In[2]:= Solve[p == 0]
```

```
Out[2]= {{x -> 1}, {x -> 2}, {x -> 3}}
```

When solving nonlinear ODEs using Mathematica, it is necessary to form a matrix and there are several commands that can be used to create matrices.

D[X,Y]

This command takes the partial derivative of an expression (X) with respect to a variable (Y) defined by the user. The first term in the square brackets is the expression you wish to differentiate, the second is the variable you wish to differentiate with respect to.

AppendRows[column1,column2]

This command creates a matrix by combining two columns. In order to use this command you must first load the Matrix Manipulation package using the command
<<LinearAlgebra`MatrixManipulation`

M = {{x1,x2,x3},{y1,y2,y3},{z1,z2,z3}}

This command creates a matrix, in this case a 3x3 matrix.

MatrixForm[X]

This command displays a specified matrix in matrix form.

These commands will allow us to proceed with the linearization of the CSTR problem shown below.

```

Cstr_examp1.nb

dCa = f1 = (m / (rho * V)) * (Ca0 - Ca) - k0 * Ca * Exp[-E / (R * T)]
-Ca * e^(-E / (R * T)) * k0 + (-Ca + Ca0) * m / (rho * V)

dT = f2 = (m * Cp * (T0 - T) - V * H * Ca * k0 * Exp[-E / (R * T)] + U * A * (Tc - T)) / (V * rho * Cp)
Cp * m * (-T + T0) + A * (-T + Tc) * U - Ca * e^(-E / (R * T)) * H * k0 * V / (Cp * rho * V)

k = g1 = k0 * Exp[-E / (R * T)]
e^(-E / (R * T)) * k0

M = {{f1}, {f2}}
{{-Ca * e^(-E / (R * T)) * k0 + (-Ca + Ca0) * m / (rho * V)}, {Cp * m * (-T + T0) + A * (-T + Tc) * U - Ca * e^(-E / (R * T)) * H * k0 * V / (Cp * rho * V)}}

column1 = D[M, Ca]
{{-e^(-E / (R * T)) * k0 - m / (rho * V)}, {e^(-E / (R * T)) * H * k0 / (Cp * rho)}}

column2 = D[M, T]
{{-Ca * e^(-E / (R * T)) * k0 / (R * T^2)}, {-Cp * m - A * U - Ca * e^(-E / (R * T)) * H * k0 * V / (R * T^2)}}

<< LinearAlgebra`MatrixManipulation`
J = AppendRows[column1, column2]
{{-e^(-E / (R * T)) * k0 - m / (rho * V), -Ca * e^(-E / (R * T)) * k0 / (R * T^2)}, {-e^(-E / (R * T)) * H * k0 / (Cp * rho), -Cp * m - A * U - Ca * e^(-E / (R * T)) * H * k0 * V / (R * T^2)}}

MatrixForm[J]
(
  -e^(-E / (R * T)) * k0 - m / (rho * V)   -Ca * e^(-E / (R * T)) * k0 / (R * T^2)
  -e^(-E / (R * T)) * H * k0 / (Cp * rho)   -Cp * m - A * U - Ca * e^(-E / (R * T)) * H * k0 * V / (R * T^2)
)

```

The first three commands input the equations that govern the behavior of the concentration, Ca, the temperature, T, and the rate of reaction, k. Once the equations have been entered into Mathematica a matrix, M, with one column and two rows containing the equations for Ca and T is created. Next two new matrices are created by taking the derivative of matrix M is with respect to both Ca and T. These matrices, called column1 and column2 respectively, together form the Jacobian of the system and is then displayed in matrix form. The **Jacobian matrix** is the matrix of all first-order partial derivatives of a vector-valued function. Its importance lies in the fact that it represents the best linear approximation to a differentiable function near a given point. For example, given a set $y=f(x)$ of n equations in variables x_1, x_2, \dots, x_n , the Jacobian matrix is defined as following:

$$J(x_1, \dots, x_n) = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \dots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_n}{\partial x_1} & \dots & \frac{\partial y_n}{\partial x_n} \end{bmatrix}$$

```

SS = {{Ca - Cas}, {T - Ts}}
{{Ca - Cas}, {T - Ts}}

MatrixForm[SS]

$$\begin{pmatrix} Ca - Cas \\ T - Ts \end{pmatrix}$$


JK = {D[g1, Ca], D[g1, T]}
{0,  $\frac{1 - \frac{e}{RT} k_0}{R T^2}$ }

MatrixForm[JK]

$$\begin{pmatrix} 0 \\ \frac{1 - \frac{e}{RT} k_0}{R T^2} \end{pmatrix}$$


SSk = {k - ks}
{ $e^{-\frac{E}{RT} k_0} - ks$ }

MatrixForm[SSk]

$$\left( e^{-\frac{E}{RT} k_0} - ks \right)$$


```

Now that we have the Jacobian we need to create a matrix containing the deviation from steady state for each of the variables. This matrix, SS, contains the actual concentration and temperature, C and T, minus the steady state concentration and temperature, Cas and Ts. The matrix is then displayed in matrix form. We now have both the Jacobian and the deviation matrix for the state variables. The next four commands create the Jacobian and deviation matrix for the output variable, k. The first command creates the Jacobian matrix by taking the derivative of the k equation with respect to Ca and T. The Jacobian is then shown in matrix form. Finally the deviation matrix for k is created in the same manner as above and then displayed in matrix form. Note that because k is defined above, this expression is substituted in for k in the deviation matrix. The following Mathematica file contains the code shown above with extra comments explaining why each step is performed [Media:cstr example.nb](#). It may be useful to download this file and run the program in Mathematica yourself to get a feel for the syntax. Downloading the file will also allow you to make any changes and edits to customize this example to another example of interest.

Note: This file needs to be saved to your computer, and then opened using Mathematica to properly run.

To see another example lets linearize the first 4 differential equations given in the introduction section.

Non-linear system of equations:

$$\frac{dA}{dt} = 3A^2 + 2B + C - 7D^3$$

$$\frac{dB}{dt} = A + C^2 + 2D$$

$$\frac{dC}{dt} = A + 4B^2 - C^2$$

$$\frac{dD}{dt} = 2C - D$$

After linearization (around the steady state point $\{-0.47,-0.35,0.11,0.23\}$):

$$\begin{pmatrix} A' \\ B' \\ C' \\ D' \end{pmatrix} = \begin{pmatrix} -2.83 & 2 & 1 & -1.10 \\ 1 & 0 & 0.23 & 2 \\ 1 & -2.78 & -0.23 & 0 \\ 0 & 0 & 2 & -1 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} + \begin{pmatrix} 0.50 \\ 0.01 \\ 0.47 \\ 0 \end{pmatrix}$$

```

lineODE.nb *

In[10]:= eqns = {3*a^2+2*b+c-7*d^3, a+c^2+2*d, a+4*b^2-c^2, 2*c-d};
(*solving for fixed points under s1*)
s1 = NSolve[eqns[[1]] == 0, eqns[[2]] == 0, eqns[[3]] == 0, eqns[[4]] == 0], {a, b, c, d}]

Out[11]:= {{a -> -113.663, b -> 6.92708, c -> 8.84727, d -> 17.6945}, {a -> -114.027, b -> -6.93898, c -> 8.86402, d -> 17.728},
{a -> -11.0743, b -> 1.9117, c -> 1.88257, d -> 3.76514}, {a -> -10.27, b -> -1.83233, c -> 1.77756, d -> 3.55512},
{a -> 0.308224 - 0.364633 i, b -> 0.140184 + 0.312248 i, c -> -0.0762646 + 0.0947721 i, d -> -0.152529 + 0.189544 i},
{a -> 0.308224 + 0.364633 i, b -> 0.140184 - 0.312248 i, c -> -0.0762646 - 0.0947721 i, d -> -0.152529 - 0.189544 i},
{a -> -0.470879, b -> -0.347842, c -> 0.114445, d -> 0.228891}, {a -> 0., b -> 0., c -> 0., d -> 0.}}

In[12]:= (*s1[[7]] equals {a->-0.47,b->-0.35,c->0.11,d->0.23} which is the steady state then define the Jacobian at the s1[[7]]*)
Jac = {D[eqns[[1]], a], D[eqns[[1]], b], D[eqns[[1]], c], D[eqns[[1]], d]},
{D[eqns[[2]], a], D[eqns[[2]], b], D[eqns[[2]], c], D[eqns[[2]], d]},
{D[eqns[[3]], a], D[eqns[[3]], b], D[eqns[[3]], c], D[eqns[[3]], d]},
{D[eqns[[4]], a], D[eqns[[4]], b], D[eqns[[4]], c], D[eqns[[4]], d]}/. s1[[7]];
(*The Jacobian is changed into Matrix Form*)
MatrixForm[Jac]

Out[13]/MatrixForm=

$$\begin{pmatrix} -2.82528 & 2 & 1 & -1.10021 \\ 1 & 0 & 0.228891 & 2 \\ 1 & -2.78274 & -0.228891 & 0 \\ 0 & 0 & 2 & -1 \end{pmatrix}$$


In[14]:= (*To calculate the constants aka k1 k2 k3 and k4 Define m1 as 2nd matrix on righthand side of linearization eqm*)
m1 = {a, b, c, d}
(*Execute the dot product of m1 and the Jacobian matrix*)
Jac.m1

Out[14]:= {a, b, c, d}

Out[15]:= {-2.82528 a + 2 b - c - 1.10021 d, a + 0.228891 c - 2 d, a - 2.78274 b - 0.228891 c, 2 c - d}

In[16]:= (*Determine the dot product of m1 at the steady state values*)
Jac.m1 /. s1[[7]]

Out[16]:= {0.497297, 0.0130977, 0.470879, 0.}

```

The 4 differential equations above are added into a Mathematica code as “eqns” and “s1” is the fixed points of the differentials. The steady state values found for “a, b, c, and d” are called "s1doubleBrackets(7)” After the steady state values are found, the Jacobian matrix can be found at those values.

To find “k1, k2, k3, and k4” the constants of the Linearization matrix equation, “m1” must be defined, which is the 2nd matrix on the right-hand side of the Linearization matrix equation.

To determine the k values (in matrix form), execute the dot product of "m1" and the “Jac” matrix, which is done by the "." operator. Therefore it should look like "Jac.m1"

To obtain the k values, determining the "Jac.m1" at the steady state values, which is done by the "/" operator. Therefore it should look like “Jac.m1/.s1doubleBrackets(7)”

2.7 Worked out Example 1

Let's say you have a system governed by the following system of equations:

$$\frac{dX_a}{dt} = 3 * X_a^2 + 2 * X_b + F_o$$

$$\frac{dX_b}{dt} = 6 * X_a + 9 * X_b^2 + X_a * X_b + F_o$$

$$Y = X_a^2 + 3 * F_o^2$$

In this case, X_a and X_b are state variables (they describe the state of the system at any given time), F_o is an input variable (it enters the system and is independent of all of the state variables), and Y is the output of the system and is dependent on both the state and input variables. Please linearize this system using Mathematica.

The solution to this Example can be found in the following Mathematica notebook: [Media:Example 1.nb](#)

2.8 Worked out Example 2

Use the Mathematica file presented in the article to linearize the CSTR example presented in the [ODE & Excel CSTR model with heat exchange](#) wiki around the steady state ($T = 368.4\text{K}$ and $C_a = 6.3\text{mol/L}$). Use the constants presented in their example. Use the linearization to approximate C_a at 369K .

Solution: The linear approximation gives concentration of a (C_a) of 7.13 mol/L . The Mathematica file used to solve this problem can be downloaded here.

[Media:LinearizationExample.nb](#) If you are having trouble running the Mathematica file try right clicking the link and using the Save Target As option.

2.9 Multiple Choice Question 1

In an ODE linearization, what point in the process is the linearization generally centered around?

- Starting point
- Ending point
- Steady-state point
- Half-way point

Answer: c

2.10 Multiple Choice Question 2

What does the D[] function in Mathematica do?

- a. Find the determinant of a matrix
- b. Finds the partial derivative a function or functions
- c. Find the dot product of two matrices
- d. Integrate a matrix or function

Answer: b

2.11 Sage's Corner

Linearization of Differential Equations of a PID Controller

<http://video.google.com/googleplayer.swf?docId=-9126622911731373374>

You will most likely need to download the powerpoint to see the fine details of the equations.

[Media:linearizingODEnoaud.ppt](#)

Linearizing O to the D to the E's


<http://video.google.com/googleplayer.swf?docId=3810028888296877515>

[Media:Anchor2PIDmodel.xls](#)

2.12 References

- Bequette, B. Wayne. *Process Dynamics: Modeling, Analysis, and Simulation*. Prentice- Hall PTR, Upper Saddle River, NJ 07458 (c) 2006.
- Kravaris, Costas. *Chemical Process Control: A Time Domain Approach, Appendix A*. Department of Chemical Engineering, University of Michigan, Ann Arbor, MI.
- Bhatti, M. Asghar. *Practical Optimization Methods With Mathematica Applications*. Springer Telos.

Section 3. Eigenvalues and Eigenvectors

Note:  [Video lecture](#) available for this section!

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- [First round reviews for this page](#)
- [Rebuttal for this page](#)

3.1 What are Eigenvectors and Eigenvalues?

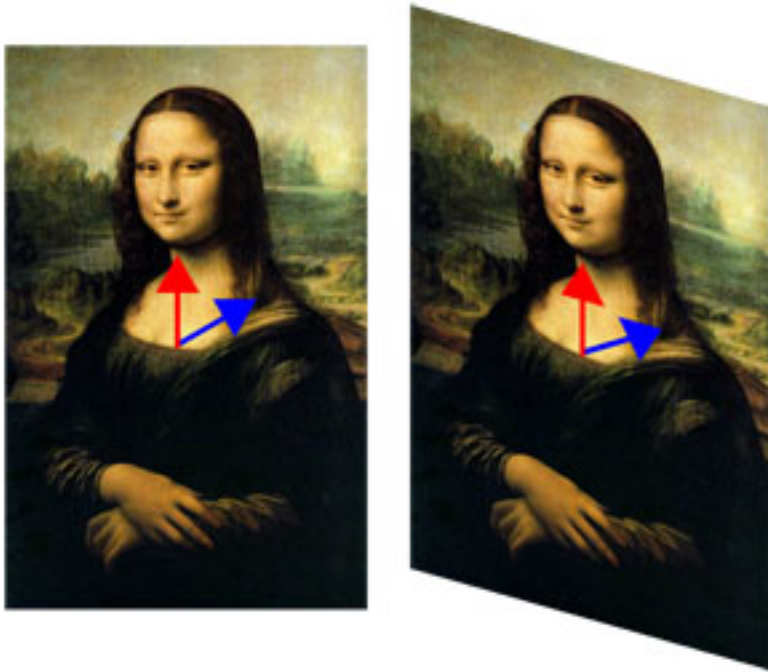
Eigenvectors(\mathbf{V}) and Eigenvalues(λ) are mathematical tools used in a wide-range of applications. They are used to solve differential equations, harmonics problems, population models, etc. In Chemical Engineering they are mostly used to solve differential equations and to analyze the stability of a system.

Defintion of Eigenvector and Eigenvalues:

An **Eigenvector** is a vector that maintains its direction after undergoing a linear transformation.

An **Eigenvalue** is the scalar value that the eigenvector was multiplied by during the linear transformation.

Eigenvectors and Eigenvalues are best explained using an example. Take a look at the picture below.



In the left picture, two vectors were drawn on the Mona Lisa. The picture then underwent a linear transformation and is shown on the right. The red vector maintained its direction; therefore, it's an eigenvector for that linear transformation. The blue vector did not maintain its direction during the transformation; thus, it is not an eigenvector. The eigenvalue for the red vector in this example is 1 because the arrow was not lengthened or shortened during the transformation. If the red vector, on the right, were twice the size than the original vector then the eigenvalue would be 2. If the red vector were pointing directly down and remained the size in the picture, the eigenvalue would be -1.

Now that you have an idea of what an eigenvector and eigenvalue are we can start talking about the mathematics behind them.

Fundamental Equation

The following equation must hold true for Eigenvectors and Eigenvalues given a square matrix \mathbf{A} :

$$\mathbf{A} \cdot \mathbf{v} = \lambda \cdot \mathbf{v}$$

Where:

\mathbf{A} is a square matrix

\mathbf{v} is the Eigenvector

λ is the Eigenvalue

Let's go through a simple example so you understand the fundamental equation better.

Question:

Is $\mathbf{v} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}$ an eigenvector with the corresponding $\lambda = 0$ for the matrix $\mathbf{A} = \begin{bmatrix} 6 & 3 \\ -2 & -1 \end{bmatrix}$?

Answer:

$$\mathbf{A} \cdot \mathbf{v} = \lambda \cdot \mathbf{v}$$

$$\begin{bmatrix} 6 & 3 \\ -2 & -1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ -2 \end{bmatrix} = 0 \begin{bmatrix} 1 \\ -2 \end{bmatrix}$$

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Therefore, it is true that \mathbf{v} and λ are an eigenvector and eigenvalue respectively, for \mathbf{A} . (See section on Matrix operations, i.e. matrix multiplication)

3.2 Calculating Eigenvalues and Eigenvectors

Calculation of the eigenvalues and the corresponding eigenvectors is completed using several principles of linear algebra. This can be done by hand, or for more complex situations a multitude of software packages (i.e. Mathematica) can be used. The following discussion will work for any $n \times n$ matrix; however for the sake of simplicity, smaller and more manageable matrices are used. Note also that throughout this article, **boldface** type is used to distinguish matrices from other variables.

3.2.1 Linear Algebra Review

For those who are unfamiliar with linear algebra, this section is designed to give the necessary knowledge used to compute the eigenvalues and eigenvectors. For a more extensive discussion on linear algebra, please consult the references.

Basic Matrix Operations

An $m \times n$ **matrix** \mathbf{A} is a rectangular array of mn numbers (or elements) arranged in horizontal **rows** (m) and vertical **columns** (n):

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{1j} & a_{1n} \\ a_{i1} & a_{ij} & a_{in} \\ a_{m1} & a_{mj} & a_{mn} \end{bmatrix}$$

To represent a matrix with the element a_{ij} in the i th row and j th column, we use the abbreviation $\mathbf{A} = [a_{ij}]$. Two $m \times n$ matrices $\mathbf{A} = [a_{ij}]$ and $\mathbf{B} = [b_{ij}]$ are said to be equal if corresponding elements are equal.

Addition and subtraction

We can add \mathbf{A} and \mathbf{B} by adding corresponding elements: $\mathbf{A} + \mathbf{B} = [a_{ij}] + [b_{ij}] = [a_{ij} + b_{ij}]$. This will give the element in row i and column j of $\mathbf{C} = \mathbf{A} + \mathbf{B}$ to have $c_{ij} = a_{ij} + b_{ij}$.

More detailed addition and subtraction of matrices can be found in the example below.

$$\begin{bmatrix} 1 & 2 & 6 \\ 4 & 5 & 10 \\ 5 & 3 & 11 \end{bmatrix} + \begin{bmatrix} 8 & 3 & 5 \\ 5 & 4 & 4 \\ 3 & 0 & 6 \end{bmatrix} = \begin{bmatrix} 1+8 & 2+3 & 6+5 \\ 4+5 & 5+4 & 10+4 \\ 5+3 & 3+0 & 11+6 \end{bmatrix} = \begin{bmatrix} 9 & 5 & 11 \\ 9 & 9 & 14 \\ 8 & 3 & 17 \end{bmatrix}$$

Multiplication

Multiplication of matrices are NOT done in the same manner as addition and subtraction. Let's look at the following matrix multiplication:

$$\mathbf{A} * \mathbf{B} = \mathbf{C}$$

\mathbf{A} is an $m \times n$ matrix, \mathbf{B} is an $n \times p$ matrix, and \mathbf{C} is an $m \times p$ matrix. Therefore the resulting matrix, \mathbf{C} , has the same number of rows as the first matrix and the same number of columns as the second matrix. Also the number of columns in the first is the same as the number of rows in the second matrix.

The value of an element in \mathbf{C} (row i , column j) is determined by the general formula:

$$c_{i,j} = \sum_{k=1}^n a_{i,k} b_{k,j}$$

Thus,

$$\begin{bmatrix} 1 & 2 & 6 \\ 4 & 5 & 10 \\ 5 & 3 & 11 \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 1 \\ 5 & 1 \end{bmatrix} = \begin{bmatrix} 1 \times 3 + 2 \times 0 + 6 \times 5 & 1 \times 0 + 2 \times 1 + 6 \times 1 \\ 4 \times 3 + 5 \times 0 + 10 \times 5 & 4 \times 0 + 5 \times 1 + 10 \times 1 \\ 5 \times 3 + 3 \times 0 + 11 \times 5 & 5 \times 0 + 3 \times 1 + 11 \times 1 \end{bmatrix} = \begin{bmatrix} 33 & 8 \\ 62 & 15 \\ 70 & 14 \end{bmatrix}$$

It can also be seen that multiplication of matrices is not commutative ($\mathbf{A} \mathbf{B} \neq \mathbf{B} \mathbf{A}$).

Multiplication of a matrix by a scalar is done by multiplying each element by the scalar.

$$c\mathbf{A} = \mathbf{A}c = [ca_{ij}]$$

$$2 \begin{bmatrix} 1 & 2 & 6 \\ 4 & 5 & 10 \\ 5 & 3 & 11 \end{bmatrix} = \begin{bmatrix} 2 & 4 & 12 \\ 8 & 10 & 20 \\ 10 & 6 & 22 \end{bmatrix}$$

Identity Matrix

The identity matrix is a special matrix whose elements are all zeroes except along the primary diagonal, which are occupied by ones. The identity matrix can be any size as long as the number of rows equals the number of columns.

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Determinant

The determinant is a property of any square matrix that describes the degree of coupling between equations. For a 2x2 matrix the determinant is:

$$\det(\mathbf{A}) = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

Note that the vertical lines around the matrix elements denotes the determinant. For a 3x3 matrix the determinant is:

$$\det(\mathbf{A}) = \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a \begin{vmatrix} e & f \\ h & i \end{vmatrix} - b \begin{vmatrix} d & f \\ g & i \end{vmatrix} + c \begin{vmatrix} d & e \\ g & h \end{vmatrix} = a(ei - fh) - b(di - fg) + c(dh - eg)$$

Larger matrices are computed in the same way where the element of the top row is multiplied by the determinant of matrix remaining once that element's row and column are removed. Terms where the top elements in odd columns are added and terms where the top elements in even rows are subtracted (assuming the top element is positive). For matrices larger than 3x3 however; it is probably quickest to use math software to do these calculations since they quickly become more complex with increasing size.

3.2.2 Solving for Eigenvalues and Eigenvectors

The eigenvalues (λ) and eigenvectors (\mathbf{v}), are related to the **square** matrix \mathbf{A} by the following equation. (Note: In order for the eigenvalues to be computed, the matrix must have the same number of rows as columns.)

$$(\mathbf{A} - \lambda\mathbf{I}) \cdot \mathbf{v} = 0$$

This equation is just a rearrangement of the equation $\mathbf{A} \cdot \mathbf{v} = \lambda \cdot \mathbf{v}$ that was seen above. To solve this equation, the eigenvalues are calculated first by setting $\det(\mathbf{A} - \lambda\mathbf{I})$ to zero and then solving for λ . The determinant is set to zero in order to ensure non-trivial solutions for \mathbf{v} , by a fundamental theorem of linear algebra.

$$\mathbf{A} = \begin{bmatrix} 4 & 1 & 4 \\ 1 & 7 & 1 \\ 4 & 1 & 4 \end{bmatrix}$$

$$\mathbf{A} - \lambda \mathbf{I} = \begin{bmatrix} 4 & 1 & 4 \\ 1 & 7 & 1 \\ 4 & 1 & 4 \end{bmatrix} + \begin{bmatrix} -\lambda & 0 & 0 \\ 0 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{bmatrix}$$

$$\det(\mathbf{A} - \lambda \mathbf{I}) = \begin{vmatrix} 4-\lambda & 1 & 4 \\ 1 & 7-\lambda & 1 \\ 4 & 1 & 4-\lambda \end{vmatrix} = 0$$

$$-54\lambda + 15\lambda^2 - \lambda^3 = 0$$

$$-\lambda(\lambda-6)(\lambda-9) = 0$$

$$\lambda = 0, 6, 9$$

For each of these eigenvalues, an eigenvector is calculated which will satisfy the equation $(\mathbf{A} - \lambda \mathbf{I})\mathbf{v} = 0$ for that eigenvalue. To do this, an eigenvalue is substituted into $\mathbf{A} - \lambda \mathbf{I}$, and then the system of equations is used to calculate the eigenvector. For $\lambda = 6$

$$(\mathbf{A} - 6\mathbf{I})\mathbf{v} = \begin{bmatrix} 4-6 & 1 & 4 \\ 1 & 7-6 & 1 \\ 4 & 1 & 4-6 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -2 & 1 & 4 \\ 1 & 1 & 1 \\ 4 & 1 & -2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = 0$$

Using multiplication we get a system of equations that can be solved.

$$-2x + y + 4z = 0 \longrightarrow y = 2x - 4z \quad (1)$$

$$x + y + z = 0 \longrightarrow y = -x - z \quad (2)$$

$$4x + y - 2z = 0 \longrightarrow y = -4x + 2z \quad (3)$$

Equating (1) and (3) ...

$$2x - 4z = -4x + 2z$$

$$6x = 6z$$

$$x = z$$

Plugging this into (2)...

$$y = -x - x = -2x$$

There is one degree of freedom in the system of equations, so we have to choose a value for one variable. By convention we choose $x = 1$ then

$$x = 1$$

$$y = -2$$

$$z = 1$$

$$\mathbf{v} = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

A degree of freedom always occurs because in these systems not all equations turn out to be independent, meaning two different equations can be simplified to the same equation. In this case a small number was chosen ($x = 1$) to keep the solution simple. However, it is okay to pick any number for x , meaning that each eigenvalue potentially has an infinite number of possible eigenvectors that are scaled based on the initial value of x chosen. Said another way, the eigenvector only points in a direction, but the magnitude of this pointer does not matter. For this example, getting an eigenvector that is

$$\mathbf{v} = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

is identical to getting an eigenvector that is

$$\mathbf{v} = \begin{bmatrix} 2 \\ -4 \\ 2 \end{bmatrix}$$

or an eigenvector that is scaled by some constant, in this case 2.

Finishing the calculations, the same method is repeated for $\lambda = 0$ and $\lambda = 9$ to get their corresponding eigenvectors.

$$\mathbf{v} = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$

For $\lambda = 0$,

$$\mathbf{v} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

For $\lambda = 9$,

In order to check your answers you can plug your eigenvalues and eigenvectors back into the governing equation $\mathbf{A} \cdot \mathbf{v} = \lambda \cdot \mathbf{v}$. For this example, $\lambda = 6$ and

$$\mathbf{v} = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

was double checked.

$$\begin{bmatrix} 4 & 1 & 4 \\ 1 & 7 & 1 \\ 4 & 1 & 4 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} = 6 \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 4 - 2 + 4 \\ 1 - 14 + 1 \\ 4 - 2 + 4 \end{bmatrix} = \begin{bmatrix} 6 \\ -12 \\ 6 \end{bmatrix}$$

$$\mathbf{v} = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

Therefore, $\lambda = 6$ and $\begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$ are both an eigenvalue-eigenvector pair for the

matrix $\mathbf{A} = \begin{bmatrix} 4 & 1 & 4 \\ 1 & 7 & 1 \\ 4 & 1 & 4 \end{bmatrix}$.

3.3 Calculating Eigenvalues and Eigenvectors using Numerical Software

3.3.1 Eigenvalues in Mathematica

For larger matrices (4x4 and larger), solving for the eigenvalues and eigenvectors becomes very lengthy. Therefore software programs like Mathematica are used. The example from the last section will be used to demonstrate how to use Mathematica. First we can generate the matrix \mathbf{A} . This is done using the following syntax:

- $A = \{\{4,1,4\},\{1,7,1\},\{4,1,4\}\}$

It can be seen that the matrix is treated as a list of rows. Elements in the same row are contained in a single set of brackets and separated by commas. The set of rows are also contained in a set of brackets and are separated by commas. A screenshot of this is seen below. (Note: The "MatrixForm[]" command is used to display the matrix in its standard form. Also in Mathematica you must hit Shift + Enter to get an output.)

```

In[1]:= A = {{4, 1, 4}, {1, 7, 1}, {4, 1, 4}}
Out[1]= {{4, 1, 4}, {1, 7, 1}, {4, 1, 4}}

In[2]:= MatrixForm[A]
Out[2]/MatrixForm=

$$\begin{pmatrix} 4 & 1 & 4 \\ 1 & 7 & 1 \\ 4 & 1 & 4 \end{pmatrix}$$


```

Next we find the determinant of matrix $A - \lambda I$, by first subtracting the matrix λI from A (Note: This new matrix, $A - \lambda I$, has been called $A2$).

```

In[9]:= i = {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}
Out[9]= {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

In[10]:= MatrixForm[i]
Out[10]/MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$


In[14]:= A2 = A - λ * i
Out[14]= {{4 - λ, 1, 4}, {1, 7 - λ, 1}, {4, 1, 4 - λ}}

In[15]:= MatrixForm[A2]
Out[15]/MatrixForm=

$$\begin{pmatrix} 4 - \lambda & 1 & 4 \\ 1 & 7 - \lambda & 1 \\ 4 & 1 & 4 - \lambda \end{pmatrix}$$

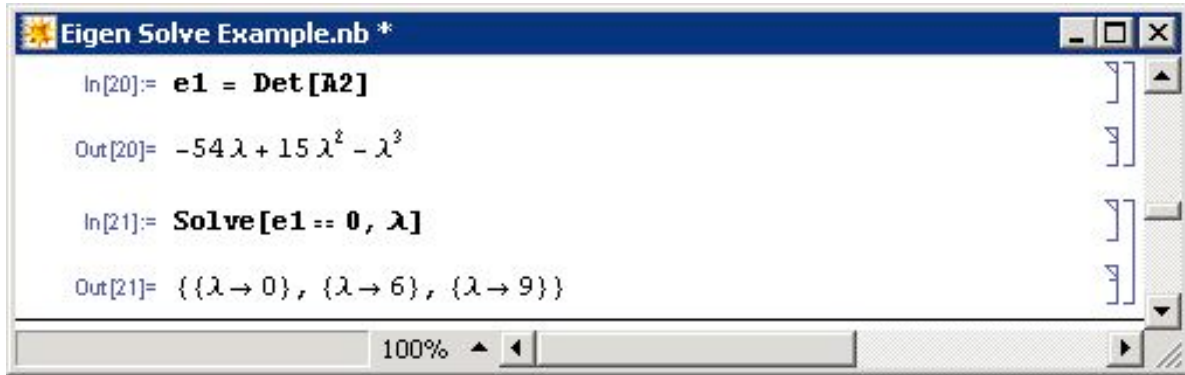

```

The command to find the determinant of a matrix A is:

- `Det[A]`

For our example the result is seen below. By setting this equation to 0 and solving for λ , the eigenvalues are found. The `Solve[]` function is used to do this. Notice in the syntax that the use of two equal signs (`==`) is used to show equivalence whereas a single equal sign is used for defining a variable.

- `Solve[{set of equations},{variables being solved}]`



```
Eigen Solve Example.nb *
In[20]:= e1 = Det[A2]
Out[20]= -54 λ + 15 λ2 - λ3
In[21]:= Solve[e1 == 0, λ]
Out[21]= {{λ → 0}, {λ → 6}, {λ → 9}}
```

Alternatively the eigenvalues of a matrix **A** can be solved with the Mathematica `Eigenvalue[]` function:

- `Eigenvalues[A]`

Note that the same results are obtained for both methods.

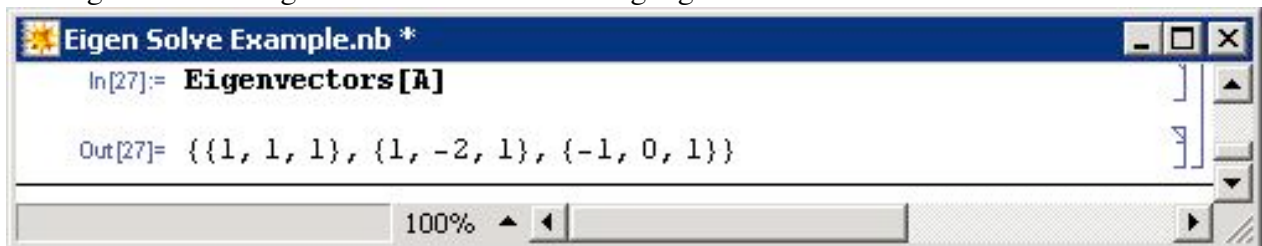


```
Eigen Solve Example.nb *
In[22]:= Eigenvalues[A]
Out[22]= {9, 6, 0}
```

To find the eigenvectors of a matrix **A**, the `Eigenvector[]` function can be used with the syntax below.

- `Eigenvectors[A]`

The eigenvectors are given in order of descending eigenvalues.

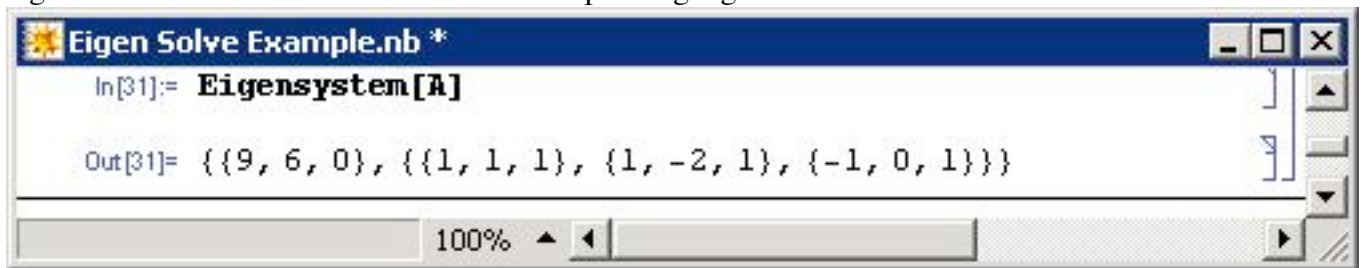


```
Eigen Solve Example.nb *
In[27]:= Eigenvectors[A]
Out[27]= {{1, 1, 1}, {1, -2, 1}, {-1, 0, 1}}
```


One more function that is useful for finding eigenvalues and eigenvectors is Eigensystem[]. This function is called with the following syntax.

- Eigensystem[A]

In this function, the first set of numbers are the eigenvalues, followed by the sets of eigenvectors in the same order as their corresponding eigenvalues.



The Mathematica file used to solve the example can be found at this link. [Media:Eigen Solve Example.nb](#)

3.3.2 Microsoft Excel

Microsoft Excel is capable of solving for Eigenvalues of symmetric matrices using its Goal Seek function. A symmetric matrix is a square matrix that is equal to its transpose and always has real, not complex, numbers for Eigenvalues. In many cases, complex Eigenvalues cannot be found using Excel. Goal Seek can be used because finding the Eigenvalue of a symmetric matrix is analogous to finding the root of a polynomial equation. The following procedure describes how to calculate the Eigenvalue of a symmetric matrix in the Mathematica tutorial using MS Excel.

(1) Input the values displayed below for matrix A then click menu INSERT-NAME-DEFINE “matrix_A” to name the matrix.

matrix_A		
4	1	4
1	7	1
4	1	4

This is the matrix.

(2) Similarly, define identity matrix I by entering the values displayed below then naming it “matrix_I.”

matrix_I		
1	0	0
0	1	0
0	0	1

This is the identity matrix.

(3) Enter an initial guess for the Eigenvalue then name it “lambda.”

lambda	6
--------	---

(4) In an empty cell, type the formula =matrix_A-lambda*matrix_I. Highlight three cells to the right and down, press F2, then press CTRL+SHIFT+ENTER. Name this matrix “matrix_A_lambda_I.”

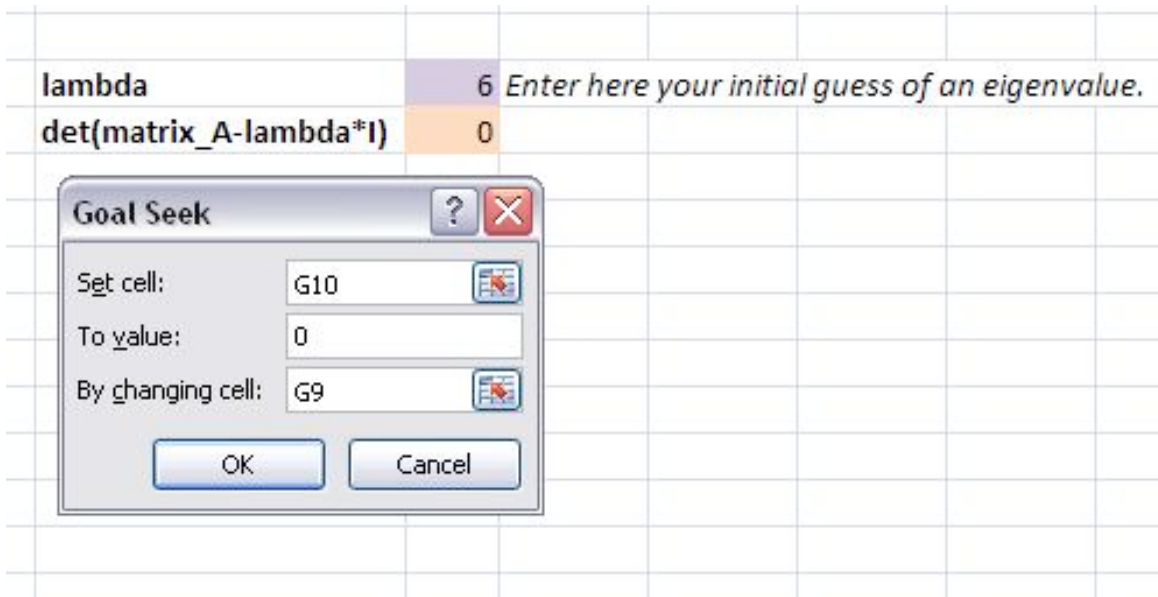
matrix_A_lambda_I		
-2	1	4
1	1	1
4	1	-2

*This is matrix_A-lambda*I.*

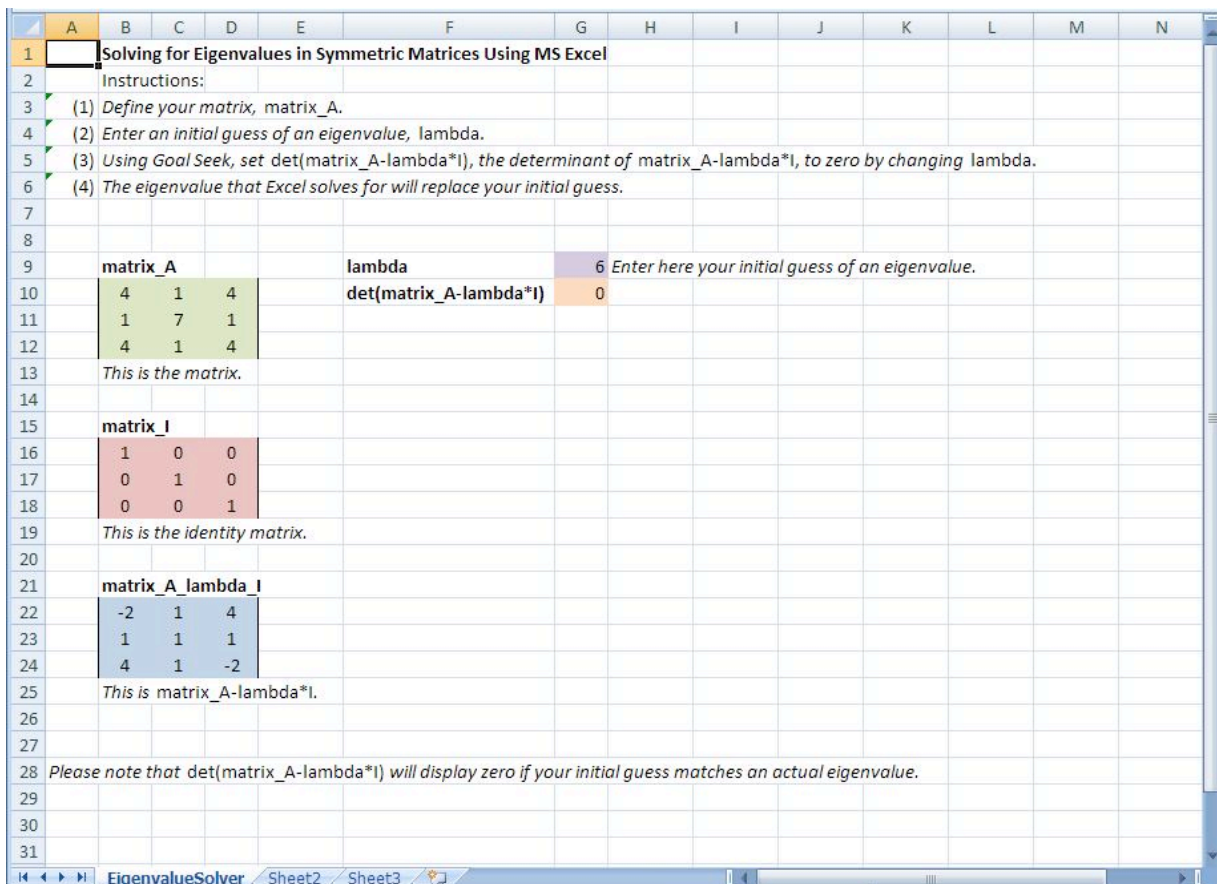
(5) In another cell, enter the formula =MDETERM(matrix_A_lambda_I). This is the determinant formula for matrix_A_lambda_I.

det(matrix_A-lambda*I)	0
------------------------	---

(6) Click menu Tools-Goal Seek... and set the cell containing the determinant formula to zero by changing the cell containing lambda.



(7) To obtain all three Eigenvalues for matrix A, re-enter different initial guesses. Excel calculates the Eigenvalue nearest to the value of the initial guess. The Eigenvalues for matrix A were determined to be 0, 6, and 9. For instance, initial guesses of 1, 5, and 13 will lead to Eigenvalues of 0, 6, and 9, respectively.



The MS Excel spreadsheet used to solve this problem, seen above, can be downloaded from this link: [Media:ExcelSolveEigenvalue.xls](#).

3.4 Chemical Engineering Applications

The eigenvalue and eigenvector method of mathematical analysis is useful in many fields because it can be used to solve homogeneous linear systems of differential equations with constant coefficients. Furthermore, in chemical engineering many models are formed on the basis of systems of differential equations that are either linear or can be linearized and solved using the eigenvalue eigenvector method. In general, most ODEs can be linearized and therefore solved by this method. [Linearizing ODEs](#) For example, a PID control device can be modeled with ODEs that may be linearized where the eigenvalue eigenvector method can then be implemented. If we have a system that can be modeled with linear differential equations involving temperature, pressure, and concentration as they change with time, then the system can be solved using eigenvalues and eigenvectors:

$$\frac{dP}{dt} = 4P - 4T + C$$

$$\frac{dT}{dt} = 4P - T + 3C$$

$$\frac{dC}{dt} = P + 5T - C$$

Note: This is not a real model and simply serves to introduce the eigenvalue and eigenvector method.

A is just the matrix that represents the coefficients in the above linear differential equations. However, when setting up the matrix, **A**, the order of coefficients matters and must remain consistent. Namely, in the following representative matrix, the first column corresponds to the coefficients of **P**, the second column to the coefficients of **T**, and the third column corresponds to the coefficients of **C**. The same goes for the rows. The first

row corresponds to $\frac{dP}{dt}$, the second row corresponds to $\frac{dT}{dt}$, and the third row corresponds to $\frac{dC}{dt}$:

$$\mathbf{A} = \begin{bmatrix} 4 & -4 & 1 \\ 4 & -1 & 3 \\ 1 & 5 & -1 \end{bmatrix}$$

It is noteworthy that matrix \mathbf{A} is only filled with constants for a linear system of differential equations. This turns out to be the case because each matrix component is the partial differential of a variable (in this case P, T, or C). It is this partial differential that yields a constant for linear systems. Therefore, matrix \mathbf{A} is really the Jacobian matrix for a linear differential system.

Now, we can rewrite the system of ODE's above in matrix form.

$$\mathbf{x}' = \mathbf{A}\mathbf{x}$$

$$\mathbf{x}(t) = \begin{bmatrix} P(t) \\ T(t) \\ C(t) \end{bmatrix}$$

Where

We guess trial solutions of the form

$$\mathbf{x} = \mathbf{v}e^{\lambda t}$$

since when we substitute this solution into the matrix equation, we obtain

$$\lambda \mathbf{v}e^{\lambda t} = \mathbf{A}\mathbf{v}e^{\lambda t}$$

After cancelling the nonzero scalar factor $e^{\lambda t}$, we obtain the desired eigenvalue problem.

$$\mathbf{A}\mathbf{v} = \lambda \mathbf{v}$$

Thus, we have shown that $\mathbf{x}=\mathbf{v}e^{\lambda t}$ will be a nontrivial solution for the matrix equation as long as \mathbf{v} is a nonzero vector and λ is a constant associated with \mathbf{v} that satisfies the eigenvalue problem.

In order to solve for the eigenvalues and eigenvectors, we rearrange the equation $\mathbf{A}\mathbf{v}=\lambda\mathbf{v}$ to obtain the following:

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = 0 \quad \longrightarrow \quad \begin{bmatrix} 4 - \lambda & -4 & 1 \\ 4 & -1 - \lambda & 3 \\ 1 & 5 & -1 - \lambda \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix} = 0$$

For nontrivial solutions for \mathbf{v} , the determinant of the eigenvalue matrix must equal zero, $\det(\mathbf{A} - \lambda\mathbf{I}) = 0$. This allows us to solve for the eigenvalues, λ . You should get, after simplification, a third order polynomial, and therefore three eigenvalues. (see section on Solving for Eigenvalues and Eigenvectors for more details) Using the calculated eigenvalues, one can determine the stability of the system when disturbed (see following section).

Once you have calculated the three eigenvalues, you are ready to find the corresponding eigenvectors. Plug the eigenvalues back into the equation $(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = 0$ and solve for the corresponding eigenvectors. There should be three eigenvectors, since there were three eigenvalues. (see section on Calculating Eigenvalues and Eigenvectors for more details)

The solution will look like the following:

$$\begin{bmatrix} P(t) \\ T(t) \\ C(t) \end{bmatrix} = c_1 \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} e^{\lambda_1 t} + c_2 \begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} e^{\lambda_2 t} + c_3 \begin{bmatrix} x_3 \\ y_3 \\ z_3 \end{bmatrix} e^{\lambda_3 t}$$

Where

$x_1, x_2, x_3, y_1, y_2, y_3, z_1, z_2, z_3$ are all constants from the three eigenvectors. The general solution is a linear combination of these three solution vectors because the original system of ODE's is homogeneous and linear. It is homogeneous because the derivative expressions have no cross terms, such as PC or TC , and no dependence on t . It is linear because the derivative operator is linear. To solve for c_1, c_2, c_3 there must be some given initial conditions (see Worked out Example 1).

This Wiki does not deal with solving ODEs. It only deals with solving for the eigenvalues and eigenvectors. In Mathematica the **Dsolve[]** function can be used to bypass the calculations of eigenvalues and eigenvectors to give the solutions for the differentials directly. See [Using eigenvalues and eigenvectors to find stability and solve ODEs](#) for solving ODEs using the eigenvalues and eigenvectors method as well as with Mathematica.

This section was only meant to introduce the topic of eigenvalues and eigenvectors and does not deal with the mathematical details presented later in the article.

3.5 Using Eigenvalues to Determine Effects of Disturbing a System

Eigenvalues can help determine trends and solutions with a system of differential equations. Once the eigenvalues for a system are determined, the eigenvalues can be used to describe the system's ability to return to steady-state if disturbed.

The simplest way to predict the behavior of a system if disturbed is to examine the signs of its eigenvalues. Negative eigenvalues will drive the system back to its steady-state value, while positive eigenvalues will drive it away. What happens if there are two eigenvalues present with opposite signs? How will the system respond to a disturbance in that case? In many situations, there will be one eigenvalue which has a much higher absolute value than the other corresponding eigenvalues for that system of differential equations. This is known as the "dominant eigenvalue", and it will have the greatest effect on the system when it is disturbed. However, in the case that the eigenvalues are equal and opposite sign there is no dominant eigenvalue. In this case the constants from the initial conditions are used to determine the stability.

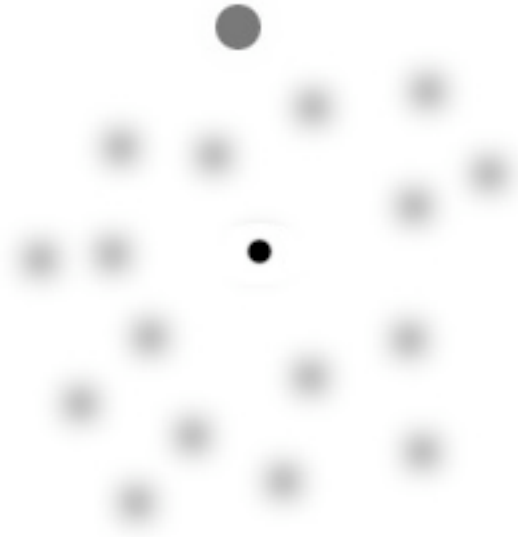
Another possible case within a system is when the eigenvalue is 0. When this occurs, the system will remain at the position to which it is disturbed, and will not be driven towards or away from its steady-state value. It is also possible for a system to have two identical eigenvalues. In this case the two identical eigenvalues produce only one eigenvector. Because of this, a situation can arise in which the eigenvalues don't give the complete story of the system, and another method must be used to analyze it, such as the [Routh Stability Analysis Method](#).

Eigenvalues can also be complex or pure imaginary numbers. If the system is disturbed and the eigenvalues are non-real number, oscillation will occur around the steady state value. If the eigenvalue is imaginary with no real part present, then the system will oscillate with constant amplitude around the steady-state value. If it is complex with a positive real part, then the system will oscillate with increasing amplitude around the function, driving the system further and further away from its steady-state value. Lastly, if the eigenvalue is a complex number with a negative real part, then the system will oscillate with decreasing amplitude until it eventually reaches its steady state value again.

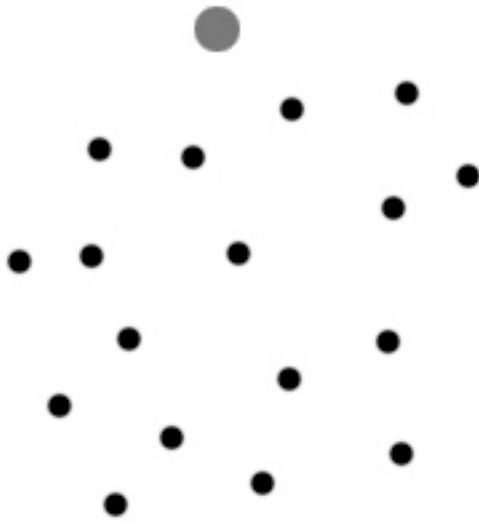
Below is a table of eigenvalues and their effects on a differential system when disturbed. It should be noted that the eigenvalues developed for a system should be reviewed as a system rather than as individual values. That is to say, the effects listed in the table below do not fully represent how the system will respond. If you were to pretend that eigenvalues were nails on a Plinko board, knowing the location and angle of one of those nails would not allow you to predict or know how the Plinko disk would fall down the wall, because you wouldn't know the location or angle of the other nails. If you have information about all of the nails on the Plinko board, you could develop a prediction based on that information. More information on using eigenvalues for stability analysis

can be seen here, [Using eigenvalues and eigenvectors to find stability and solve ODEs Wiki](#).

Eigenvalue	Effect on system when disturbed
Positive real number	Driven away from steady-state value
Negative real number	Driven back to steady-state value
0	Remains at position to which it was disturbed
Identical to another eigenvalue	Effects can not be determined
Complex, positive real number	Oscillates around steady-state value with increasing amplitude
Complex, negative real number	Oscillates around steady-state value with decreasing amplitude
Imaginary	Oscillates around steady-state value with constant amplitude



The above picture is of a plinko board with only one nail position known. Without knowing the position of the other nails, the Plinko disk's fall down the wall is unpredictable.



Knowing the placement of all of the nails on this Plinko board allows the player to know general patterns the disk might follow.

3.5.1 Repeated Eigenvalues

A final case of interest is repeated eigenvalues. While a system of N differential equations must also have N eigenvalues, these values may not always be distinct. For example, the system of equations:

$$\frac{dC_A}{dt} = f_{A \text{ in}} C_{A \text{ in}} - f_{out} C_A \sqrt{V_1} - V_1 k_1 C_A C_B$$

$$\frac{dC_B}{dt} = f_{B \text{ in}} C_{B \text{ in}} - f_{out} C_B \sqrt{V_1} - V_1 k_1 C_A C_B$$

$$\frac{dC_C}{dt} = -f_{out} C_C \sqrt{V_1} + V_1 k_1 C_A C_B$$

$$\frac{dV_1}{dt} = f_{A \text{ in}} + f_{B \text{ in}} - f_{out} \sqrt{V_1}$$

$$\frac{dV_2}{dt} = f_{out} \sqrt{V_1} - f_{customer} \sqrt{V_2}$$

$$\frac{dC_{C2}}{dt} = f_{out} C_C \sqrt{V_1} - f_{customer} C_{C2} \sqrt{V_2}$$

May yield the eigenvalues: $\{-82, -75, -75, -75, -0.66, -0.66\}$, in which the roots ‘-75’ and ‘-0.66’ appear multiple times. Repeat eigenvalues bear further scrutiny in any analysis because they might represent an edge case, where the system is operating at some extreme. In mathematical terms, this means that linearly independent eigenvectors cannot be generated to complete the matrix basis without further analysis. In “real-world” engineering terms, this means that a system at an edge case could distort or fail unexpectedly.

However, for the general solution:

$$Y(t) = k_1 \exp(\lambda t)V_1 + k_2 \exp(\lambda t)(tV_1 + V_2)$$

If $\lambda < 0$, as t approaches infinity, the solution approaches 0, indicating a stable sink, whereas if $\lambda > 0$, the solution approaches infinity in the limit, indicating an unstable source. Thus the rules above can be roughly applied to repeat eigenvalues, that the system is still likely stable if they are real and less than zero and likely unstable if they are real and positive. Nonetheless, one should be aware that unusual behavior is possible. This course will not concern itself with resultant behavior of repeat eigenvalues, but for further information, see:

http://en.wikipedia.org/wiki/Edge_case

<http://math.rwinters.com/S21b/supplements/newbasis.pdf>

<http://www.sosmath.com/diffeq/system/linear/eigenvalue/repeated/repeated.html>

3.6 Worked out Example 1

Your immediate supervisor, senior engineer Captain Johnny Goonewadd, has brought you in on a project dealing with a new silicone-based sealant that is on the ground level of research. Your job is to characterize the thermal expansion of the sealant with time given a constant power supply. Luckily, you were given a series of differential equations that relate temperature and volume in terms of one another with respect to time (Note: T and V are both dimensionless numbers with respect to their corresponding values at $t=0$). Solve the system of differentials and determine the equations for both Temperature and Volume in terms of time.

You are given the initial condition at time $t=0$, $T=1$ and $V=1$

$$\begin{aligned} \frac{dT}{dt} &= 4T - 3V \\ \frac{dV}{dt} &= 3T + 4V \end{aligned}$$

By defining a matrix for both the coefficients and dependant variables we are able to rewrite the above series of differentials in matrix form

$$A = \begin{bmatrix} 4 & -3 \\ 3 & 4 \end{bmatrix}$$

$$X = \begin{bmatrix} T \\ V \end{bmatrix}$$

$$A * X = \begin{bmatrix} \frac{dT}{dt} \\ \frac{dV}{dt} \end{bmatrix}$$

Lambda is inserted into the A matrix to determine the Eigenvalues

$$\det(A - \lambda I) = 0$$

$$\det \begin{bmatrix} 4 - \lambda & -3 \\ 3 & 4 - \lambda \end{bmatrix} = 0$$

$$(4 - \lambda)^2 + 9 = 0$$

$$\lambda_1 = 4 - 3i$$

$$\lambda_2 = 4 + 3i$$

For each eigenvalue, we must find the eigenvector. Let us start with $\lambda_1 = 4 - 3i$

$$(A - \lambda I)v = 0$$

$$\begin{bmatrix} 4 - (4 - 3i) & -3 \\ 3 & 4 - (4 - 3i) \end{bmatrix}$$

$$3iT - 3V = 0$$

$$3T + 3iV = 0$$

$$v_1 = \begin{bmatrix} 1 \\ i \end{bmatrix}$$

Now we find the eigenvector for the eigenvalue $\lambda_2 = 4 + 3i$

$$\begin{aligned}
(A - \lambda I)v &= 0 \\
\begin{bmatrix} 4 - (4 + 3i) & -3 \\ 3 & 4 - (4 + 3i) \end{bmatrix} \\
-3iT - 3V &= 0 \\
3T - 3iV &= 0 \\
v_1 &= \begin{bmatrix} 0 \\ 0 \end{bmatrix}
\end{aligned}$$

The general solution is in the form

$$\begin{aligned}
x(t) &= c_1 e^{\lambda_1 t} v_1 + c_2 e^{\lambda_2 t} v_2 \\
\begin{bmatrix} T(t) \\ V(t) \end{bmatrix} &= c_1 \begin{bmatrix} 1 \\ i \end{bmatrix} e^{(4-3i)t} + c_2 \begin{bmatrix} 0 \\ 0 \end{bmatrix} e^{(4+3i)t} \\
\begin{bmatrix} T(t) \\ V(t) \end{bmatrix} &= c_1 \begin{bmatrix} 1 \\ i \end{bmatrix} e^{(4-3i)t}
\end{aligned}$$

A mathematical proof, [Euler's formula](#), exists for transforming complex exponentials into functions of $\sin(t)$ and $\cos(t)$

$$e^{(a+bi)t} = e^{at} (\cos(bt) - i \sin(bt))$$

Thus

$$\begin{bmatrix} T(t) \\ V(t) \end{bmatrix} = c_1 \begin{bmatrix} 1 \\ i \end{bmatrix} e^{4t} (\cos(3t) - i \sin(3t))$$

Simplifying

$$\begin{bmatrix} T(t) \\ V(t) \end{bmatrix} = e^{4t} \begin{bmatrix} c_1 \cos(3t) - c_1 i \sin(3t) \\ c_1 i \cos(3t) + c_1 \sin(3t) \end{bmatrix}$$

Since we already don't know the value of c_1 , let us make this equation simpler by making the following substitution

$$\begin{aligned}c_3 &= c_1 \\c_4 &= c_1 i\end{aligned}$$

Thus, we get have our solution in terms of real numbers

$$\begin{bmatrix} T(t) \\ V(t) \end{bmatrix} = e^{4t} \begin{bmatrix} c_3 \cos(3t) - c_4 \sin(3t) \\ c_4 \cos(3t) + c_3 \sin(3t) \end{bmatrix}$$

Or, rewriting the solution in scalar form

$$\begin{aligned}T(t) &= e^{4t} (c_3 \cos(3t) - c_4 \sin(3t)) \\V(t) &= e^{4t} (c_3 \sin(3t) + c_4 \cos(3t))\end{aligned}$$

Now that we have our solutions, we can use our initial conditions to find the constants c_3 and c_4

First initial condition: $t=0, T=1$

$$\begin{aligned}T(t) &= e^{4t} (c_3 \cos(3t) - c_4 \sin(3t)) \\1 &= e^{4*0} (c_3 \cos(3 * 0) - c_4 \sin(3 * 0)) \\1 &= 1 * (c_3 * 1 - c_4 * 0) \\c_3 &= 1\end{aligned}$$

First initial condition: $t=0, V=1$

$$\begin{aligned}V(t) &= e^{4t} (c_3 \sin(3t) + c_4 \cos(3t)) \\1 &= e^{4*0} (c_3 \sin(3 * 0) + c_4 \cos(3 * 0)) \\1 &= 1 * (c_3 * 0 + c_4 * 1) \\c_4 &= 1\end{aligned}$$

We have now arrived at our solution

$$T(t) = e^{4t}(\cos(3t) - \sin(3t))$$

$$V(t) = e^{4t}(\sin(3t) + \cos(3t))$$

See [Using eigenvalues and eigenvectors to find stability and solve ODEs Wiki](#) for solving ODEs using the eigenvalues and eigenvectors.

3.7 Worked out Example 2

Process Engineer, Dilbert Pickel, has started his first day for the Helman's Pickel Brine Factory. His first assignment is with a pre-startup team formulated to start up a new plant designed to make grousley sour pickle brine. Financial constraints have demanded that the process begin to produce good product as soon as possible. However, you are forced to reflux the process until you reach the set level of sourness. You have equations that relate all of the process variable in terms of one another with respect to time. Therefore, it is Dill Pickles job to characterize all of the process variables in terms of time (dimensionless Sourness, Acidity, and Water content; S, A, & W respectively). Below is the set of differentials that will be used to solve the equation.

$$\frac{dS}{dt} = S + A + 10W$$

$$\frac{dA}{dt} = S + 5A + 2W$$

$$\frac{dW}{dt} = 4S + 3A + 8W$$

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 10 \\ 1 & 5 & 2 \\ 4 & 3 & 8 \end{bmatrix}$$

Thus the coefficient matrix

Using mathematica it is easy to input the coefficients of the system of equations into a matrix and determine both the eigenvalues and eigenvectors.

```
In[6]:= A = {{1, 1, 10}, {1, 5, 2}, {4, 3, 8}}; MatrixForm[A]
Eigenvalues[A]
Eigenvectors[A]

Out[6]/MatrixForm=

$$\begin{pmatrix} 1 & 1 & 10 \\ 1 & 5 & 2 \\ 4 & 3 & 8 \end{pmatrix}$$

Out[7]= {5 +  $\sqrt{59}$ , 4, 5 -  $\sqrt{59}$ }
Out[8]= {{- $\frac{116}{55}$  +  $\frac{13}{55}$  (5 +  $\sqrt{59}$ ),  $\frac{8}{55}$  +  $\frac{1}{55}$  (5 +  $\sqrt{59}$ ), 1}, {2, -4, 1}, {- $\frac{116}{55}$  +  $\frac{13}{55}$  (5 -  $\sqrt{59}$ ),  $\frac{8}{55}$  +  $\frac{1}{55}$  (5 -  $\sqrt{59}$ ), 1}}
```

The eigenvectors can then be used to determine the final solution to the system of differentials. Some data points will be necessary in order to determine the constants.

$$\begin{bmatrix} S \\ A \\ W \end{bmatrix} = C_1 \begin{bmatrix} 0.88 \\ 0.38 \\ 1 \end{bmatrix} e^{(5+\sqrt{59})t} + C_2 \begin{bmatrix} 2 \\ -4 \\ 1 \end{bmatrix} e^{4t} + C_3 \begin{bmatrix} -2.74 \\ 0.10 \\ 1 \end{bmatrix}$$

See [Using eigenvalues and eigenvectors to find stability and solve ODEs Wiki](#) for solving ODEs using the eigenvalues and eigenvectors.

3.8 Worked Out Example 3

It is possible to find the Eigenvalues of more complex systems than the ones shown above. Doing so, however, requires the use of advanced math manipulation software tools such as Mathematica. Using Mathematica, it is possible to solve the system of ODEs shown below.

$$\frac{dX}{dt} = 8X + \frac{10XYZ}{X + Z}$$

$$\frac{dY}{dt} = 4F - Y - Z - \frac{3XY}{X + Y}$$

$$\frac{dZ}{dt} = 9X - 2Z + F$$

Obviously, this system of ODEs has 4 variables and only 3 equations.

Obviously, this is a more complex set of ODEs than the ones shown above. And even though they will create a more complex set of Eigenvalues, they are solved for in the same way when using Mathematica.

Using the code shown below:

```
In[39]:= eqns =
{
  8 * X + 10 * X * Y * F / (Y + Z) ,
  4 * F - Y - Z - 3 * X * Y / (X + Y) ,
  9 * X - 2 * Z + F
}
```

```
Out[39]= {8 X +  $\frac{10 F X Y}{Y + Z}$ , 4 F - Y -  $\frac{3 X Y}{X + Y}$  - Z, F + 9 X - 2 Z}
```

The equations can be entered into Mathematica. The equations are shown again in the output

Then, using the next bit of code:


```

In[37]:= eqns =
{
  8 * X + 10 * X * Y + F / (Y + Z),
  4 * F - Y - Z - 3 * X * Y / (X + Y),
  9 * X - 2 * Z + F
};

s = Solve[{eqns[[1]] == 0, eqns[[2]] == 0, eqns[[3]] == 0}, {X, Y, Z}]

```

```

Out[38]= {{Z -> F/2, X -> 0, Y -> 7 F/2},
{Z -> 1/4 * (-496 F / (-48 - 130 F + 25 F^2) - 440 F^2 / (-48 - 130 F + 25 F^2) + 225 F^3 / (-48 - 130 F + 25 F^2) - 4 * Sqrt[7] * Sqrt[2416 F^2 - 1000 F^3 + 175 F^4] / (-48 - 130 F + 25 F^2) - 5 * Sqrt[7] * F * Sqrt[2416 F^2 - 1000 F^3 + 175 F^4] / (-48 - 130 F + 25 F^2)),
X -> 1/18 * (-2 F - 496 F / (-48 - 130 F + 25 F^2) - 440 F^2 / (-48 - 130 F + 25 F^2) + 225 F^3 / (-48 - 130 F + 25 F^2) - 4 * Sqrt[7] * Sqrt[2416 F^2 - 1000 F^3 + 175 F^4] / (-48 - 130 F + 25 F^2) - 5 * Sqrt[7] * F * Sqrt[2416 F^2 - 1000 F^3 + 175 F^4] / (-48 - 130 F + 25 F^2)),
Y -> (124 F - 45 F^2 + Sqrt[7] * Sqrt[2416 F^2 - 1000 F^3 + 175 F^4]) / (-48 - 130 F + 25 F^2)},
{Z -> 1/4 * (-496 F / (-48 - 130 F + 25 F^2) - 440 F^2 / (-48 - 130 F + 25 F^2) + 225 F^3 / (-48 - 130 F + 25 F^2) + 4 * Sqrt[7] * Sqrt[2416 F^2 - 1000 F^3 + 175 F^4] / (-48 - 130 F + 25 F^2) + 5 * Sqrt[7] * F * Sqrt[2416 F^2 - 1000 F^3 + 175 F^4] / (-48 - 130 F + 25 F^2)),
X -> 1/18 * (-2 F - 496 F / (-48 - 130 F + 25 F^2) - 440 F^2 / (-48 - 130 F + 25 F^2) + 225 F^3 / (-48 - 130 F + 25 F^2) + 4 * Sqrt[7] * Sqrt[2416 F^2 - 1000 F^3 + 175 F^4] / (-48 - 130 F + 25 F^2) + 5 * Sqrt[7] * F * Sqrt[2416 F^2 - 1000 F^3 + 175 F^4] / (-48 - 130 F + 25 F^2)),
Y -> (124 F - 45 F^2 - Sqrt[7] * Sqrt[2416 F^2 - 1000 F^3 + 175 F^4]) / (-48 - 130 F + 25 F^2)}}}

```

The it is possible to find where the equations are equal to 0 (i.e. the fixed points). The results of this is also shown in the image above. It's notable that 3 solutions are found. This makes sense as the system is 3 ODEs.

The Jacobian can then be found by simply using the code shown below.

```

In[42]:= eqns =
{
  8 * X + 10 * X * Y + F / (Y + Z),
  4 * F - Y - Z - 3 * X * Y / (X + Y),
  9 * X - 2 * Z + F
};

s = Solve[{eqns[[1]] == 0, eqns[[2]] == 0, eqns[[3]] == 0}, {X, Y, Z}];

Jac = {
  {D[eqns[[1]], X], D[eqns[[1]], Y], D[eqns[[1]], Z]},
  {D[eqns[[2]], X], D[eqns[[2]], Y], D[eqns[[2]], Z]},
  {D[eqns[[3]], X], D[eqns[[3]], Y], D[eqns[[3]], Z]}
}

```

```

Out[44]= {{8 + 10 F Y / (Y + Z), -10 F X Y / (Y + Z)^2 + 10 F X / (Y + Z), -10 F X Y / (Y + Z)^2}, {3 X Y / (X + Y)^2 - 3 Y / (X + Y), -1 + 3 X Y / (X + Y)^2 - 3 X / (X + Y), -1}, {9, 0, -2}}

```

The results of finding the Jacobian are shown in the equation above.

Finally, to find one of the Eigenvalues, one can simply use the code shown below.

```

In[57]:= eqns =
  {
    8 * X + 10 * X * Y * F / (Y + Z),
    4 * F - Y - Z - 3 * X * Y / (X + Y),
    9 * X - 2 * Z + F
  };

s = Solve[{eqns[[1]] == 0, eqns[[2]] == 0, eqns[[3]] == 0}, {X, Y, Z}];

Jac = {
  {D[eqns[[1]], X], D[eqns[[1]], Y], D[eqns[[1]], Z]},
  {D[eqns[[2]], X], D[eqns[[2]], Y], D[eqns[[2]], Z]},
  {D[eqns[[3]], X], D[eqns[[3]], Y], D[eqns[[3]], Z]}
};

t1 = Simplify[Eigenvalues[Jac /. s[[1]]]]

```

```

Out[60]= {-2, -1, 8 +  $\frac{35 F}{4}$ }

```

This gives the Eigenvalue when the first fixed point (the first solution found for "s") is applied. The other two solutions could be found by simply changing the fixed blade that is referred to when finding t1. The other Eigenvalues are not shown because of their large size.

3.9 Multiple Choice Questions

3.9.1 Question 1

What are the eigenvalues for the matrix A?

$$\mathbf{A} = \begin{bmatrix} 4 & 2 \\ 3 & -1 \end{bmatrix}$$

a) $\lambda_1 = -2 \quad \lambda_2 = 5$

- b) $\lambda_1 = 2$ $\lambda_2 = -5$
- c) $\lambda_1 = 2$ $\lambda_2 = 5$
- d) $\lambda_1 = -2$ $\lambda_2 = -5$

3.9.2 Question 2

When a differential system with a real negative eigenvalue is disturbed, the system is...

- a) Driven away from the steady state value
- b) Unchanged and remains at the disturbed value
- c) Driven back to the steady state value
- d) Unpredictable and the effects can not be determined

3.10 Multiple Choice Answers

3.10.1 Question 1 Answer

```
In[1]:= A = {{4, 2}, {3, -1}};
```

```
MatrixForm[A]
```

```
Out[2]/MatrixForm=
```

$$\begin{pmatrix} 4 & 2 \\ 3 & -1 \end{pmatrix}$$

```
In[3]:= Eigenvalues[A]
```

```
Out[3]= {5, -2}
```

a. $\lambda_1 = -2$ $\lambda_2 = 5$

[#Calculating Eigenvalues and Eigenvectors using Numerical Software](#)

3.10.2 Question 2 Answer

c. A real negative eigenvalue is indicative of a stable system that will return to the steady state value after it is disturbed.

[#Using Eigenvalues to Determine Effects of Disturbing a System](#)

3.11 Sage's Corner

<http://video.google.com/googleplayer.swf?docId=5005666994126795748>

Click here for an electronic version of the slideshow [PDF of slides from Presentation 1](#)

<http://video.google.com/googleplayer.swf?docId=-3334285703170917951>
[PDF Eigenvalues Presentation](#)


Also [here is a lecture on eigenvalues and eigenvectors](#) from Spring 2005 from MIT. Note that this lecture is in real media requiring a player.

3.12 References

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Section 4. Using eigenvalues and eigenvectors to find stability and solve ODEs

Title: Using eigenvalues and eigenvectors to find stability and solve ODEs

Note:  [Video lecture](#) available for this section!

Authors: Daniel Katzman, Jessica Moreno, Jason Noelanders, and Mark Winston-Galant

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

4.1 Introduction

Eigenvalues and eigenvectors are very useful in the modeling of chemical processes. When designing the controls for a process it is necessary to create a program to operate these controls. Differential equations are used in these programs to operate the controls based on variables in the system. These equations can either be solved by hand or by using a computer program. The solutions for these differential equations will determine the stability of the system. After finding this stability, you can show whether the system will be stable and damped, unstable and undamped (so that there is constant fluctuation in the system), or as an unstable system in which the amplitude of the fluctuation is always increasing. For the first case, a stable and damped system, if there is a change, the system will adjust itself properly to return to steady state. For the other two cases, the system will not be able to return to steady state. For the undamped situation, the constant fluctuation will be hard on the system and can lead to equipment failure. The final situation, with the ever increasing amplitude of the fluctuations will lead to a catastrophic failure.

There are a couple ways to develop the differential equation used to determine stability. First, you can create a differential equation to guide the system where the variables are the readings from the sensors in the system. A second method would be using actual data found from running the system. You could fit a differential equation to this data and use that equation for stability determination.

In this section on Eigenvalue Stability, we will first show how to use eigenvalues to solve a system of linear ODEs. Next, we will use the eigenvalues to show us the stability of the system. After that, another method of determining stability, the Routh stability test, will be introduced. For the Routh stability test, calculating the eigenvalues is unnecessary which is a benefit since sometimes that is difficult. Finally, the advantages and disadvantages of using eigenvalues to evaluate a system's stability will be discussed.

4.2 Solving ODEs

Eigenvalues and eigenvectors can be used as a method for solving linear systems of ordinary differential equations (ODEs). The method is rather straight-forward and not too tedious for smaller systems. See [The Eigenvector Eigenvalue Method](#) for solving systems by hand and [Linearizing ODEs](#) for a linear algebra/Jacobian matrix review. When trying to solve large systems of ODEs however, it is usually best to use some sort of mathematical computer program. Mathematica is a program that can be used to solve systems of ordinary differential equations when doing them by hand is simply too tedious. Once one overcomes the syntax of Mathematica, solving enormous systems of ordinary linear differential equations becomes a piece of cake!

4.2.1 Using Eigenvalues to Solve a System

A linear system will be solve by hand and using Eigenvalues[] expression in Mathematica simultaneously. Note that, in the Mathematica inputs below, "In[:]=" is not literally typed into the program, only what is after it. The syntax needed to be typed is the line following "In[:]=" . The term is used here to more accurately demonstrate coding in Mathematica. To find a general solution of the linear system of ordinary differential equation:

$$\begin{aligned}\frac{dx}{dt} &= 4x + 8y \\ \frac{dy}{dt} &= 10x + 2y\end{aligned}$$

We first put the system in matrix form:

$$A = \begin{bmatrix} \frac{dx}{dt} \\ \frac{dy}{dt} \end{bmatrix} = \begin{bmatrix} 4 & 8 \\ 10 & 2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$
$$A = \begin{bmatrix} 4 & 8 \\ 10 & 2 \end{bmatrix}$$

Where we can see that

In mathematica, we can use the following code to represent A:

In[1]:= **MatrixForm** [{{4,8},{10,2}}

$$\text{Out[1]} := \begin{bmatrix} 4 & 8 \\ 10 & 2 \end{bmatrix}$$

The eigenvalues λ_1 and λ_2 , are found using the characteristic equation of the matrix A, $\det(A - \lambda I) = 0$.

$$\begin{aligned} \det(A - \lambda I) &= 0 \\ \det\left(\begin{bmatrix} 4 & 8 \\ 10 & 2 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right) &= 0 \\ \det\begin{bmatrix} 4 - \lambda & 8 \\ 10 & 2 - \lambda \end{bmatrix} &= 0 \\ (4 - \lambda)(2 - \lambda) - 80 &= 0 \\ (\lambda - 12)(\lambda + 6) &= 0 \end{aligned}$$

Therefore, $\lambda_1 = 12$ and $\lambda_2 = -6$

We can use Mathematica to find the eigenvalues using the following code:

In[2]:= **Eigenvalues** [{{4,8},{10,2}}

Out[2]:= {12,-6}

Now, for each eigenvalue ($\lambda_1=12$ and $\lambda_2=-6$), an eigenvector associated with it can be

found using $(A - \lambda I)\vec{v} = 0$, where \vec{v} is an eigenvector such that $A\vec{v} = \lambda\vec{v}$

i) For $\lambda_1=12$

$$\begin{aligned} (A - \lambda_1 I)\vec{v} &= 0 \\ \begin{bmatrix} 4 - 12 & 8 - 0 \\ 10 - 0 & 2 - 12 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} &= 0 \end{aligned}$$

$$\begin{bmatrix} -8 & 8 \\ 10 & -10 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 0$$

This will lead to the equations (1) &(2):

$$\begin{aligned} -8x + 8y &= 0 & \text{(1)} \\ +10x - 10y &= 0 & \text{(2)} \end{aligned}$$

The Mathematica input is:

In[3]:= **eqn1= -8x+8y==0**

In[4]:= **eqn2= 10x-10y==0**

In[5]:= **Solve[{eqn1,eqn2},{x,y}]**

Out[5]:= **{{ y -> x }}**

Equations (1) & (2) lead to the solution $y = x$

ii) For $\lambda_2=-6$,

$$\begin{aligned} (A - \lambda_2 I)\vec{v} &= 0 \\ \begin{bmatrix} 4 + 6 & 8 - 0 \\ 10 - 0 & 2 + 6 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} &= 0 \\ \begin{bmatrix} 10 & 8 \\ 10 & 8 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} &= 0 \end{aligned}$$

This will lead to the equations (3) & (4):

$$\begin{aligned} 10x + 8y &= 0 & \text{(3)} \\ 10x + 8y &= 0 & \text{(4)} \end{aligned}$$

The Mathematica input is:

In[6]:= **eqn3= 10x+8y==0**

In[7]:= **eqn4= 10x+8y==0**

In[8]:= `Solve[{eqn3,eqn4},{x,y}]`

Out[8]:= $\left\{ \left\{ y \rightarrow -\frac{5}{4}x \right\} \right\}$

Equations (3) & (4) lead to the solution $y = -\frac{5}{4}x$.

Recall that the direction of a vector such as $\begin{bmatrix} 1 \\ 2 \end{bmatrix}$ is the same as the vector $\begin{bmatrix} 4 \\ 8 \end{bmatrix}$ or any other scalar multiple. Therefore, to get the eigenvector, we are free to choose for either the value x or y.

i) For $\lambda_1 = 12$

We have arrived at $y = x$. As mentioned earlier, we have a degree of freedom to choose for either x or y. Let's assume that $x=1$. Then, $y=1$ and the eigenvector \vec{v}_1 associated

$$\vec{v}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

with the eigenvalue λ_1 is

ii) For $\lambda_2 = -6$

We have arrived at $y = -\frac{5}{4}x$. Let's assume that $x = 4$. Then, $y = -5$ and the

$$\vec{v}_2 = \begin{bmatrix} 4 \\ -5 \end{bmatrix}$$

eigenvector associated with the eigenvalue λ_2 is

These two eigenvalues and associated eigenvectors yield the solution:

$$\begin{bmatrix} x(t) \\ y(t) \end{bmatrix} = c_1 \begin{bmatrix} 1 \\ 1 \end{bmatrix} e^{12t} + c_2 \begin{bmatrix} 4 \\ -5 \end{bmatrix} e^{-6t}$$

Hence a general solution of the linear system in scalar form is:

$$x(t) = c_1 e^{12t} + c_2 4e^{-6t}$$

$$y(t) = c_1 e^{12t} - c_2 5e^{-6t}$$

4.2.2 Solving a System Using DSolve

Using the same linear system of ordinary differential equations:

$$\frac{dx}{dt} = 4x + 8y$$

$$\frac{dy}{dt} = 10x + 2y$$

We input the differential equations to Mathematica with the following command:

In:= `ODEs={x'[t]==4x[t]+8y[t],y'[t]==10x[t]+2y[t]}`

where $x'[t] = \frac{dx}{dt}$ and $y'[t] = \frac{dy}{dt}$

After entering the equations, we use the DSolve function:

In:= `DSolve[ODEs, {x[t], y[t]}, t]`

Mathematica will output the solution:

Out:= {{

$$x[t] \rightarrow \frac{1}{9}e^{-6t}(4 + 5e^{18t})C[1] + \frac{4}{9}e^{-6t}(-1 + e^{18t})C[2]$$

,

$$y[t] \rightarrow \frac{5}{9}e^{-6t}(-1 + e^{18t})C[1] + \frac{1}{9}e^{-6t}(5 + 4e^{18t})C[2]$$

}}

This set of equations, although looks more complicated than the first one, is actually the same.

4.3 Stability

Eigenvalues can be used to determine whether a fixed point (also known as an equilibrium point) is stable or unstable. A stable fixed point is such that a system can be initially disturbed around its fixed point yet eventually return to its original location and remain there. A fixed point is unstable if it is not stable. To illustrate this concept, imagine a round ball in between two hills. If left alone, the ball will not move, and thus its position is considered a fixed point. If we were to disturb the ball by pushing it a little bit up the hill, the ball will roll back to its original position in between the two hills. This is a stable fixed point. Now imagine that the ball is at the peak of one of the hills. If left undisturbed, the ball will still remain at the peak, so this is also considered a fixed point. However, a disturbance in any direction will cause the ball to roll away from the top of the hill. The top of the hill is considered an unstable fixed point.

The eigenvalues of a system linearized around a fixed point can determine the stability behavior of a system around the fixed point. The particular stability behavior depends upon the existence of real and imaginary components of the eigenvalues, along with the signs of the real components and the distinctness of their values. We will examine each of the possible cases below.

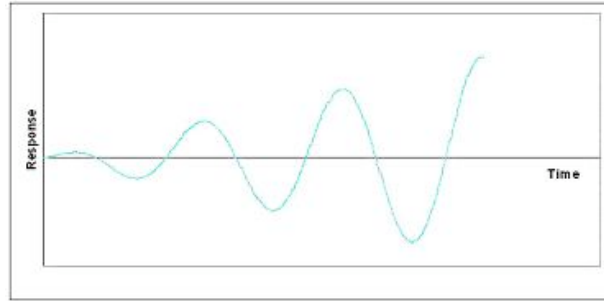
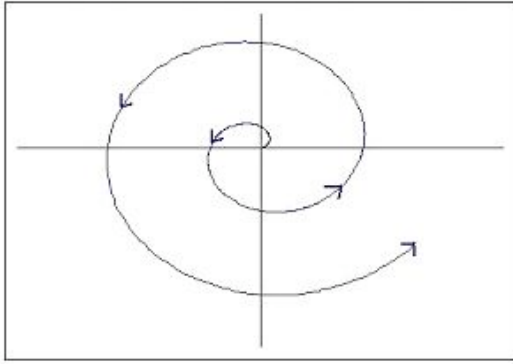
4.3.1 Imaginary (or Complex) Eigenvalues

When eigenvalues are of the form $a + bi$, where a and b are real scalars and i is the imaginary number $\sqrt{-1}$, there are three important cases. These three cases are when the real part a is positive, negative, and zero. In all cases, when the complex part of an eigenvalue is non-zero, the system will be oscillatory.

Positive Real Part

When the real part is positive, the system is unstable and behaves as an unstable oscillator. This can be visualized as a vector tracing a spiral away from the fixed point. The plot of response with time of this situation would look sinusoidal with ever-increasing amplitude, as shown below.

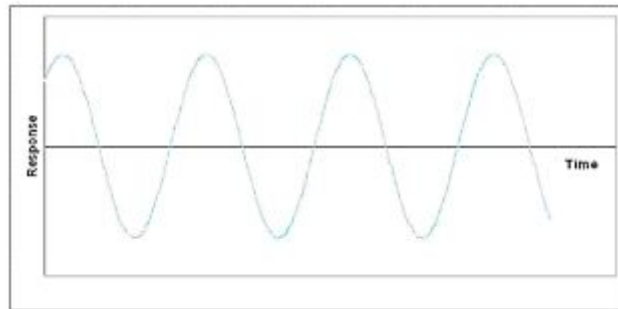
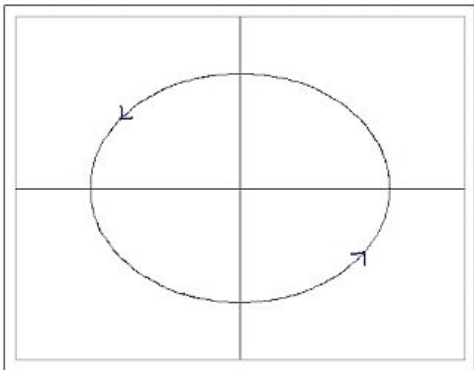
This situation is usually undesirable when attempting to control a process or unit. If there is a change in the process, arising from the process itself or from an external disturbance, the system itself will not go back to steady state.



Zero Real Part

When the real part is zero, the system behaves as an undamped oscillator. This can be visualized in two dimensions as a vector tracing a circle around a point. The plot of response with time would look sinusoidal. The figures below should help in understanding.

Undamped oscillation is common in many control schemes arising out of competing controllers and other factors. Even so, this is usually undesirable and is considered an unstable process since the system will not go back to steady state following a disturbance.

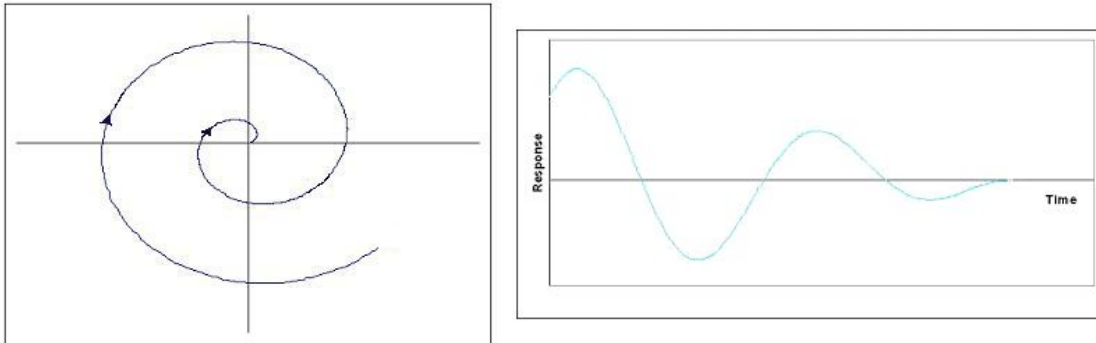


Negative Real Part

When the real part is negative, then the system is stable and behaves as a damped oscillator. This can be visualized as a vector tracing a spiral toward the fixed point. The plot of response with time of this situation would look sinusoidal with ever-decreasing amplitude, as shown below.

This situation is what is generally desired when attempting to control a process or unit. This system is stable since steady state will be reached even after a disturbance to the system. The oscillation will quickly bring the system back to the setpoint, but will overshoot, so if overshooting is a large concern, increased damping would be needed.

While discussing complex eigenvalues with negative real parts, it is important to point out that having all negative real parts of eigenvalues is a necessary and sufficient condition of a stable system.



Complex Part of Eigenvalues

As previously noted, the stability of oscillating systems (i.e. systems with complex eigenvalues) can be determined entirely by examination of the real part. Although the sign of the complex part of the eigenvalue may cause a phase shift of the oscillation, the stability is unaffected.

4.3.2 Real Eigenvalues

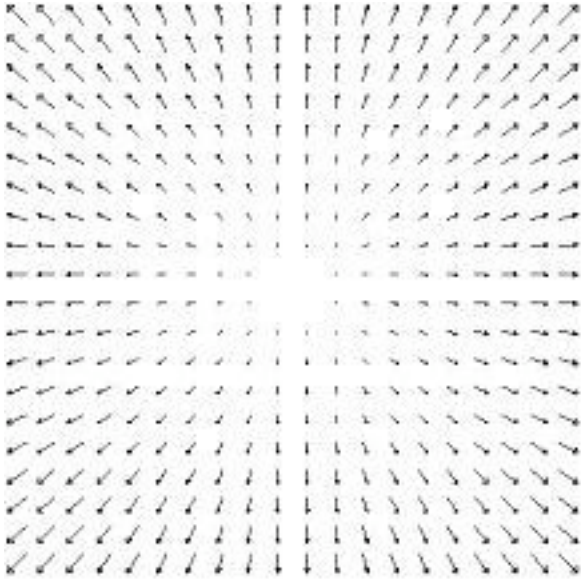
We've seen how to analyze eigenvalues that are complex in form, now we will look at eigenvalues with only real parts.

Zero Eigenvalues

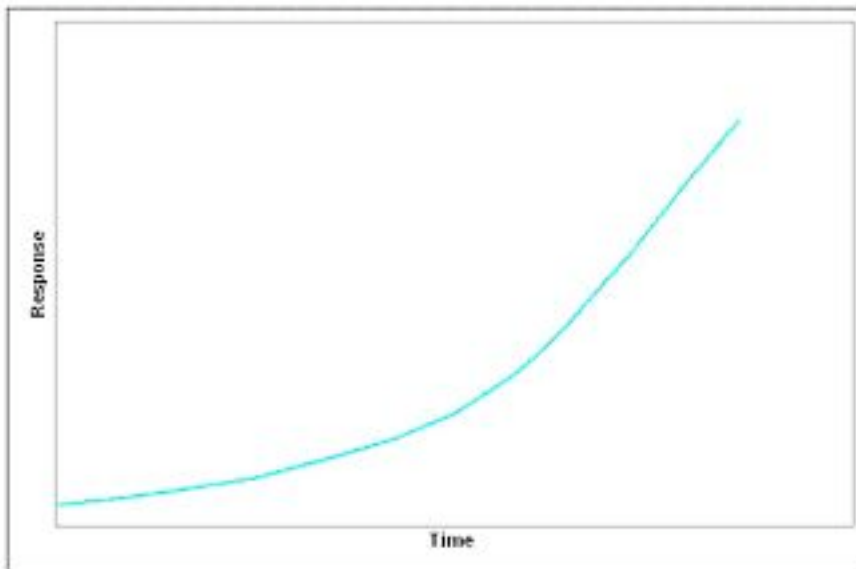
If an eigenvalue has no imaginary part and is equal to zero, the system will be unstable, since, as mentioned earlier, a system will not be stable if its eigenvalues have any non-negative real parts. This is just a trivial case of the complex eigenvalue that has a zero part.

Positive Eigenvalues

When all eigenvalues are real, positive, and distinct, the system is unstable. On a gradient field, a spot on the field with multiple vectors circularly surrounding and pointing out of the same spot (a node) signifies all positive eigenvalues. This is called a source node.

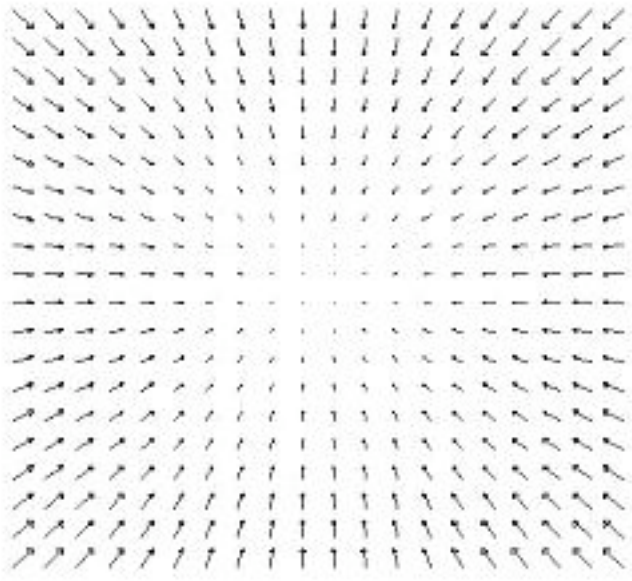


Graphically, real and positive eigenvalues will show a typical exponential plot when graphed against time.

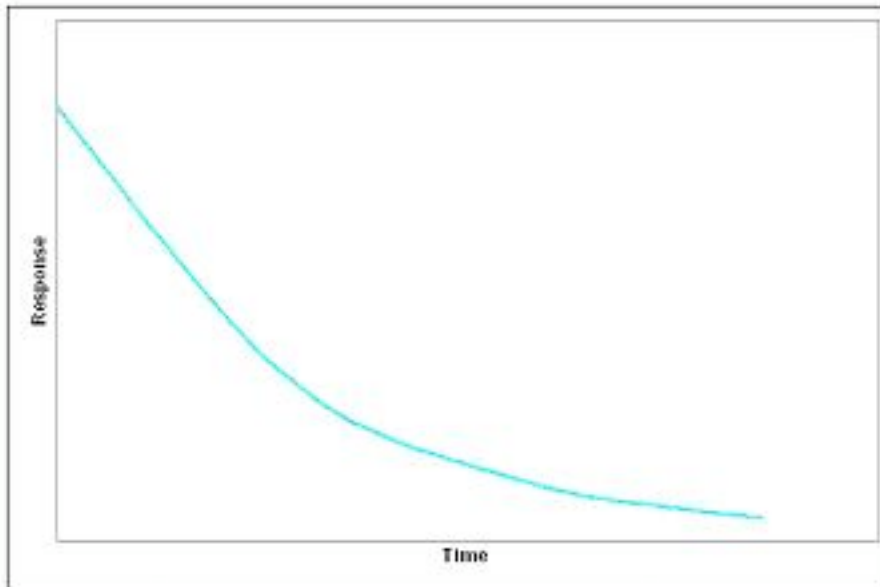


Negative Eigenvalues

When all eigenvalues are real, negative, and distinct, the system is unstable. Graphically on a gradient field, there will be a node with vectors pointing toward the fixed point. This is called a sink node.

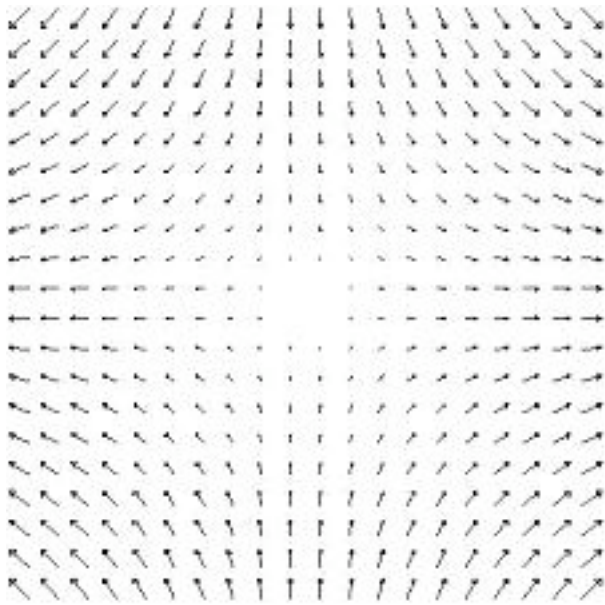


Graphically, real and negative eigenvalues will output an inverse exponential plot.



Positive and Negative Eigenvalues

If the set of eigenvalues for the system has both positive and negative eigenvalues, the fixed point is an unstable saddle point. A saddle point is a point where a series of minimum and maximum points converge at one area in a gradient field, without hitting the point. It is called a saddle point because in 3 dimensional surface plot the function looks like a saddle.

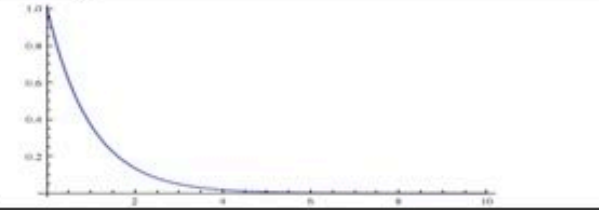
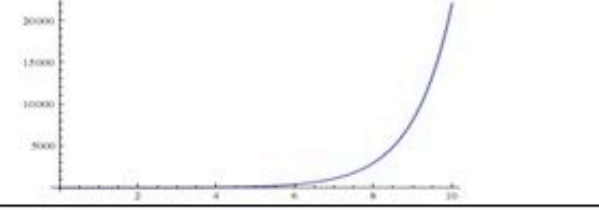
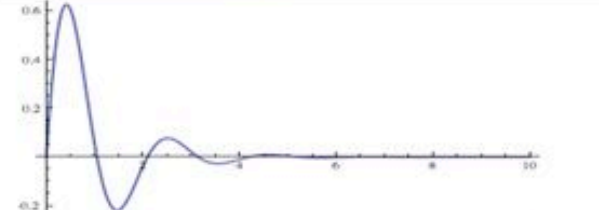
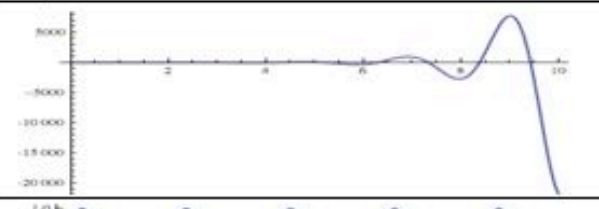
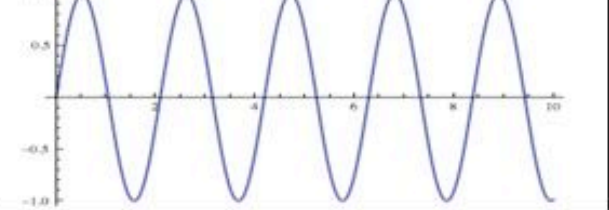


4.3.3 Repeated Eigenvalues

If the set of eigenvalues for the system has repeated real eigenvalues, then the stability of the critical point depends on whether the eigenvectors associated with the eigenvalues are linearly independent, or orthogonal. This is the case of degeneracy, where more than one eigenvector is associated with an eigenvalue. In general, the determination of the system's behavior requires further analysis. For the case of a fixed point having only *two* eigenvalues, however, we can provide the following two possible cases. If the two repeated eigenvalues are positive, then the fixed point is an unstable source. If the two repeated eigenvalues are negative, then the fixed point is a stable sink.

4.3.4 Summary of Eigenvalue Graphs

Below is a table summarizing the visual representations of stability that the eigenvalues represent.

Eigenvalues	Graph
All real and negative	
All real and one or more are positive	
All real eigenvalues are negative and there are imaginary parts	
One or more eigenvalues have a positive real part and there are imaginary parts	
Real parts of the eigenvalues are zero and there are imaginary parts	

Note that the graphs from Peter Woolf's lecture from Fall'08 titled Dynamic Systems Analysis II: Evaluation Stability, Eigenvalues were used in this table.

4.4 Another method of determining stability

The process of finding eigenvalues for a system of linear equations can become rather tedious at times and to remedy this, a British mathematician named Edward Routh came up with a handy little short-cut.

First, recall that an unstable eigenvalue will have a positive or zero real part and that a stable eigenvalue will have a negative real part.

The first test is to take an n-th degree polynomial of interest:

$$P(\lambda) = a_0\lambda^n + a_1\lambda^{n-1} + \dots + a_{n-1}\lambda + a_n$$

and look to see if any of the coefficients are negative or zero. If so, there is at least one value with a positive or zero real part which refers to an unstable node.

The way to test exactly how many roots will have positive or zero real parts is by performing the complete Routh array. Referring to the previous polynomial, it works as follows:

Row					
1	a_0	a_2	a_4	a_6	...
2	a_1	a_3	a_5	a_7	...
3	b_1	b_2	b_3	b_4	...
4	c_1	c_2	c_3	c_4	...
	\vdots	\vdots	\vdots	\vdots	
n-1	p_1	p_2			
n	q_1				
n+1	v_1				

An array of n+1 rows and the coefficients placed as above. After the first two rows, the values are obtained as below:

$$b_1 = \frac{a_1a_2 - a_0a_3}{a_1}, b_2 = \frac{a_1a_4 - a_0a_5}{a_1}, b_3 = \frac{a_1a_6 - a_0a_7}{a_1}, \dots$$

$$c_1 = \frac{b_1a_3 - a_1b_2}{b_1}, c_2 = \frac{b_1a_5 - a_1b_3}{b_1}, c_3 = \frac{b_1a_7 - a_1b_4}{b_1}, \dots$$

Routh's theorem says:

1. For all of the roots of the polynomial to be stable, all the values in the first column of the Routh array must be positive.
2. If any of the values in the first column are negative, then the number of roots with a positive real part equals the number of sign changes in the first column.

So considering the following example,

$$f(x) = 9x^4 + 14x^3 + 7x + 10$$

Preliminary test: All of the coefficients are positive, however, there is a zero coefficient for x^2 so there should be at least one point with a negative or zero real part.

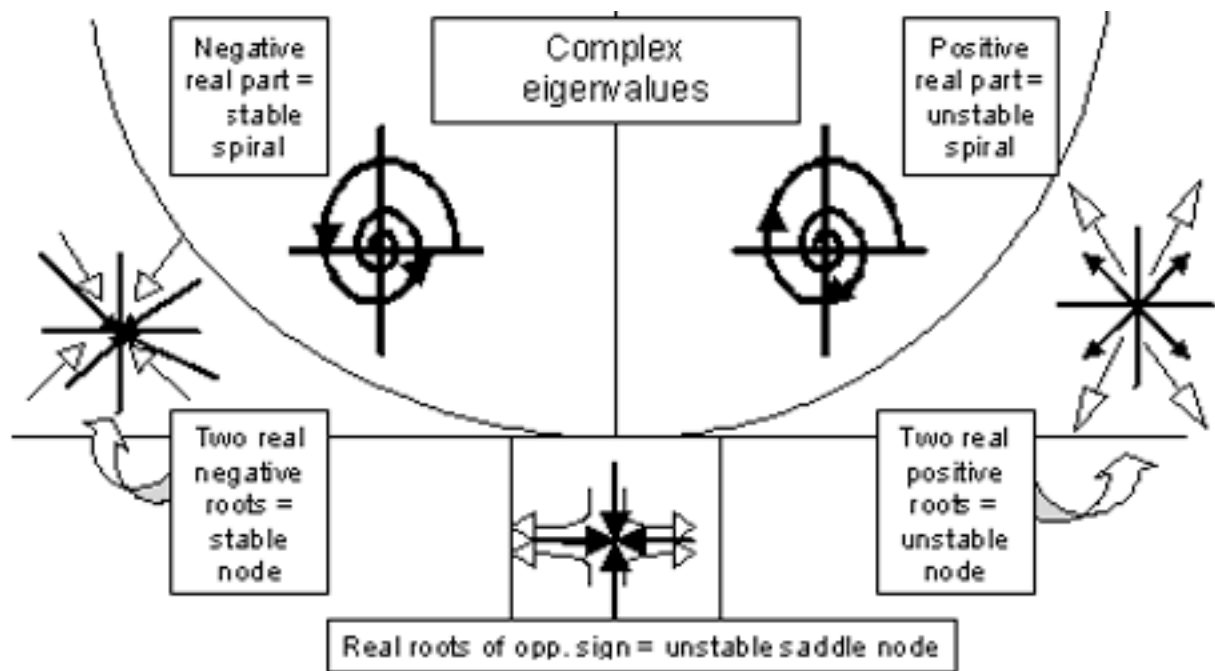
Routh array:

Row			
1	9	0	10
2	14	7	
3	-4.5	10	
4	38.1		
5	10		

Since Row 3 has a negative value, there is a sign change from Row 2 to Row 3 and again from Row 3 to Row 4. Thus, there are 2 roots with positive or zero real part.

4.5 Stability Summary

The following image can work as a quick reference to remind yourself of what vector field will result depending on the eigenvalue calculated.



The table below gives a complete overview of the stability corresponding to each type of eigenvalue.

Eigenvalue Type	Stability	Oscillatory Behavior	Notation
All Real and +	Unstable	None	Unstable Node
All Real and -	Stable	None	Stable Node
Mixed + & - Real	Unstable	None	Unstable saddle point
+a + bi	Unstable	Undamped	Unstable spirral
-a + bi	Stable	Damped	Stable spirral
0 + bi	Unstable	Undamped	Circle
Repeated values	Depends on orthogonality of eigenvectors		

4.6 Advantages and Disadvantages of Eigenvalue Stability

There are several advantages of using eigenvalues to establish the stability of a process compared to trying to simulate the system and observe the results. However, there are situations where eigenvalue stability can break down for some models.

4.6.1 Advantages

1. High accuracy for linear systems.
2. General method that can be applied to a variety of processes.
3. Can be used even if all variables are not defined, such as control parameters.

4.6.2 Disadvantages

1. Only applicable for linear models.
2. Linear approximations of nonlinear models break down away from the fixed point of approximation.

4.7 Worked out Example 1

For the system described by:

$$\frac{dx}{dt} = y$$

$$\frac{dy}{dt} = 2x + y$$

Find the fixed points and determine their stability.

4.7.1 Solution

Step 1. Determining the fixed points

At the fixed points, nothing is changing with respect to time. Therefore, set the derivatives to zero to find the fixed points.

$$\begin{aligned}0 &= y \\ 0 &= 2x + y\end{aligned}$$

Solving these two equations simultaneously, we see that we have one fixed point at $\{0,0\}$

Step 2. Determine the eigenvalue of this fixed point

First, let us rewrite the system of differentials in matrix form.

$$\begin{bmatrix} \frac{dx}{dt} \\ \frac{dy}{dt} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

Next, find the eigenvalues by setting $\det(A - \lambda I) = 0$

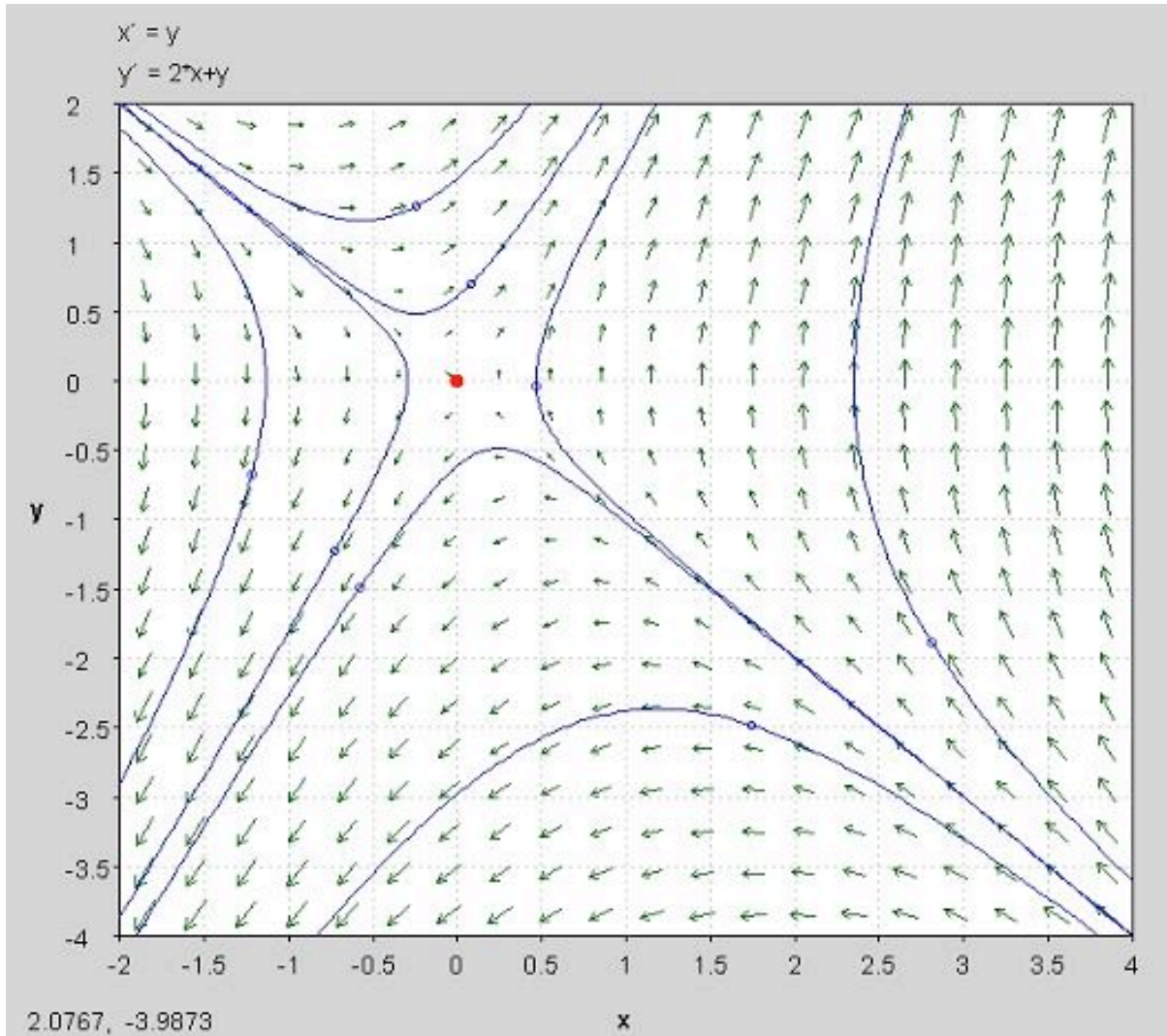
$$\begin{aligned}\det \begin{bmatrix} 0 - \lambda & 1 \\ 2 & 1 - \lambda \end{bmatrix} &= 0 \\ -\lambda(1 - \lambda) - 2 &= 0 \\ \lambda^2 - \lambda - 2 &= 0\end{aligned}$$

Using the quadratic formula, we find that $\lambda_1 = 2$ and $\lambda_2 = -\frac{1}{2}$

Step 3. Determine the stability based on the sign of the eigenvalue

The eigenvalues we found were both real numbers. One has a positive value, and one has a negative value. Therefore, the point $\{0, 0\}$ is an unstable saddle node.

The stability can be observed in the image below. The fixed point is seen at $(0,0)$. All solutions that do not start at $(0,0)$ will travel away from this unstable saddle point. The solution was found by using the two-dimensional system in PPlane 2005.10 [PPlane](#).



4.8 Worked out Example 2

Determine the Routh array and the number of positive or zero roots of the following equation.

$$f(x) = 6x^5 + 12x^4 + 5x^3 + 3x^2 + 17x$$

4.8.1 Solution

Routh Array:

Row

1	6	5	17
2	12	3	0
3	3.5	17	
4	-26.1		
5	17		
6	0		

Since you go from a positive value in row three, to a negative value in row four, and back to a positive value in row five, you will have a positive or zero real part for two of your roots.

4.9 Worked out Example 3

Use Mathematica to find the eigenvalues of the system defined by:

$$\frac{dx_1}{dt} = 8x_1 + 15x_2 - 3x_3 + 7x_4 + 2x_5$$

$$\frac{dx_2}{dt} = -22x_1 - 21x_2 + 3x_3 - 12x_4 + 11x_5$$

$$\frac{dx_3}{dt} = 10x_1 + 6x_2 + 24x_3 + 3x_4 - 6x_5$$

$$\frac{dx_4}{dt} = 0x_1 - 2x_2 + 21x_3 + 0x_4 + 4x_5$$

$$\frac{dx_5}{dt} = 4x_1 + 9x_2 + x_3 - 22x_4 - 7x_5$$

And comment on the stability of this system

4.9.1 Solution

The matrix that corresponds with this system is the square matrix:

$$\begin{bmatrix} 8 & 15 & -3 & 7 & 2 \\ -22 & -21 & 3 & -12 & 11 \\ 10 & 6 & 24 & 3 & -6 \\ 0 & -2 & 21 & 0 & 4 \\ 4 & 9 & 1 & -22 & -7 \end{bmatrix}$$

Using the Eigenvalues[] function in Mathematica the input is:

```
In[1]:= Eigenvalues[{{8, 15, -3, 7, 2}, {-22, -21, 3, -12, 11}, {10, 6, 24, 3, -6}, {0, -2, 21, 0, 4}, {4, 9, 1, -22, -7}}]
```

```
In[2]:= N[%]          This step produces numerical results
```

The output contains the 5 eigenvalues:

```
out[2]:= {27.0612, -10.7653 + 10.0084 i, -10.7653 - 10.0084 i, -0.765272 + 7.71127 i, -0.765272 - 7.71127 i }
```

So the five eigenvalues are:

27.0612

$$-10.7653 + 10.0084i$$

$$-10.7653 - 10.0084i$$

$$-0.765272 + 7.71127i$$

$$-0.765272 - 7.71127i$$

Looking at these eigenvalues it is clear that the system as a whole is unstable. This is because one of the eigenvalues has a positive real part.

4.10 Multiple Choice Question 1

A system is stable if and only if all of the system's eigenvalues:

- a. are real
- b. are complex
- c. have negative real parts
- d. have negative imaginary parts

Answer: c

4.11 Multiple Choice Question 2

What would the following set of eigenvalues predict for the system's behavior?

$$-4, -2 + 3i, -2 - 3i, 3$$

- a. An unstable oscillation
- b. A damped oscillation
- c. An undamped oscillation
- d. A source

e. A saddle point

Answer: d

4.12 Sage's Corner

Eigenvalues & Eigenvectors: Math That Happens in Vegas, Stays in Vegas

<http://video.google.com/googleplayer.swf?docId=2359424877194610618>


[File:EigenvaluesAndEigenvectors.ppt Slides Without Narration](#)

4.13 References

- Kravaris, Costas. *Chemical Process Control: A Time Domain Approach*.
- Liptak, Bela G., *Process Control and Optimization. Vol. II*. New York: Taylor & Francis.

Section 5. Phase plane analysis: attractors, spirals, limit cycles

Title: Phase Plane Analysis

Note:  [Video lecture](#) available for this section!

Authors: Erin Knight, Dipti Sawalka, Matt Russell, Spencer Yendell

Stewards: Eric Black, Megan Boekeloo, Daniel Carter, Stacy Young

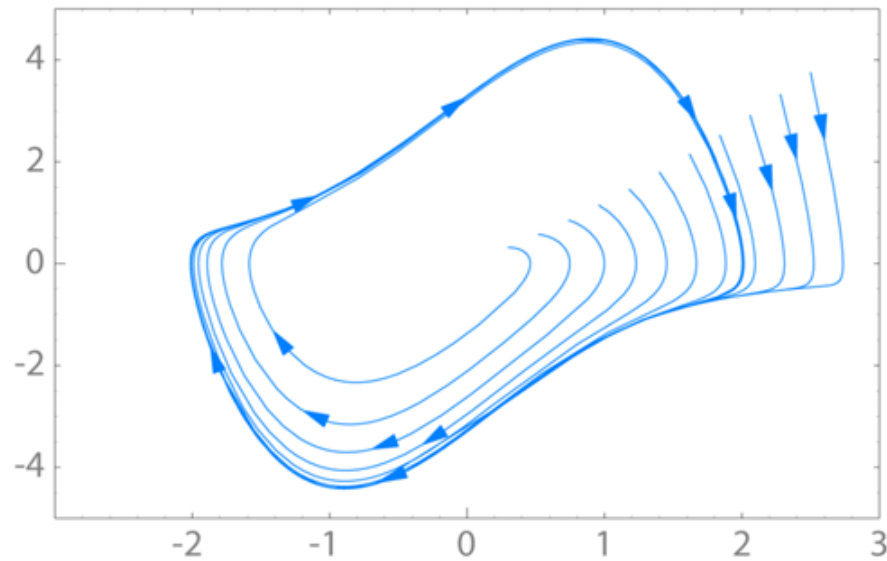
Date created: 10/23/06; updated: 10/24/07

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

5.1 Introduction to Attractors, Spirals and Limit Cycles

We often use differential equations to model a dynamic system such as a valve opening or tank filling. Without a driving force, dynamic systems would stop moving. At the same time dissipative forces such as internal friction and thermodynamic losses are taking away from the driving force. Together the opposing forces cancel any interruptions or initial conditions and cause the system to settle into typical behavior. Attractors are the location that the dynamic system is drawn to in its typical behavior. Attractors can be fixed points, limit cycles, spirals or other geometrical sets.

Limit cycles are much like sources or sinks, except they are closed trajectories rather than points. Once a trajectory is caught in a limit cycle, it will continue to follow that cycle. By definition, at least one trajectory spirals into the limit cycle as time approaches either positive or negative infinity. Like a sink, attractive (stable) limit cycles have the neighboring trajectories approaching the limit cycle as time approaches positive infinity. Like a source, non-attractive (unstable) limit cycles have the neighboring trajectories approaching the limit cycle as time approaches negative infinity. Below is an illustration of a limit cycle [1].



Spirals are a similar concept. The attractor is a spiral if it has complex eigenvalues. If the real portion of the complex eigenvalue is positive (i.e. $3 + 2i$), the attractor is unstable and the system will move away from steady-state operation given a disturbance. If the real portion of the eigenvalue is negative (i.e. $-2 + 5i$), the attractor is stable and will return to steady-state operation given a disturbance.

Given the following set of linear equations we will walk through an example that produces a spiral:

$$\frac{dx}{dt} = 2x + 5y$$

$$\frac{dy}{dt} = -5x + 2y$$

The Jacobian matrix would be the coefficients:

$$A = \begin{vmatrix} 2 & 5 \\ -5 & 2 \end{vmatrix}$$

Next we found the eigenvalues:

$$(A - \lambda I) = \begin{vmatrix} 2 & 5 \\ -5 & 2 \end{vmatrix} - \lambda \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} = \begin{vmatrix} (2 - \lambda) & 5 \\ -5 & (2 - \lambda) \end{vmatrix}$$

where I is the identity matrix

$$\det(A - \lambda I) = (2 - \lambda)^2 + 25 = 0$$

Eigenvalues: $\lambda = 2 \pm 5i$

The system is unstable because the real portion of the complex eigenvalues is positive.

To find the first eigenvector we continue by plugging in $2 - 5i$:

$$\begin{vmatrix} (2 - \lambda) & 5 \\ -5 & (2 - \lambda) \end{vmatrix} = \begin{vmatrix} 2 - (2 - 5i) & 5 \\ -5 & 2 - (2 - 5i) \end{vmatrix} = \begin{vmatrix} 5i & 5 \\ -5 & 5i \end{vmatrix}$$

$$(A - \lambda I)v = \begin{vmatrix} 5i & 5 \\ -5 & 5i \end{vmatrix} v = 0$$

let $v = \begin{vmatrix} x \\ y \end{vmatrix}$

$$\begin{vmatrix} 5i & 5 \\ -5 & 5i \end{vmatrix} \begin{vmatrix} x \\ y \end{vmatrix} = \begin{vmatrix} 0 \\ 0 \end{vmatrix}$$

We now have a system of equations which we can solve for x,y:

$$5ix + 5y = 0$$

$$-5x + 5iy = 0$$

Dividing both equations by 5:

$$ix + y = 0$$

$$-x + iy = 0$$

$$v_1 = \begin{pmatrix} -1 \\ i \end{pmatrix}$$

Solution:

Following the same procedure using the second eigenvalue of $2 + 5i$, we find the second eigenvector to be:

$$v_2 = \begin{pmatrix} i \\ -1 \end{pmatrix}$$

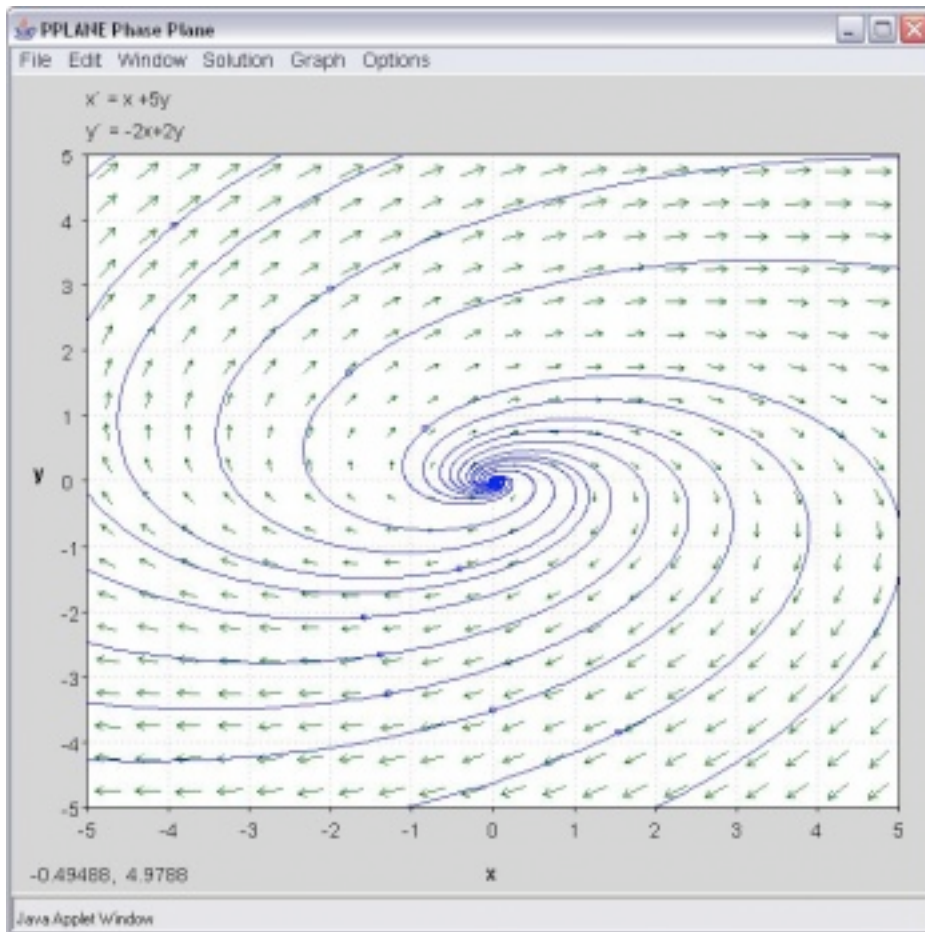
Now plugging both eigenvalues and eigenvectors into the characteristic equation:

$$x(t) = e^{2t}(C_1 \cos 5t + C_2 \sin 5t)$$

$$y(t) = e^{2t}(C_3 \cos 5t + C_4 \sin 5t)$$

For more on this procedure, see: [Eigenvalues and Eigenvectors](#)

The phase-plane plot is shown below:



5.2 Introduction to Pplane

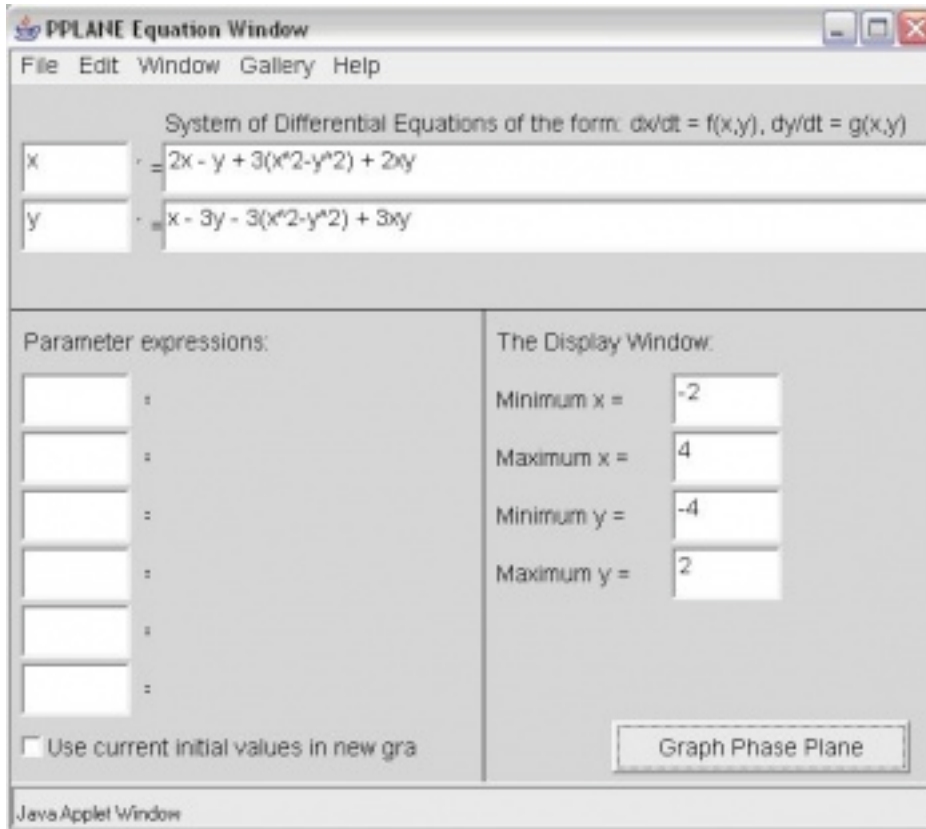
Phase-plane analysis is an important tool in studying the behavior of nonlinear systems since there is often no analytical solution for a nonlinear system model.

[PPlane](#) is a JAVA applet for phase plane analysis of two-dimensional systems. It starts in your web browser and you can directly input your equations and parameter values. PPLANE plots vector fields for systems of differential equations. At each point, (x,y) , of a grid, PPLANE draws an arrow indicating the direction and magnitude of the vector (x',y') . This vector equals $dy/dt / dx/dt = dy/dx$, and is independent of t ; therefore, it must be tangent to any solution curve through (x,y) .

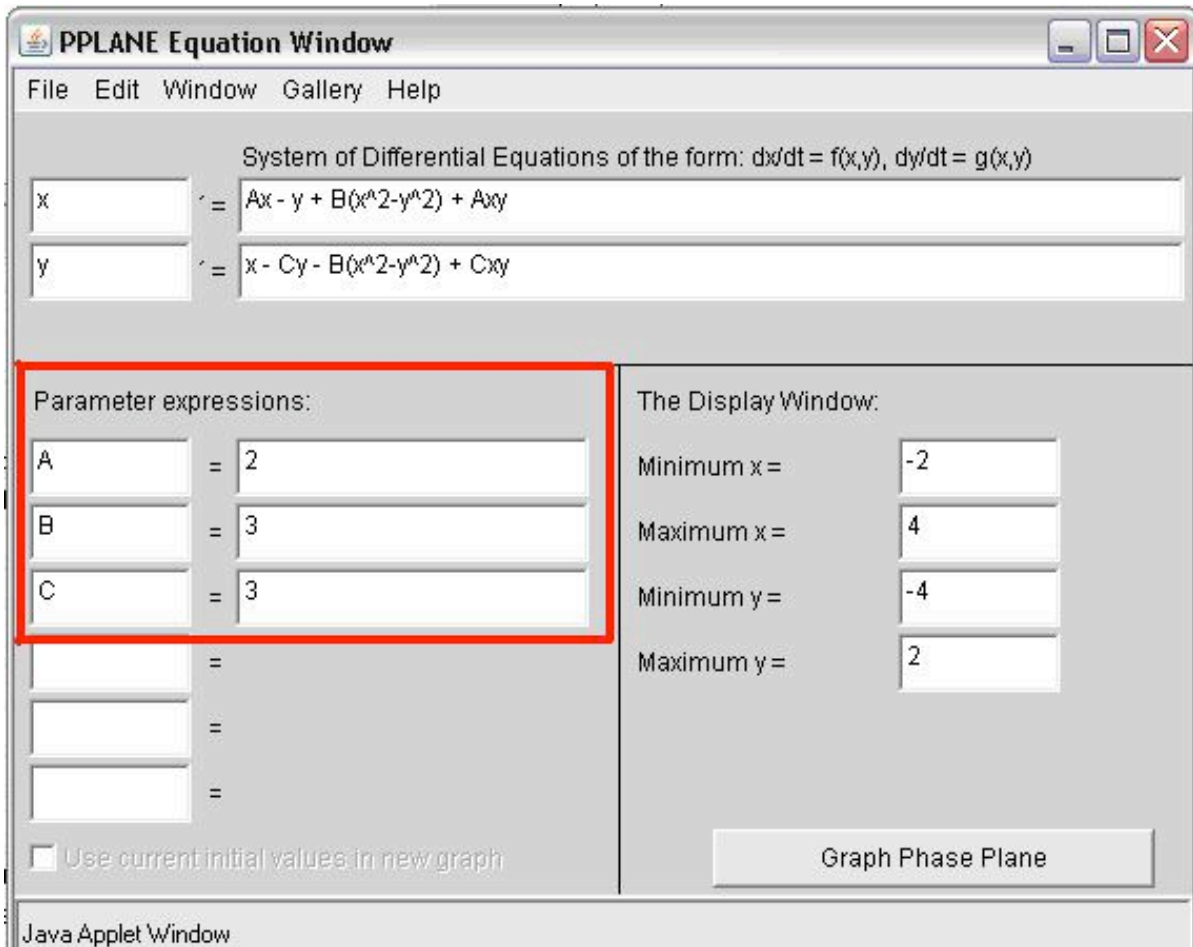
It allows the user to plot solution curves in the phase plane by simple clicking on them. It also enables the user to plot these solutions in a variety of plots. There are a number of advanced features, including finding equilibrium points, eigenvalues and nullclines, that you will find useful later.

5.2.1 How to use Pplane

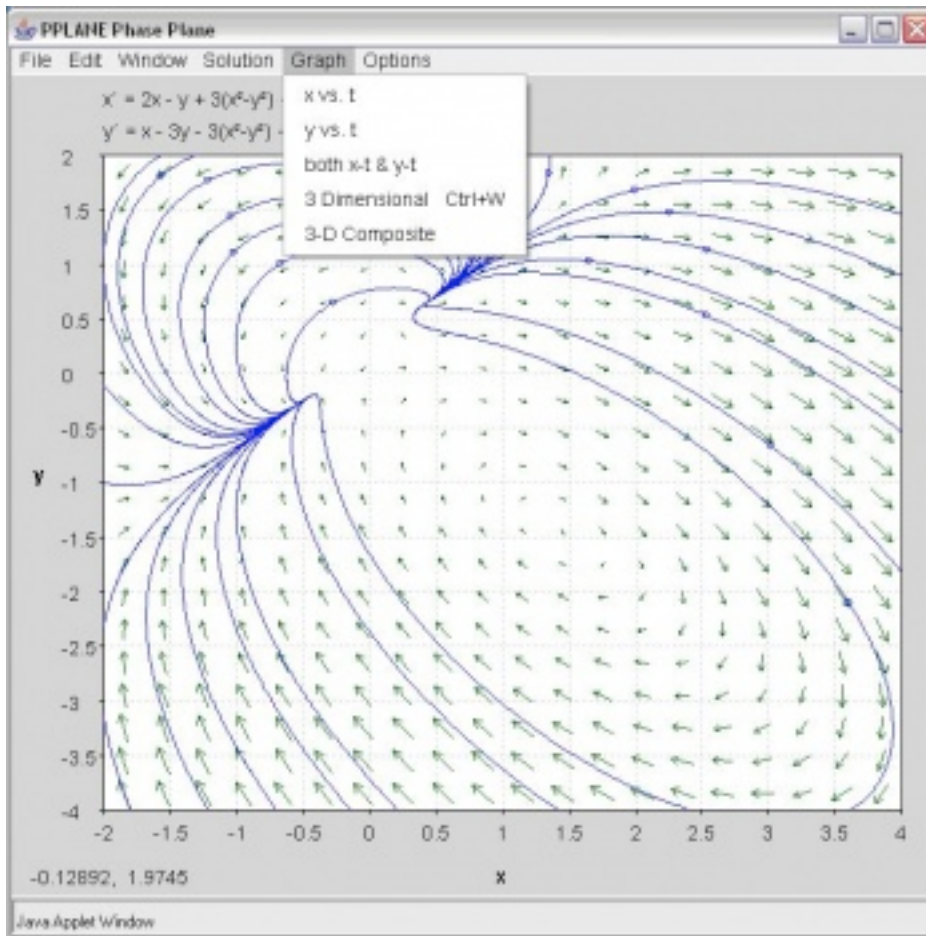
In the PPlane equation window you can enter a system of differential equations of the form $dx/dt = f(x,y)$ and $dy/dt = g(x,y)$, define parameters and resize the display window. Under the Gallery pull down from the menu, you can switch to a linear system.



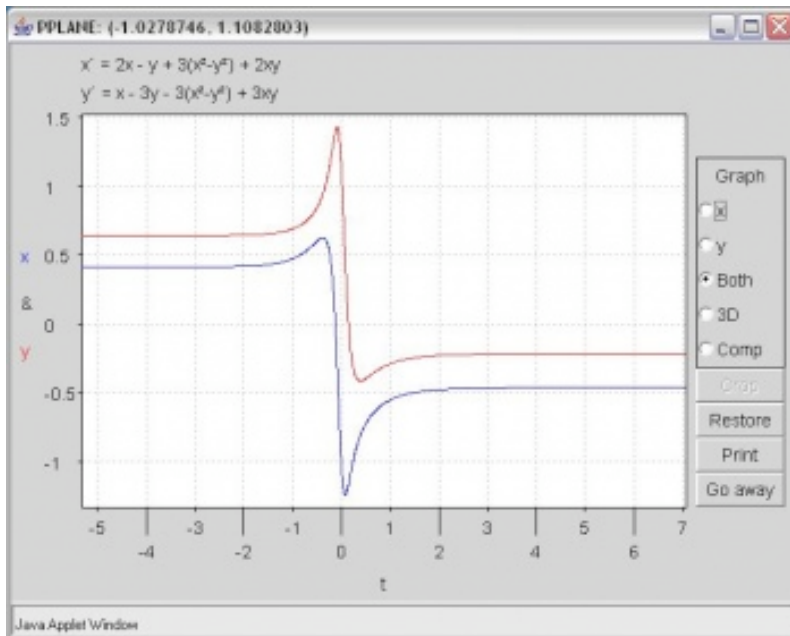
Note, if your differential equations contain constant parameters, you can enter them in the "Parameter Expressions" boxes below the differential equations as seen in the figure below (A, B, and C are used as example parameters). This is a convenient feature to use when considering the effect of changed parameters on the steady state of a system because it eliminates the redundancy of re-entering the parameter values multiple times within the differential equations.



In the PPlane Phase Plane window below you will see the vector fields for the system. By clicking on the field you will plot solution curves in the phase plane. If you are interested in a plot of your solution vs. time or a 3-D view, click on graph:



If you choose the x-t and y-t option, you have to pick a specific solution curve. The result will look like this:



Use the crop function to zoom in on a point of interest

Choose Find Equilibrium Point under the Solution pull down menu. Then when you click on an orbit in the phaseplane, the Pplane Messages window will display the eigenvalues and possible equilibrium points.

Additional Things you can Change in PPlane

Changing the Slope Field

By clicking on the "Options" tab, then by selecting "Direction Field Settings," you can change the number of rows and columns plotted, the way the field is made up, as well as the computational settings of PPlane.

Erasing Made Orbits

On the "Edit" tab, there are options that say "Delete Orbit" or "Delete All Orbits". These options act as their names imply.

Changing the Direction of Graphing

By clicking on the "Options" tab, then by selecting the "Solution Direction" option, you can then change the way that PPlane graphs a line when you click on the field. You can

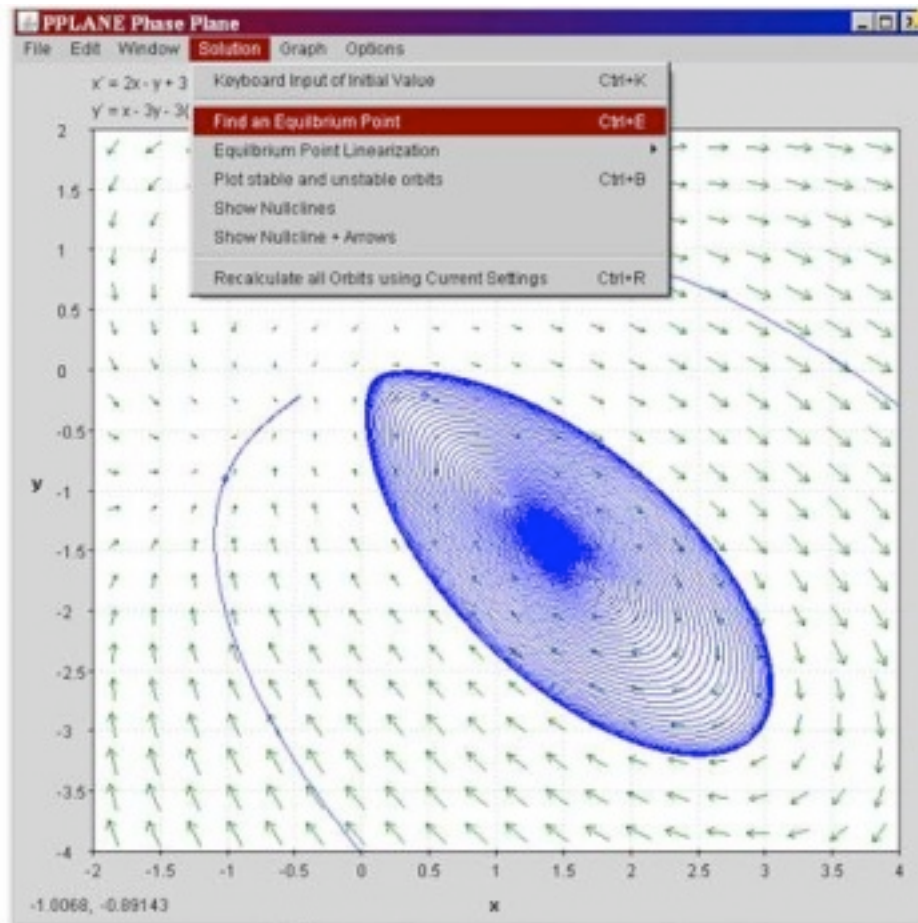
change the graphing to plot forwards (for values of $t > 0$), backwards (for values of $t < 0$) or in both directions of t .

5.2.2 More Uses for PPLANE

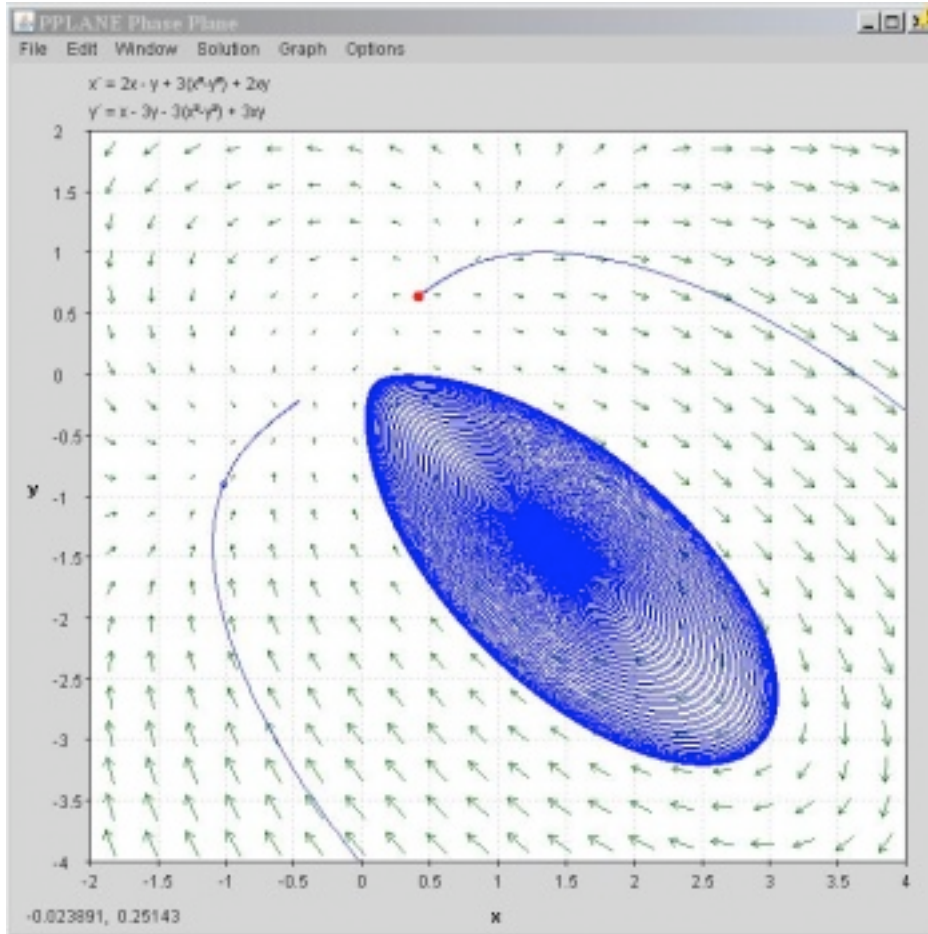
Of the many uses that PPLANE has to offer, some of the most helpful functions involve:

Finding eigenvalues/eigenvectors for an equilibrium point.

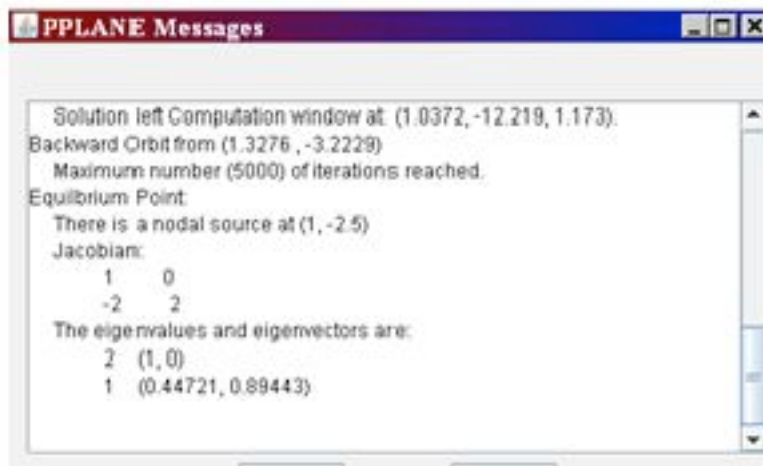
After graphing a series of differential equations, find a particular equilibrium point within the graphed data (“Find an Equilibrium Point,” under the Solution tab)



Now, by selecting a point on the field that has been graphed by pplane, pplane will find the closest equilibrium point on the graph, and highlight this point on the graph in red.



The PPLANE Messages box in the upper left hand corner of the screen should pop up with some new information. This information provides eigenvalues and the corresponding eigenvectors to the selected equilibrium value:



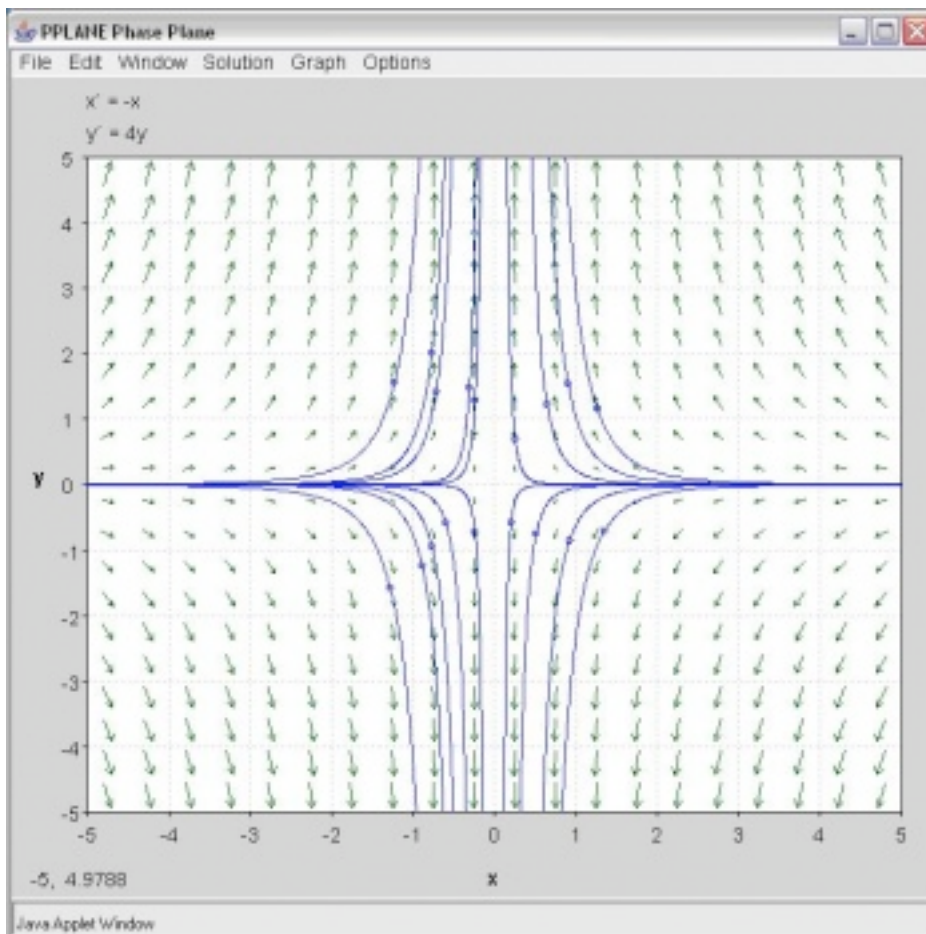
Stability of a Equilibrium Point

Similarly to before, the Messages Box will provide the stability features (ie: is it a nodal sink?) of the found equilibrium point, immediately after using the “Find an Equilibrium Point.”

5.2.3 Other concepts of phase plane analysis

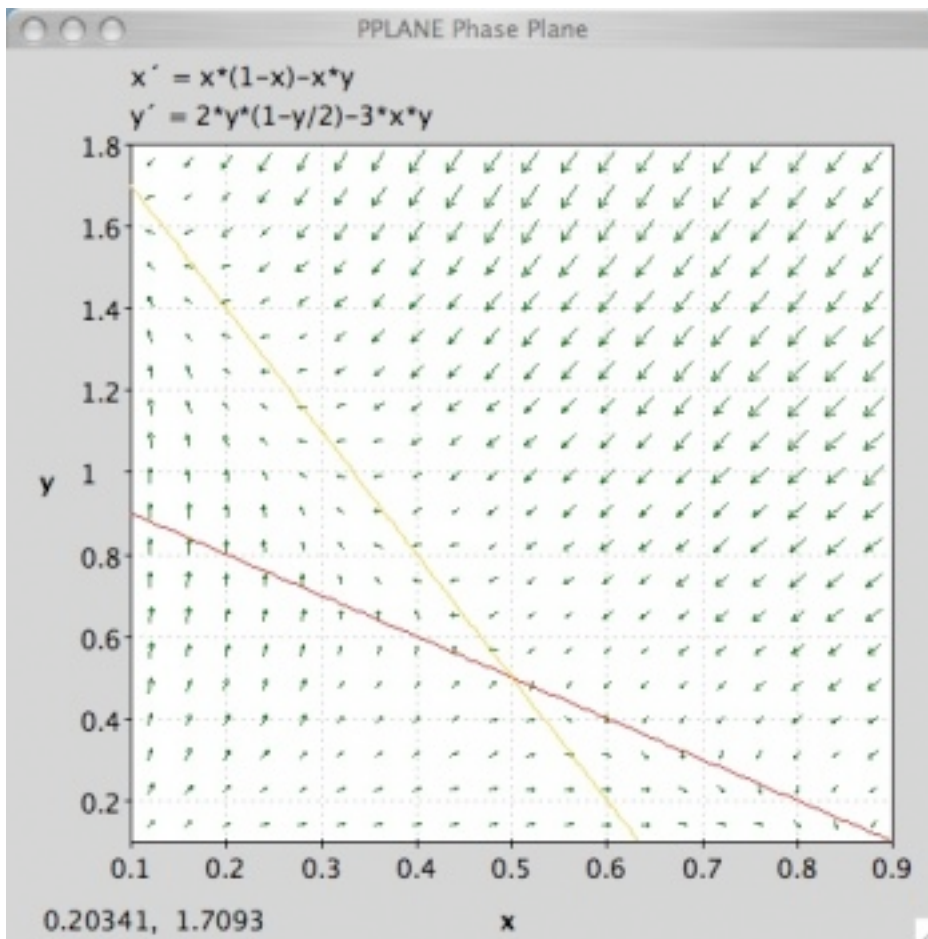
Separatrix

A separatrix is any line in the phase-plane that is not crossed by any trajectory. The unstable equilibrium point, or saddle point, below illustrates the idea of a separatrix, as neither the x or y axis is crossed by a trajectory. If you picture a topographic map, the seperatrix would be a mountain ridge; if you fall a little of the edge, you will never come back. Plotting your phase plane in Pplane would be useful to identify impossible set points, for example.



Nullclines

A nullcline is a curve where $x'=0$ or $y'=0$, thus indicating where the phase plane is completely horizontal or completely vertical. The point at which two nullclines intersect is an equilibrium point. Nullclines can also be quite useful for visualization of a phase plane diagram as they split the phase plane into regions of similar flow. To display nullclines on the Phase Plane window, select Nullclines under the Solutions drop down menu. The screenshot below is an example.

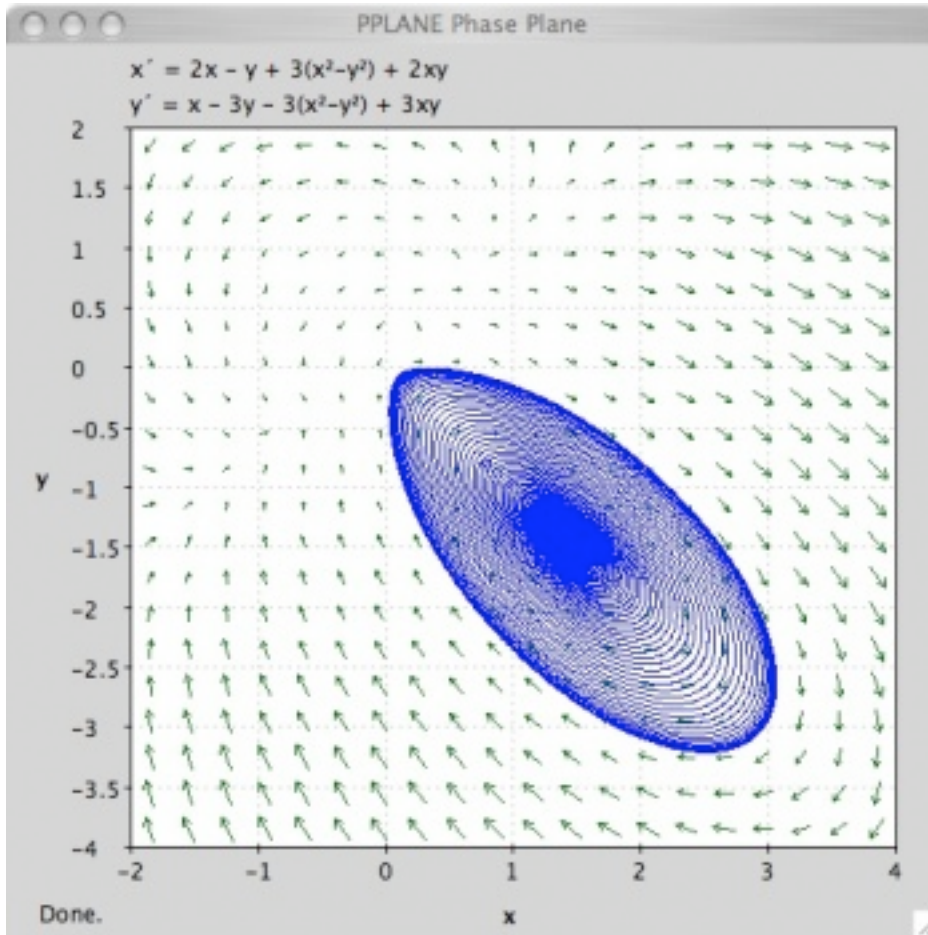


Notice that the red nullcline shows where the flow is completely vertical ($x'=0$) and the yellow nullcline shows where the flow is completely horizontal ($y'=0$).

Limit Cycle

Below you will find a solution curve for a limit cycle. The limit cycle contains the response in a set range, which is something you may want to take advantage for certain

engineering applications. On the other hand it is always rotating and may not be stable enough for your purposes.

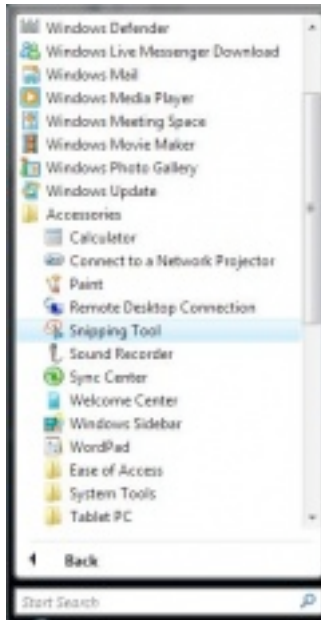


5.2.4 Taking Screen Shots to copy Pplane phase portraits

With the introduction of Windows Vista, the Snipping Tool was introduced. This tool allows much greater flexibility with taking screen shots and editing them. This article will talk about the Snipping Tool as well as the Windows Print Screen key which can be used to take photos of your computer screen. When pressing the key, your computer copies the image of your screen and onto your computer's clipboard. The image can then be pasted into multiple programs. There are many instances throughout the CHE 466 course in which taking a screen shot of your work will come in handy. Examples include copying phase portraits created in Pplane, graphs created in Mathematica, or your Mathematica code.

To enable the Snipping Tool on your Vista computer go to the Windows button in the bottom left of your screen and click Accessories -> Snipping Tool.

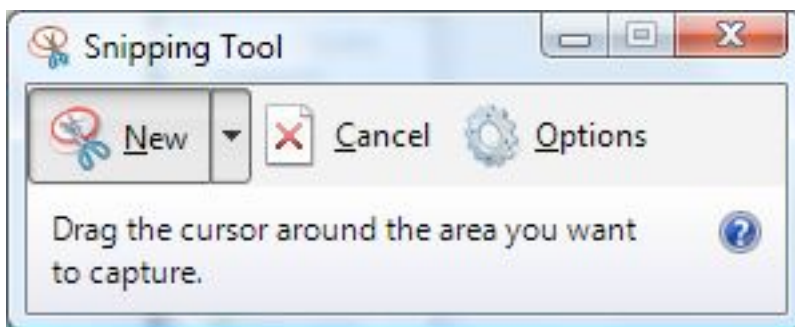
Figure 1. How to enable the Snipping Tool



A window will appear asking if you would like to add the Snipping Tool to your Quicklaunch. This provides a simple and quick way to take screenshots.

To take a picture of your graph, just press the Snipping Tool button in the Quicklaunch area and a window like this will appear:

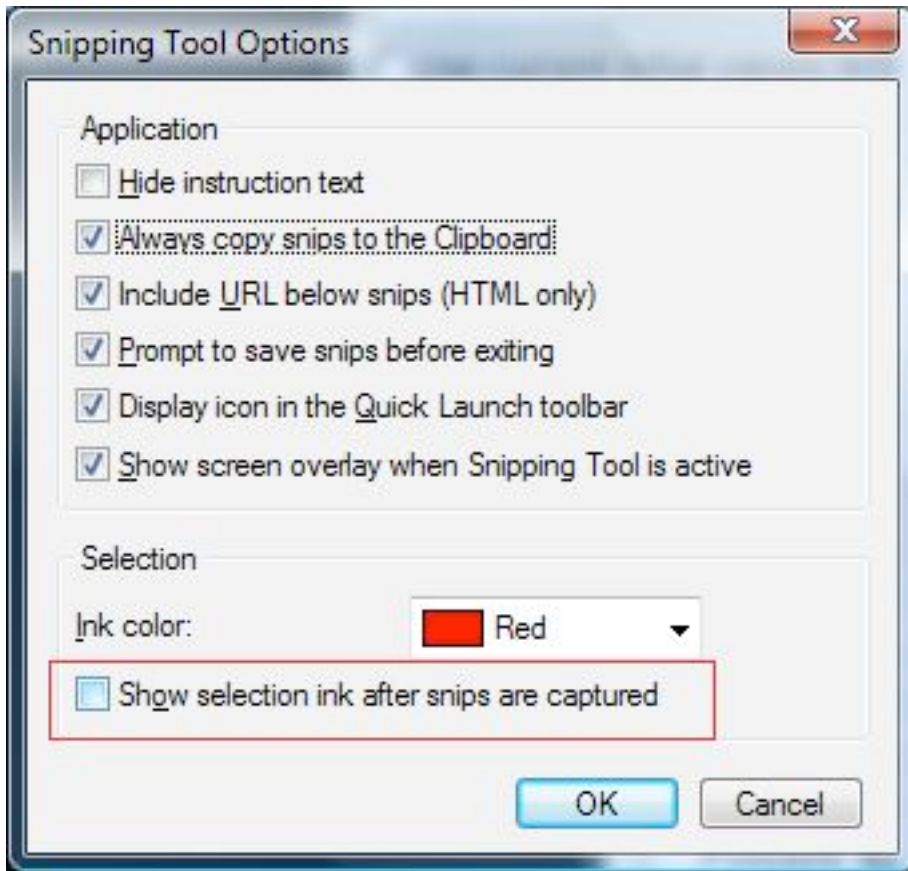
Figure 2. The Snipping Tool Window



Automatically, the Snipping Tool will default to a crosshair from which you can click and drag to make a selection of the section of the screen you would like represented by a red rectangle.

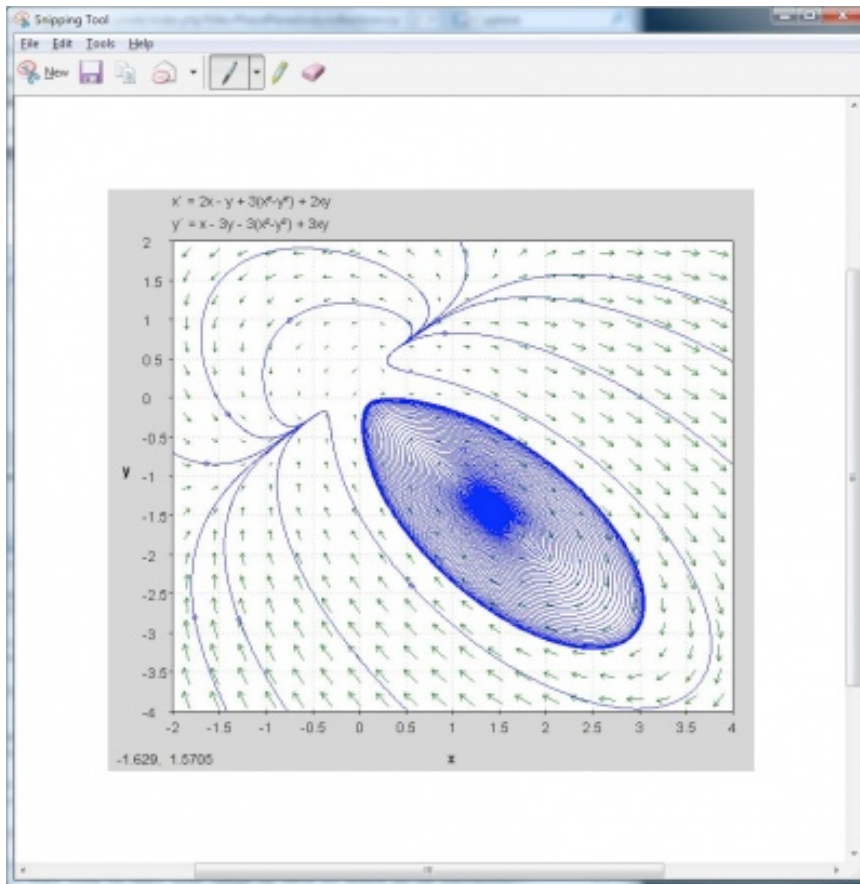
WARNING: In the Options section you should uncheck "Show selection ink after snips are captured" in order to eliminate the red edge around your photos.

Figure 3. Snipping Tool Option Menu (Uncheck the selection ink)



The Snipping Tool will open up a new window with your selection and copy the image to your clipboard. Feel free to edit your image or save it where it is convenient.

Figure 4. Snipping Tool Editing Window



If not using Windows Vista you can still use Print Screen:

Follow these simple steps to copy and paste your phase portrait into a Microsoft Word document:

1. Pull up the window containing your phase portrait so that it is displayed on the screen.
2. Find the Print Screen or PrtSc button in the upper-right hand portion of your keyboard. (The key may appear slightly different depending on your Windows keyboard manufacturer).
3. Open Microsoft Word to the document of your choice (i.e. CHE 466 Homework 7).
4. Paste the image into the Word document. Figure 1 below indicates how your phase portrait will look in Word.
5. To crop or resize the image as you like, you may use the Picture toolbar (seen in Figure 2) by selecting View -> Toolbars -> Picture.

If you prefer to take a screen shot of just your phase portrait rather than the entire computer screen, follow these simple steps:

1. Pull up the window containing your phase portrait so that it is displayed on the screen.
2. Press Alt-Print Screen to capture a photo of the window you selected.
3. Open Microsoft Word to the document of your choice (i.e. CHE 466 Homework 7).
4. Paste the image into the Word document. Figure 3 below indicates how your phase portrait image will look.

Figure 5. Initial screen shot

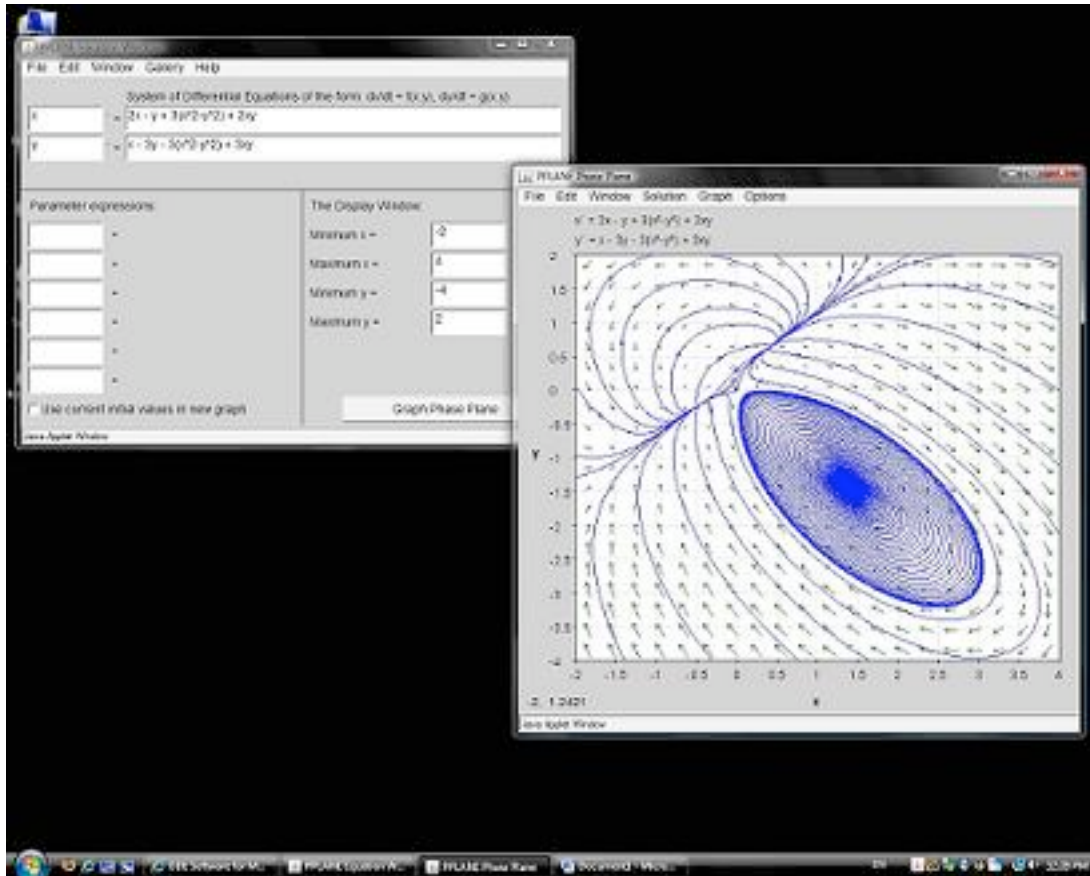


Figure 6. Microsoft Word document containing the screen shot

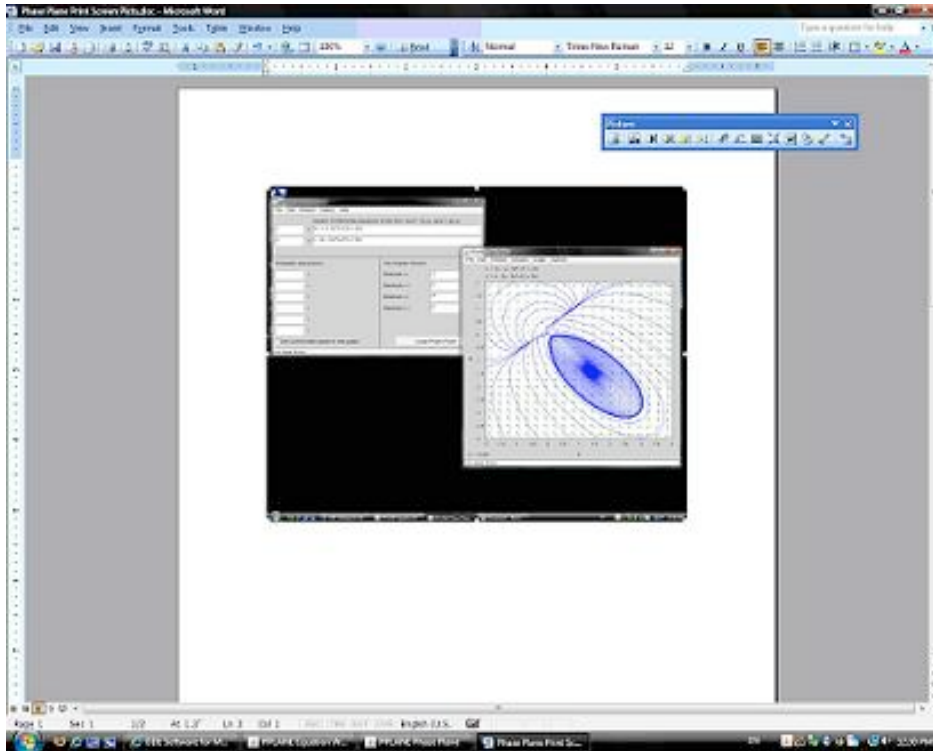
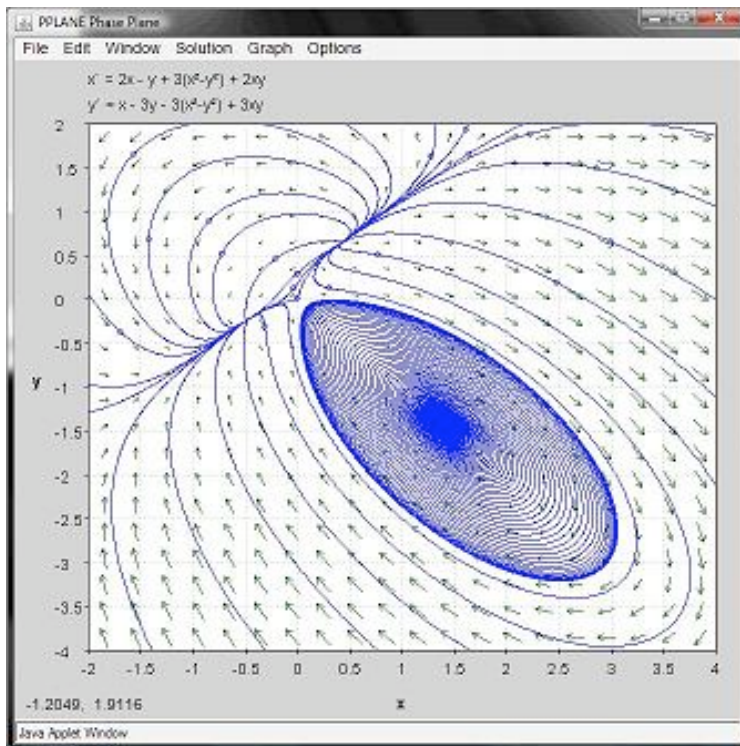


Figure 7. Screen shot of phase portrait window



5.3 Worked Out Example 1 - Linear System of Equations

Problem statement

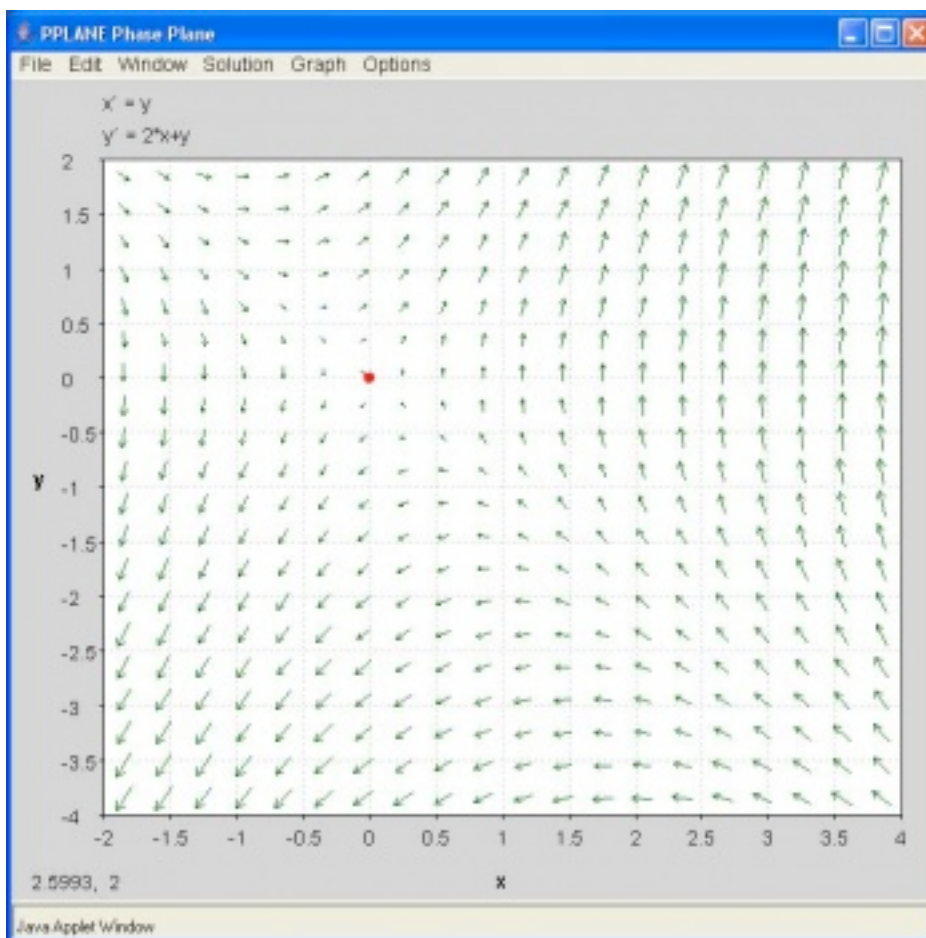
Use [PPLANE](#) to calculate the following information of the system given below: location and type of equilibrium point, Jacobian matrix, eigenvectors, and eigenvalues.

$$x' = y$$

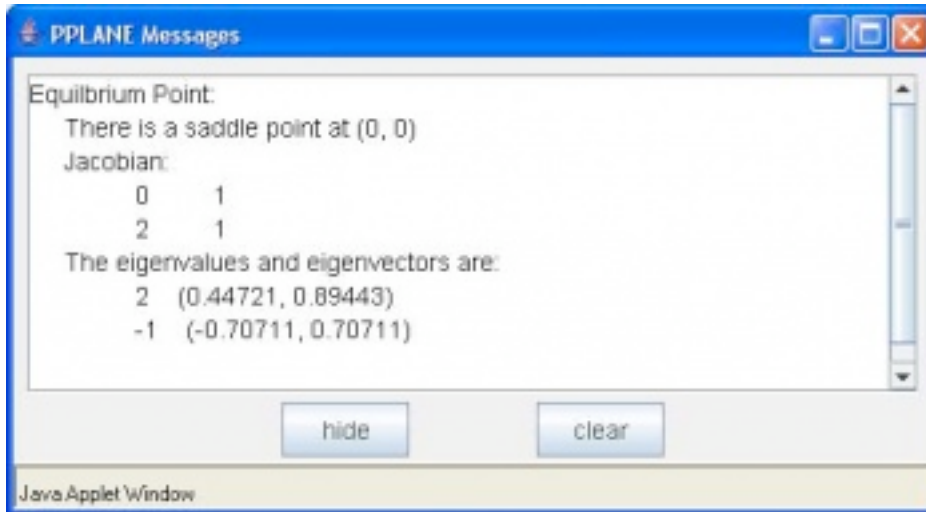
$$y' = 2x + y$$

Solution

Using PPLANE's "Find an Equilibrium Point" feature and clicking on the phase plane, the following equilibrium point will be indicated:



The location, and type of the equilibrium point is given in the "PPLANE Messages" window, along with the Jacobian matrix, eigenvectors and eigenvalues.



5.4 Worked Out Example 2 - Nonlinear System of Equations

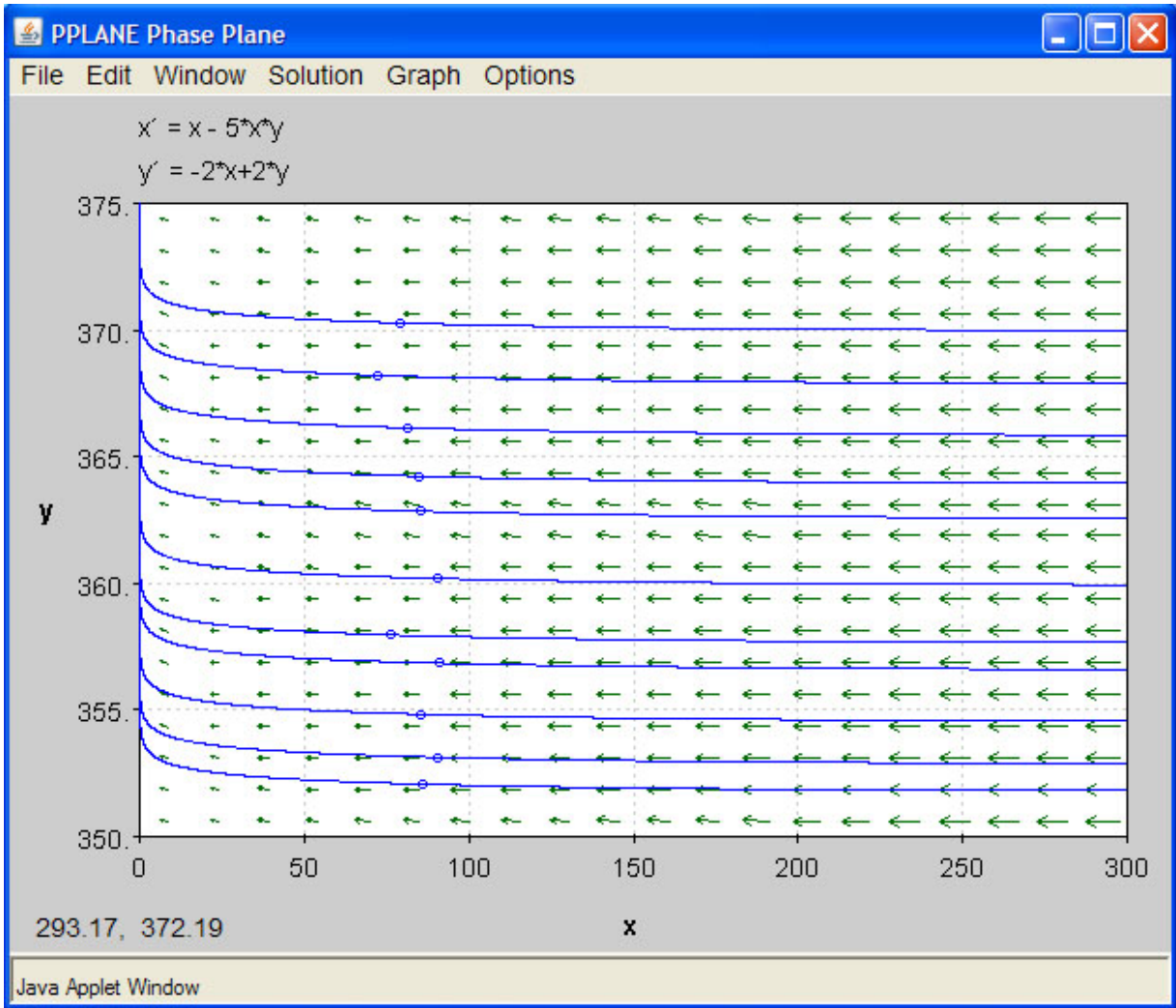
For our second example problem we would like you to try a non-linear system of equations. Solve for the set of equations on PPlane. Consider the trends of change in rate of the differential equations and subsequently solve the equations on Mathematica to compare the trends.

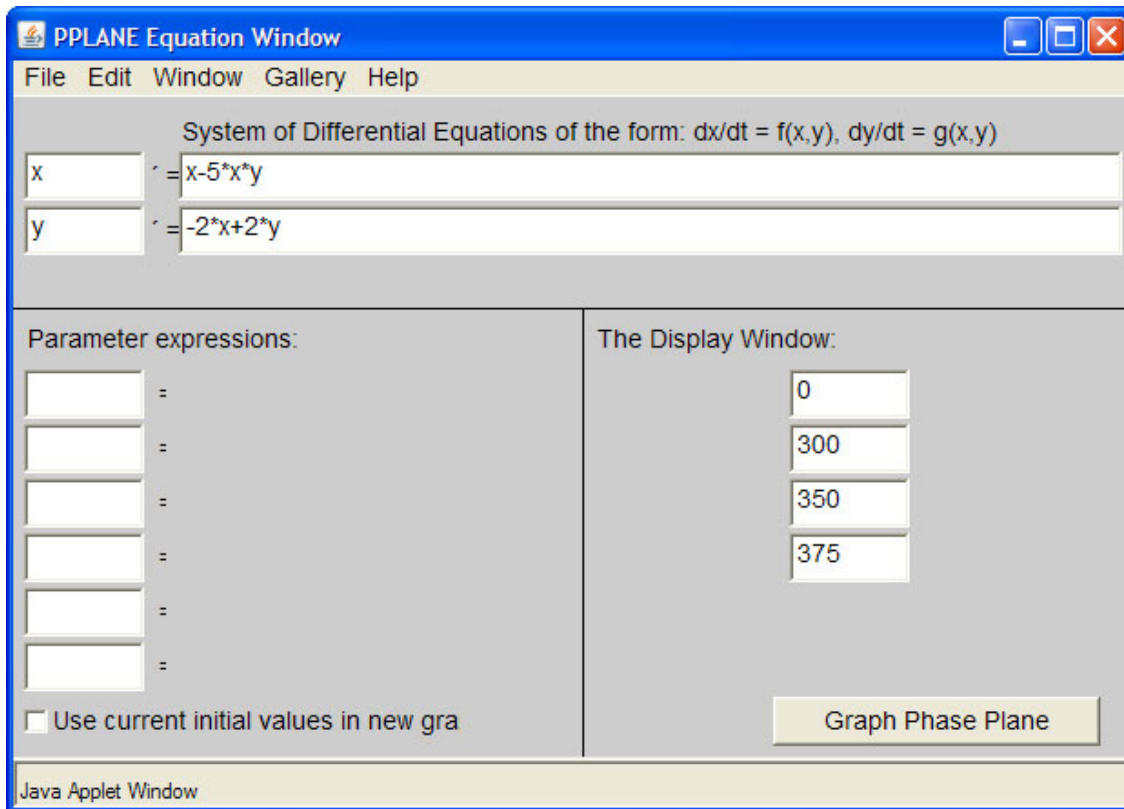
The Following two differential equations are going to be used to walk through the solutions on PPlane and Mathematica:

$$\frac{dx}{dt} = x - (5xy)$$

$$\frac{dy}{dt} = -2x + 2y$$

The above equations were put in to the PPlane window and solved. The following two windows show the solution for the set of differential equations:



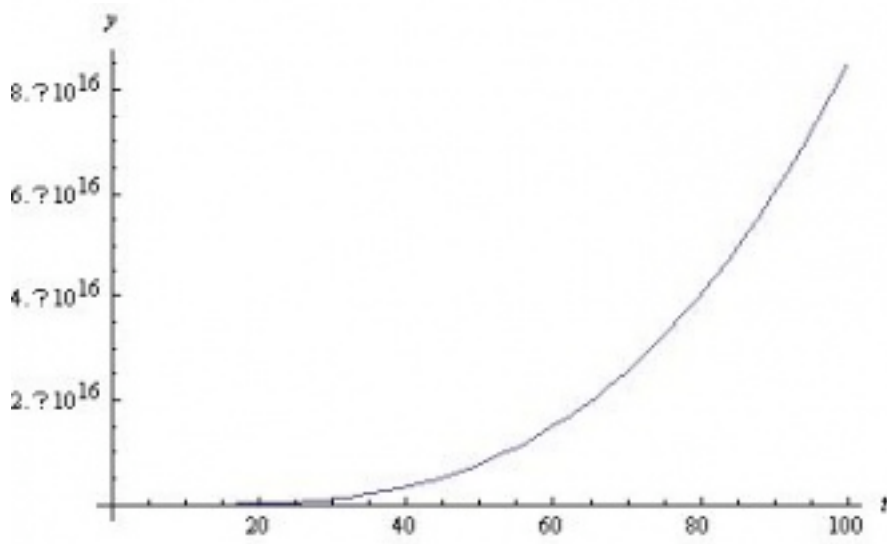
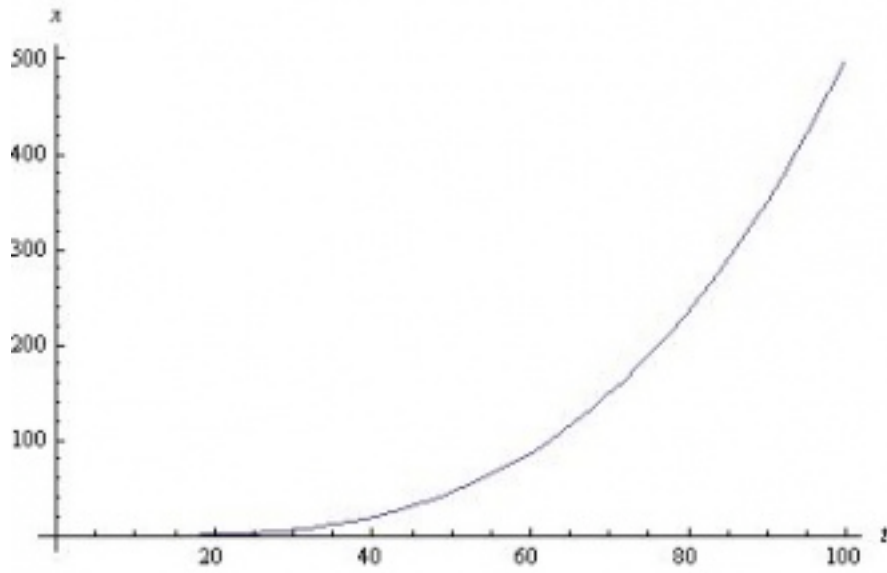


Looking at the phase-plane plot, at low values of x and y , t increases slowly. However at higher values of y , the increase in t is rapid. When x is high and y is low, however, t increases slowly. Mathematica will help us visualize the relative rates of change better.

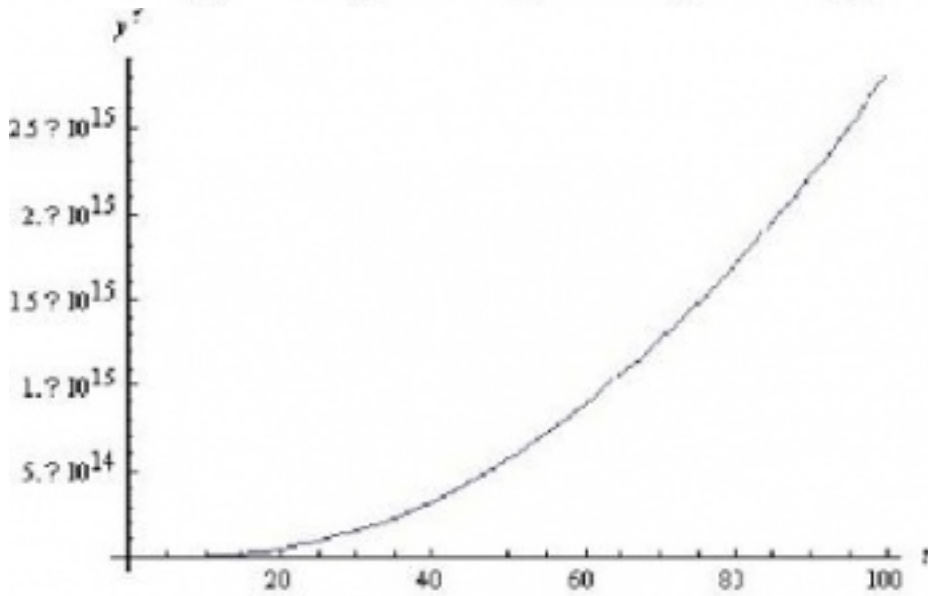
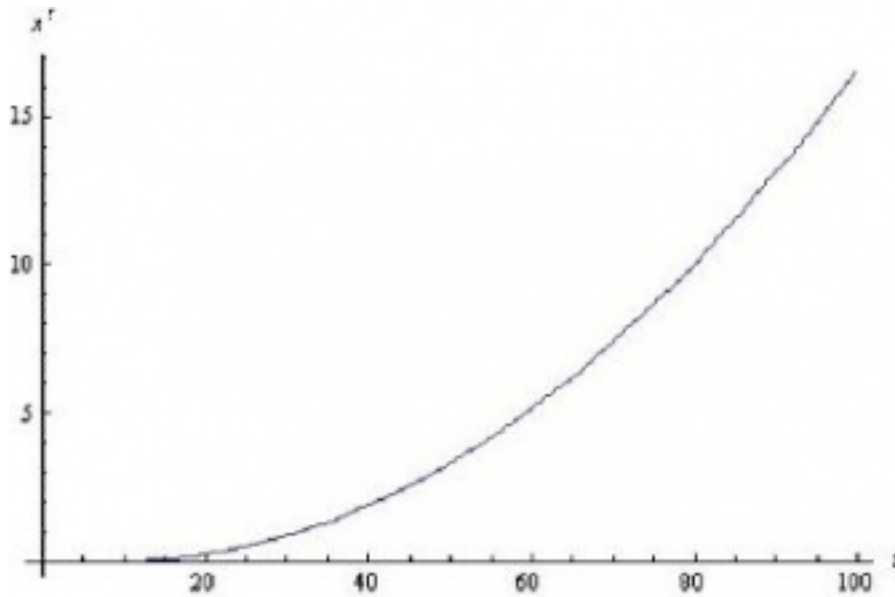
The following is the code used in Mathematica to solve and plot the set of differential equations:

```
ODEs = {x'[t] == (x[t] - 5*x[t]*y[t]), y'[t] == (-
2*x[t]) + (2*y[t]), x[0] == 9, y[0] == 370}
numericalSol = NDSolve[ODEs, {x[t], y[t]}, {t, 1, 100}]
Plot[y[t] /. numericalSol, {t, 1, 100}, PlotRange -> All]
```

The graphs obtained on Mathematica for x versus t and y versus t are shown below. Please note the difference between the axes scales.



Also, for a closer look, here are the plots of the slopes of graphs above.



Comparing the increase in t with increase in x , we see a similar trend in the PPlane diagram. Mathematica shows a constantly increasing x' with t . At higher values of x , the value for t increases in the PPlane diagram. However, as seen clearly in the PPlane diagram and the graphs of the slope of x with respect to t and the slope of y with respect to t , the slope of x does not compare to the very large slope shown for y' versus t . Therefore the results using Mathematica and PPlane are consistent.

This modeling system could be used to view trends of variables in a CSTR or any other system which can be modeled using differential equations.

5.5 Multiple Choice Questions

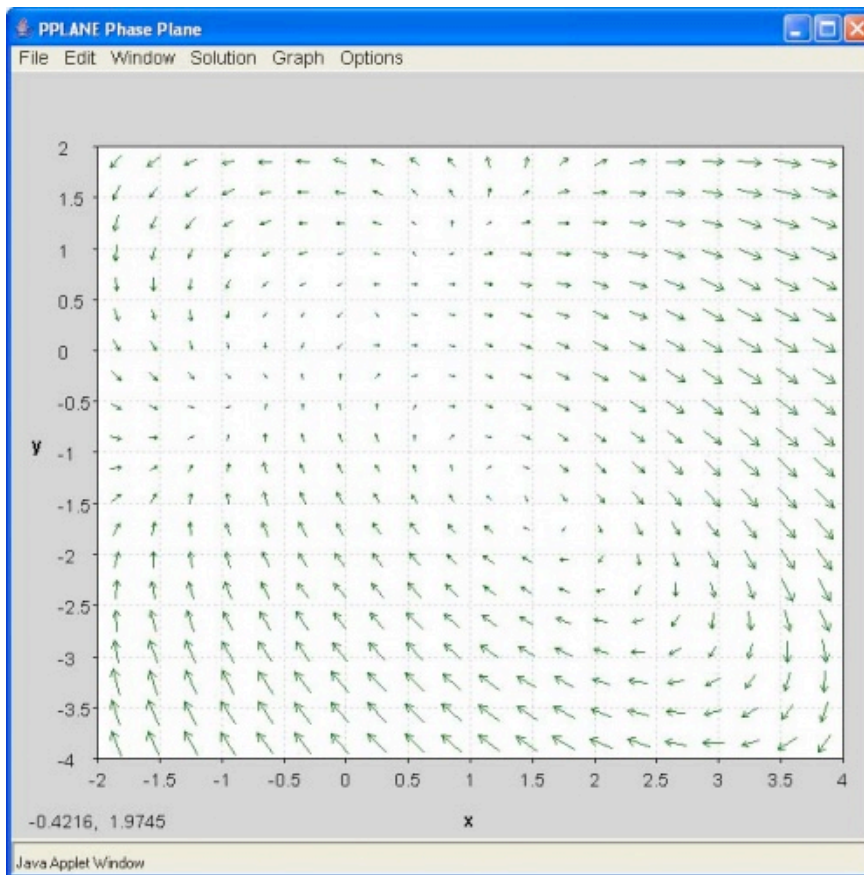
5.5.1 Question 1

Open [PPLANE](#) and enter the following equations into the PPLANE Equation Window:

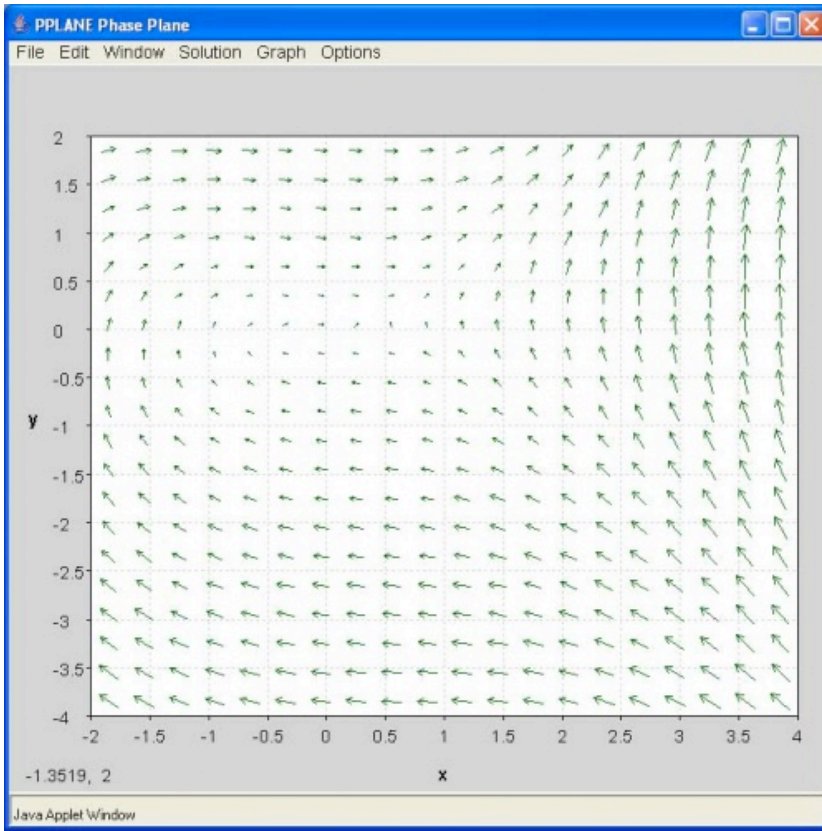
$$x' = \sin(x)$$

$$y' = \cos(y)$$

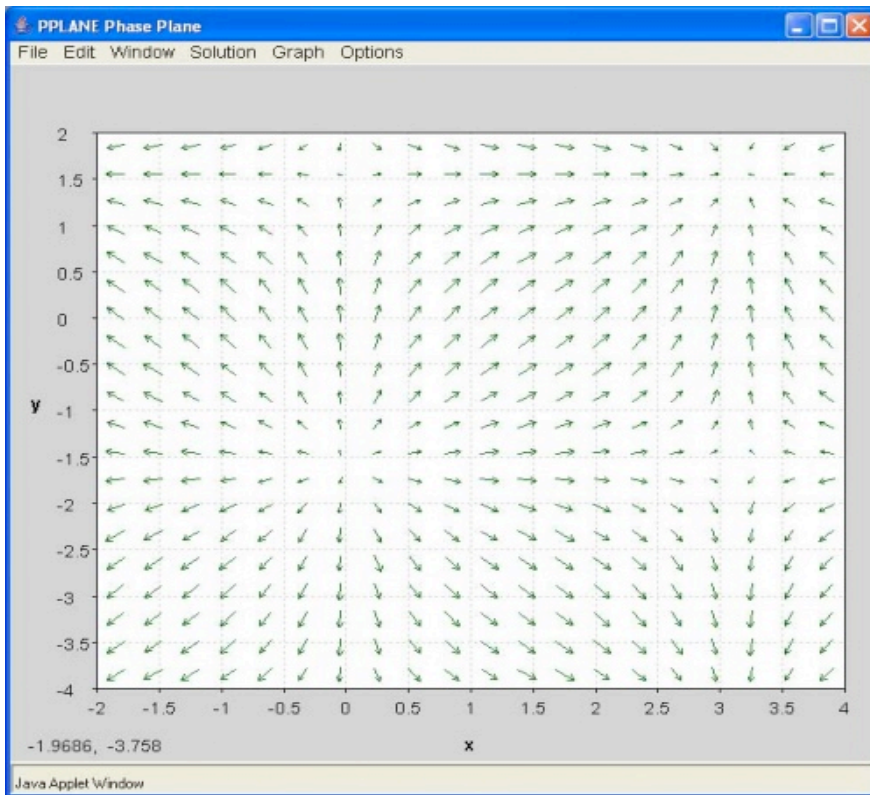
What does the resulting phase plane look like? (Note: Click on image to enlarge)



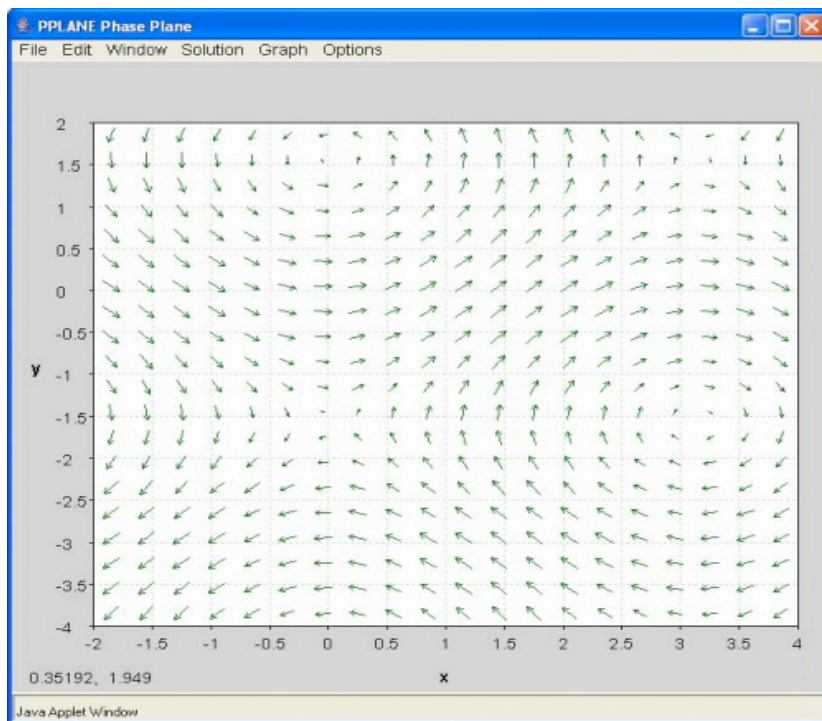
A.



B.



C.



D.

5.5.2 Question 2

If you have a disturbance in your system and the system is driven right back to equilibrium, that fixed point's eigenvalue is most likely a:

- A. complex number with negative real number component
- B. 0
- C. negative real number
- D. positive real number

5.6 Answers to the Multiple Choice Questions

Question 1: C

Question 2: A

5.7 Sage's Corner

Phase Plane Analysis Video

<http://video.google.com/googleplayer.swf?docId=-7542292834933597867>

[slides for this talk](#)

Using PPlane

<http://www.youtube.com/v/CIY3iUb094s>

5.8 References

- "Limit-cycle." http://en.wikipedia.org/wiki/Limit_cycle. Last Updated 12 September 2007.

Section 6. Root locus plots: effect of tuning

Date created: 10/23/06

Authors: Halley Crast, Andrew Laskowski, Maurice Telesford, Emily Yatch

Stewards: Victoria Cardine, Anthony Campell, David Hines, Stephen Kerns

Date Presented: Oct 16, 2006; Revised: Oct 24, 2007

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

6.1 Introduction

Root locus plots show the roots of the systems characteristic equation, (i.e. the Laplacian), as a function of the control variables such as K_c . By examining these graphs it is possible to determine the stability of different values of the control variable. A typical transfer function is of the form $G(s) = Y(s)/U(s)$.

Poles: $U(s) = 0$

Zeros: $Y(s) = 0$

In other words, after factorization the poles are the roots of the denominators and the zeros are the roots of the numerator. Stability only depends on the value of the poles. The system is stable for all values of the control variables that result in the value of the real part of every pole value being less than zero. The lines of a Root locus plot display the poles for values of the control variable(s) from zero to infinity on complex coordinate system. These plots will always have a line of symmetry at $i = 0$.

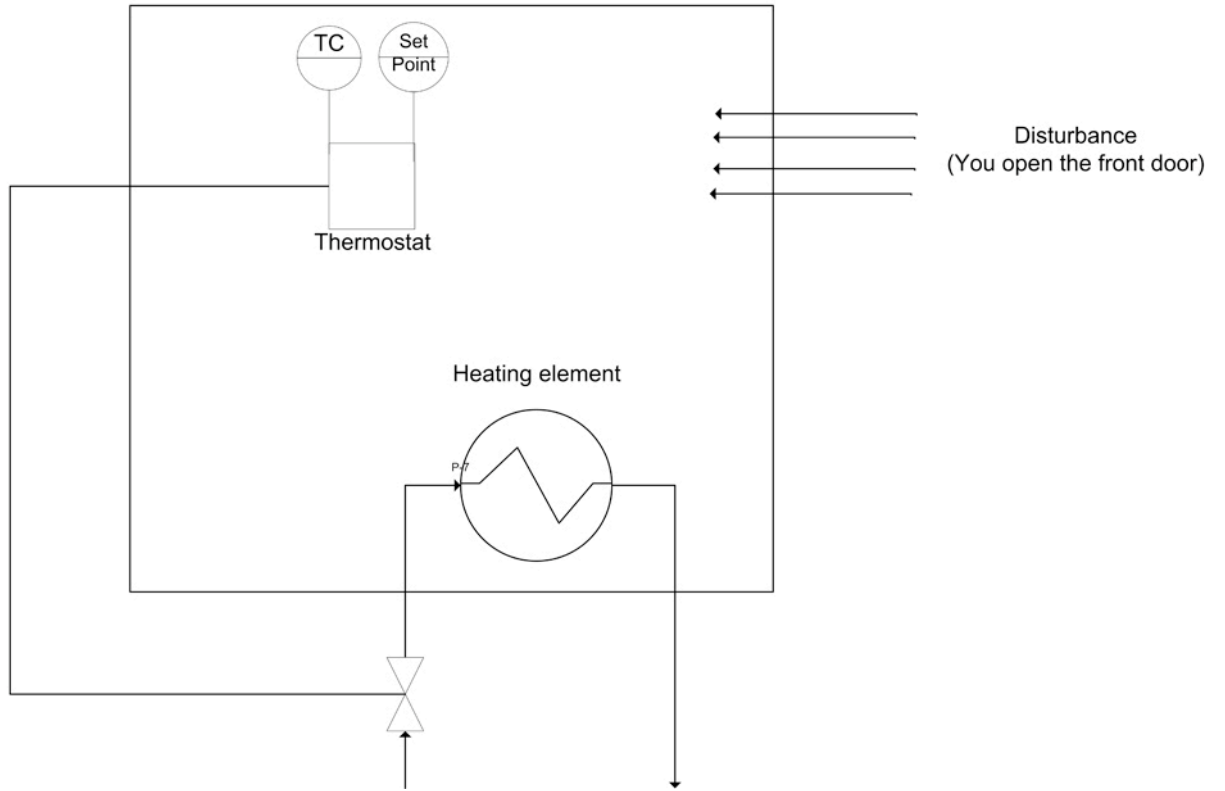
6.1.1 Closed-loop vs. Open-loop

A closed-loop system uses feedback control where the output has an effect on the input. With a closed-loop, oscillations are usually introduced, and therefore can become unstable. Unlike the open-loop systems, the closed-loop incorporates valves and controllers.

In an open-loop system, the output is not compared with and has no effect on the input. In an open-loop system, oscillations are not introduced and therefore cannot become unstable. An open-loop system, however, can be inaccurate because it does not take into account the control dynamics. Open-loop systems will include feed forward control schemes or timed control schemes. The two diagrams below depict this difference when

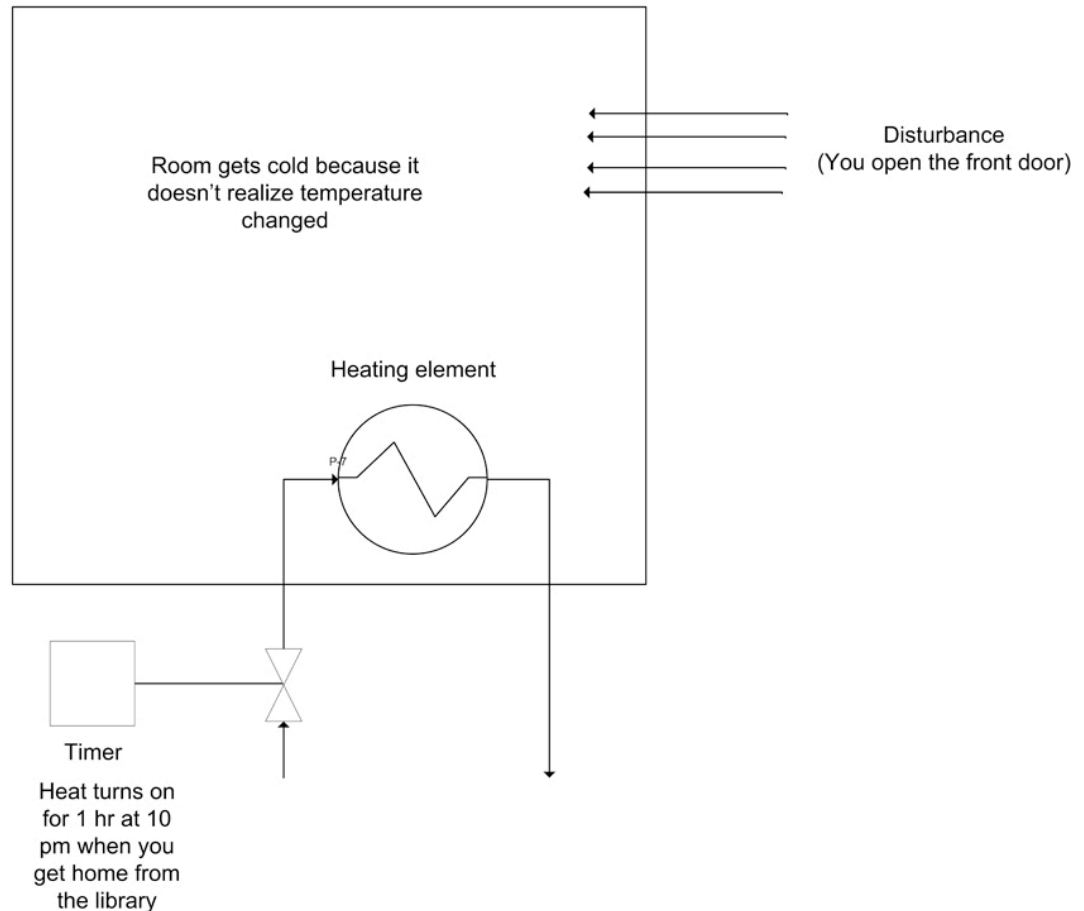
trying to control the temperature in your apartment. (Click on images for increased resolution).

Closedloop System (Winter Household Heating)



In this diagram a thermostat presents feedback to the heater to turn it on or off.

Openloop System (Winter Household Heating)



Since the heater only turns on at 10 pm, it assumes that the amount of time you open the door will be the same each day. It is considered an open system since the temperature in the room is independent of the heater controller.

Note that all the examples presented in this web page discuss closed-loop systems because they include all systems with feedback.

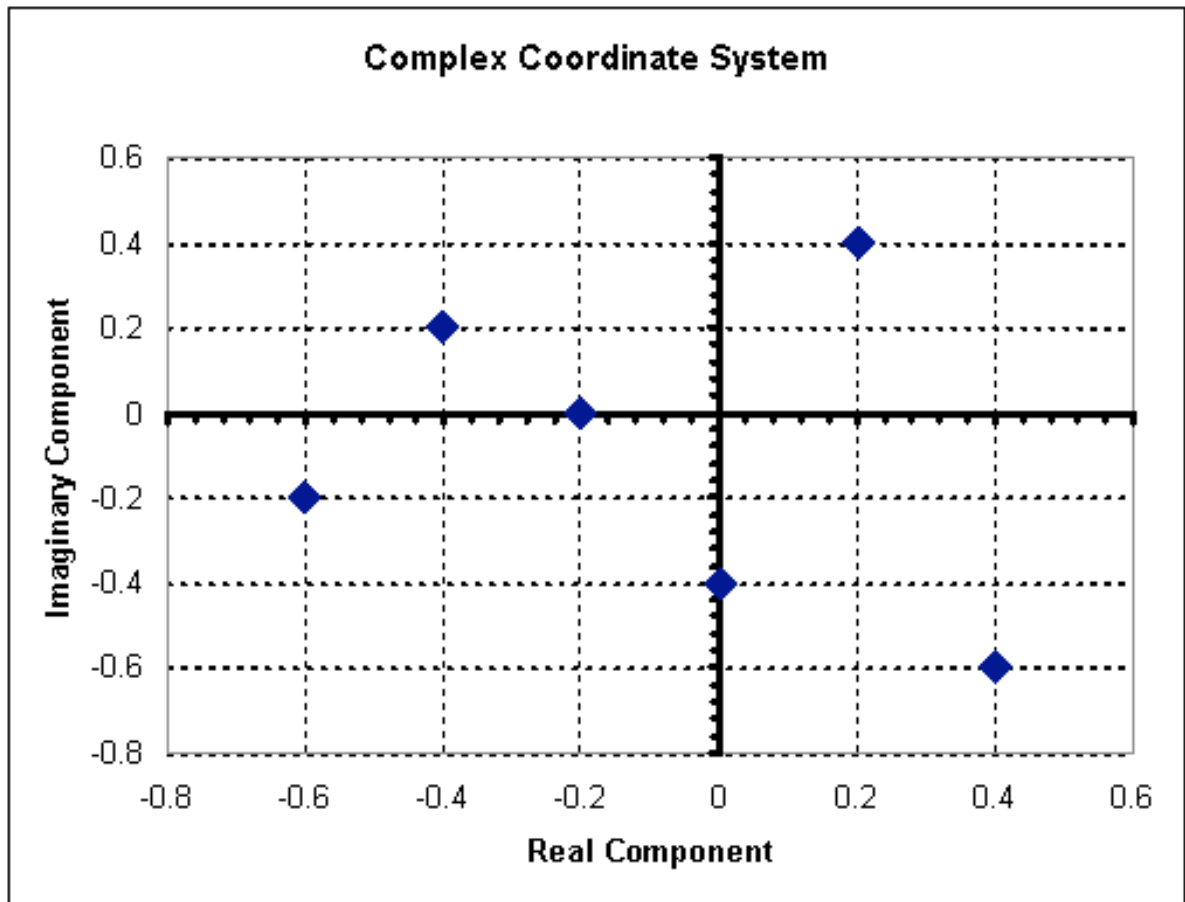
6.1.2 Complex Coordinate Systems

Root locus plots are a plot of the roots of a characteristic equation on a complex coordinate system. A complex coordinate system allows the plotting of a complex number with both real and imaginary parts. The real component is plotted on the x-axis and the imaginary component is plotted on the y-axis. When creating root locus plots imaginary roots must be solved for. These imaginary roots come in complex conjugate

pairs (this can be seen below in the section on "Plotting Poles on a Complex Coordinate System to make Root Locus Plot").

For example a plot of the following complex numbers is shown below. These complex numbers can be broken into the real and imaginary components to make it easier to plot.

Complex Number	Real Component	Imaginary Component
$-0.4 + 0.2i$	-0.4	0.2
$-0.6 - 0.2i$	-0.6	-0.2
$-0.2 + 0i$	-0.2	0
$0 - 0.4i$	0	-0.4
$0.2 + 0.4i$	0.2	0.4
$0.4 - 0.6i$	0.4	-0.6



6.1.3 Developing a Characteristic Equation

Although the focus of this article is to discuss root locus plots, it is necessary to mention briefly how to determine the characteristic equation for a system in order to obtain the root locus plot. In general, most chemical engineering processes can be described by a system of ordinary differential equations. Follow the following steps to determine the characteristic equation for the system (which will allow you to develop a root locus plot).

1. If the ODEs are not linear, linearize them. (See this link for more information on linearizing ODEs <<http://controls.engin.umich.edu/wiki/index.php/LinearizingODEs>>)
2. After linearizing the ODEs, use matrix algebra to find the eigenvalues of your system. Be careful here not to insert numerical values for your control parameters, (e.g. leave K_c as K_c , not $K_c=1$). (For more information on finding eigenvalues <<http://controls.engin.umich.edu/wiki/index.php/EigenvaluesEigenvectors>>)

3. The polynomial equation obtained for the eigenvalue should contain lambda and the control parameters. This equation is the characteristic equation. Obtain solutions to this equation by setting values for the control parameters and solving for the eigenvalues. The roots obtained will be used to create the root locus diagram.

This 3-step process is valid to obtain a characteristic equation for any closed loop control system.

A more traditional method to develop characteristic equations is by applying Laplace transforms.

Laplace Transforms

Laplace transforms are a method to change linear ordinary differential equations into transfer function. All transfer functions used in root locus plots are independent of time because the $L[f(t)] \equiv F(s)$. Formally, the equation below shows that the time function is integrated, leaving only the variable s .

$$F(s) = \int_0^{\infty} f(t) e^{-st} dt$$

s is a complex number, therefore allowing us to construct complex coordinate system graphs. The exact solution to most disturbances and controllers can be found in any controls book. Please always refer to your Ordinary differential equations mathematics book for more information on Laplace transforms.

6.1.4 Example

The stability of the series chemical reactors is to be determined. The reactors are well mixed and isothermal, and the reaction is first-order in component A. The outlet concentration of the second reactor is controlled with a PI feedback algorithm that manipulates the flow of the reactant, which is very much smaller than the flow of the solvent. The sensor and final element are assumed fast, and process data is as follows.

Process

$$V = 5\text{m}^3$$

$$F_s = 5\text{m}^3/\text{min} \gg F_A$$

$$k = 1 \text{ min}^{-1}$$

vs= 50% open

$$CA_0 = 20 \text{ mole/m}^3$$

$$CA_0(s)/v(s) = K_v = 0.40 \text{ (mole/ m}^3\text{) (\%open)}$$

PI Controller $K_c = ??$ $T_f = 1 \text{ min}$

Formulation The transfer function for the process and controller are

$$G_p(s) = \frac{K_p}{(\tau s + 1)(\tau s + 1)}$$

$$G_c(s) = K_c \left(1 + \frac{1}{T_f s} \right)$$

$$K_p = K_v \left(\frac{F}{F + V k} \right) = 0.1 \frac{\text{mole/m}^3}{\%}$$

$$\tau = \frac{V}{F + V k} = 0.5 \text{ min}$$

The individual transfer functions can be combined to give the closed-loop transfer function for a set point change, which includes the characteristic equation. (where CV= Control variable & SP = set-point signal)

$$\frac{CV(s)}{SP(s)} = \frac{G_p(s)G_v(s)G_c(s)}{1 + G_p(s)G_v(s)G_c(s)G_s(s)} = \frac{K_p \left(1 + \frac{1}{s}\right) \frac{0.1}{(0.5s + 1)^2}}{1 + K_p \left(1 + \frac{1}{s}\right) \frac{0.1}{(0.5s + 1)^2}}$$

Characteristic equation

$$0 = 1 + K_p \left(1 + \frac{1}{s}\right) \frac{0.1}{(0.5s + 1)^2}$$

6.2 Root Locus Diagrams

Root Locus plots are a method of evaluating the behavior of a control system. The creation of a root locus plot begins by determining the poles of the control system for a given set of control parameters. These poles are then plotted on a complex coordinate system as seen in the previous section and analyzed to determine the behavior of the system.

6.2.1 Determining the Poles of a Control System

The “poles” of a system are the roots of the denominator of the transfer function. In other words the poles are the values of "s" when the transfer function goes to infinity (when the denominator equals zero). For a system of differential equations, poles are the eigenvalues of the equation system. Consider the following solution to a system of differential equations:

$$f(s) = 48s^3 + 44s^2 + 12s + 1 \quad (1)$$

This equation is a third order polynomial, therefore it will have three poles (be aware that some of these poles may be imaginary numbers). These poles can be obtained by factoring the expression or using a computer program such as Maple. The three poles, or roots, of this equation are $s = -0.167, -0.25, -0.5$.

For a system of differential equations, finding the eigenvalues can be time consuming and the use of Matlab, Maple, or Mathematica is more efficient. One method would be to use the Mathematica `eigenvalues[]` function to solve the system for you. This function is explained in [Eigenvalues and Eigenvectors](#) section of the wiki text.

6.2.2 Plotting Poles on a Complex Coordinate System to make Root Locus Plot

A root locus plot is created by plotting the resulting poles on a complex coordinate system. For a system of P-only control, the governing differential equations will depend on the proportional gain, K_c . Consider the following solution to a system of differential equations:

$$f(s) = 48s^3 + 44s^2 + 12s + 1 + 6K_c \quad (2)$$

Notice that K_c is a term in this equation. Therefore, there exists a set of poles for each value of K_c . If $K_c = 0$, then equation #2 reduces to equation #1, and poles are as listed above. Table 1 lists the three poles of the system for given values of K_c . These poles

were calculated using a computer algebra system because it is impractical to try and evaluate these functions with analytical methods.

Table 1- Poles of Characteristic Equation

Kc	Pole 1	Pole 2	Pole 3
-0.028	-0.406	-0.406	-0.105
0.000	-0.167	-0.25	-0.500
0.004	-0.205	-0.205	-0.506
0.050	-.182+.126i	-.182-.126i	-0.553
0.200	-.140+.229i	-.140-.229i	-0.637
0.500	-.093+.325i	-.093-.325i	-0.731
1.000	-.045+.417i	-.045-.417i	-0.880
1.670	0-.500i	0+.500i	-0.917
2.000	.018-.532i	.018+.532i	-0.952

To create a root locus plot, each pole is broken down into its real (x-axis) and imaginary (y-axis) component (Table 2):

Table 2- Real and Imaginary Components of each Pole

Kc	Real Part	Imaginary Part
0	-0.167	0
0	-0.25	0
0	-0.5	0
0.004	-0.205	0
0.004	-0.205	0
0.004	-0.506	0
0.05	-0.182	0.126
0.05	-0.182	-0.126
0.05	-0.553	0
0.2	-0.14	0.229
0.2	-0.14	-0.229
0.2	-0.637	0
0.5	-0.093	0.325
0.5	-0.093	-0.325
0.5	-0.731	0
1	-0.045	0.417
1	-0.045	-0.417
1	-0.88	0
1.67	0	0.5
1.67	0	-0.5
1.67	-0.917	0
2	0.018	0.532
2	0.018	-0.532
2	-0.952	0

These points can now be plotted to make the root-locus diagram (Figure 1):

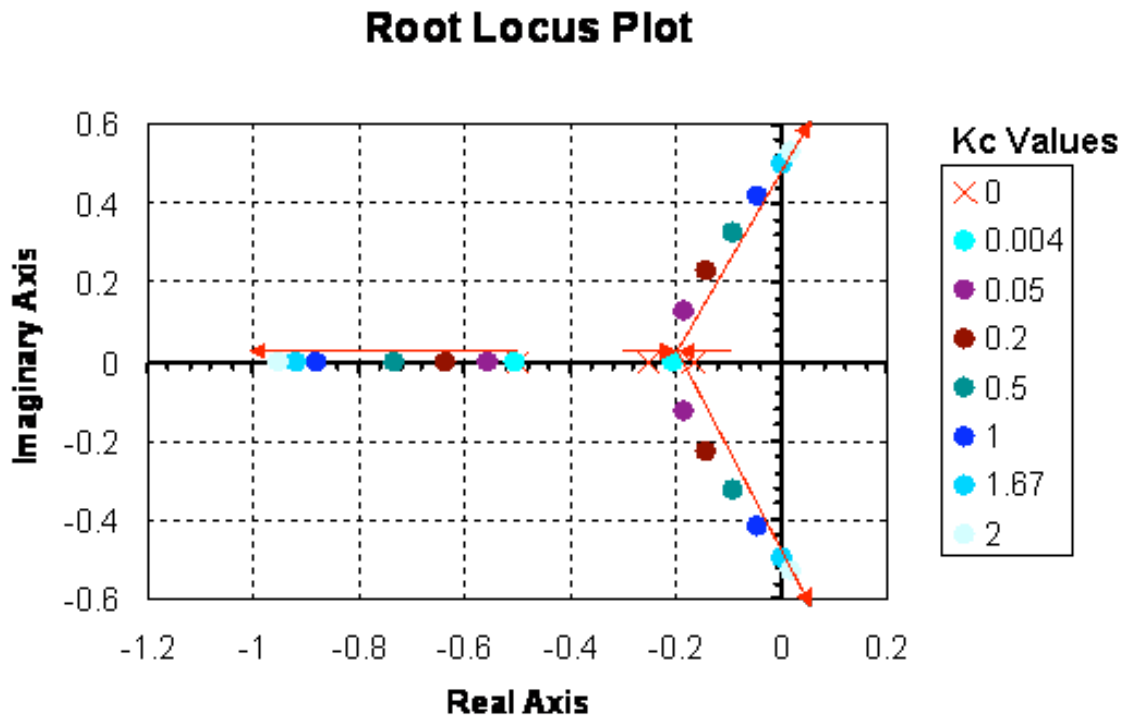


Figure 1- Root Locus Diagram of the Characteristic Equation

By convention, red arrows are drawn on the plot in the direction of increasing K_c values. They help to illustrate how the roots of the system vary by changing the K_c value. Also by convention, the points in which $K_c = 0$ are represented with 'x' marks instead of dots.

6.2.3 Interpreting a Root Locus Diagram

The primary use of a Root Locus Diagram is to evaluate how differing values of K_c affect the stability and behavior of a control system.

The stability of the control system depends on the sign of the real component of the pole. If the real components of all poles are negative, then the system is said to be stable for that value of K_c . If the real component of the pole is positive, the system is unstable for that value of K_c , meaning the output signal will diverge from the set point.

The behavior of the control system depends on the presence of an imaginary component of the pole. If any of the three poles contains an imaginary number component, then that value of K_c will cause the output signal to oscillate. If all of the poles are real (contain no imaginary components), the output signal will not oscillate at that K_c value.

Please refer back to the Root Locus diagram in Figure 1. The system becomes unstable (i.e. the real component of the poles becomes positive) for $K_c > 1.67$ and $K_c < 0$. Within the range of stability, no oscillations (i.e. no imaginary component) are observed when $0 < K_c < 0.004$.

6.3 Root Locus Diagrams for PID Control

Root Locus diagrams are much more difficult to create for PID control. The characteristic equation will contain unknown variables K_c , T_i , and T_d . Therefore, each point on the Root Locus Diagram will represent a set of tuning parameters. In order to show the progression as each tuning parameter changes, the resulting diagram will be a three-dimensional surface plot. Due to the complexity of this diagram, we will not create one, as it is beyond the scope of this text. However, stability analysis can still be applied to the characteristic equation. Take for example equation 3:

$$f(s) = \frac{48s^3 + 44s^2 + 12s + 1 + 6K_c}{T_i + 3T_d} \quad (3)$$

In this theoretical instance, equation 3 is the characteristic equation governing the same system mentioned above, only now with PID control. Notice the additional presence of the T_i and T_d terms. Under P- only control, this system was stable for K_c values between 0 and 1.67. Will the same be true if this system were tuned with PID control?

Let's suppose we want to test the conditions $K_c = 1.0$, $T_i = 0.3$ and $T_d = 0.1$. These values were randomly chosen. Using a computer software package, the three roots were determined to be: $r_1 = -0.827$, $r_2 = -0.044 + 0.417i$, $r_3 = -0.044 - 0.417i$. Therefore, since the real components are all negative, the system is still stable. Since complex roots are present, the response is expected to oscillate around the set point.

6.4 Creating Root Locus Plots with Mathematica

Mathematica allows you to develop root locus plots for polynomials since the math involved in solving for the solutions can become very tedious. Before you are able to obtain the root locus plot, you need to solve for the roots. We will use the same equation as was used in the "Determining the Poles of a Control System" section.

$$f(s) = 48s^3 + 44s^2 + 12s + 1 + 6K_c$$

The **Solve[]** function can be used to determine the roots, both real and imaginary, for each corresponding K_c value. The syntax in Mathematica is shown below for the specified equation when $K_c = 0$. It is important to note that in order to obtain an output you must press “Shift Enter.”

```

In[1]:= Solve[48 * x^3 + 44 * x^2 + 12 * x + 1 == 0, x]

Out[1]= {{x -> -1/2}, {x -> -1/4}, {x -> -1/6}}

```

The following is just to show how Mathematica formats the output when $K_c \neq 0$ and when there are imaginary roots. In this case, $K_c = -0.167$.

```

In[98]:= Solve[48 * x^3 + 44 * x^2 + 12 * x + 1 + 6 * (-.167) == 0, x]

Out[98]= {{x -> -0.458417 - 0.200017 i},
          {x -> -0.458417 + 0.200017 i}, {x -> 0.000166565}}

```

This can be done for all K_c values to obtain the corresponding real and imaginary roots. After all of the roots have been calculated, a table can be made to format the real roots (x axis) versus imaginary roots (y axis). When the syntax, **A={{x,y}{a,b}...}**, is used, you are inputting all of the x and y values and naming those values **A**. When you call **A** in the **TableForm[]** function, the table will be made according to all of the x and y values input into **A**. The syntax and corresponding outputs are shown below.

```
Mathematica Root Locus Plot cont.nb *

R = {{-0.466, 0.217}, {-0.466, -0.217}, {0.016, 0}, {-0.458, 0.2},
      {-0.458, -0.2}, {0, 0}, {-0.406, 0}, {-0.406, 0}, {-0.105, 0},
      {-0.167, 0}, {-0.25, 0}, {-0.5, 0}, {-0.205, 0}, {-0.205, 0},
      {-0.506, 0}, {-0.182, 0.126}, {-0.182, -0.126}, {-0.533, 0},
      {-0.14, 0.229}, {-0.14, -0.229}, {-0.637, 0}, {-0.093, 0.325},
      {-0.093, -0.325}, {-0.731, 0}, {-0.045, 0.417}, {-0.045, -0.417},
      {-0.88, 0}, {0, 0.5}, {0, -0.5}, {-0.917, 0}, {0.018, 0.532},
      {0.018, -0.532}, {-0.952, 0}}

Out[104]= {{-0.466, 0.217}, {-0.466, -0.217}, {0.016, 0}, {-0.458, 0.2},
            {-0.458, -0.2}, {0, 0}, {-0.406, 0}, {-0.406, 0},
            {-0.105, 0}, {-0.167, 0}, {-0.25, 0}, {-0.5, 0}, {-0.205, 0},
            {-0.205, 0}, {-0.506, 0}, {-0.182, 0.126}, {-0.182, -0.126},
            {-0.533, 0}, {-0.14, 0.229}, {-0.14, -0.229}, {-0.637, 0},
            {-0.093, 0.325}, {-0.093, -0.325}, {-0.731, 0}, {-0.045, 0.417},
            {-0.045, -0.417}, {-0.88, 0}, {0, 0.5}, {0, -0.5},
            {-0.917, 0}, {0.018, 0.532}, {0.018, -0.532}, {-0.952, 0}}
```

Mathematica Root Locus Plot cont.nb *

```
In[107]:= TableForm[A, TableAlignments -> Right,
  TableHeadings -> {Automatic, {"Real", "Imaginary"}}]
```

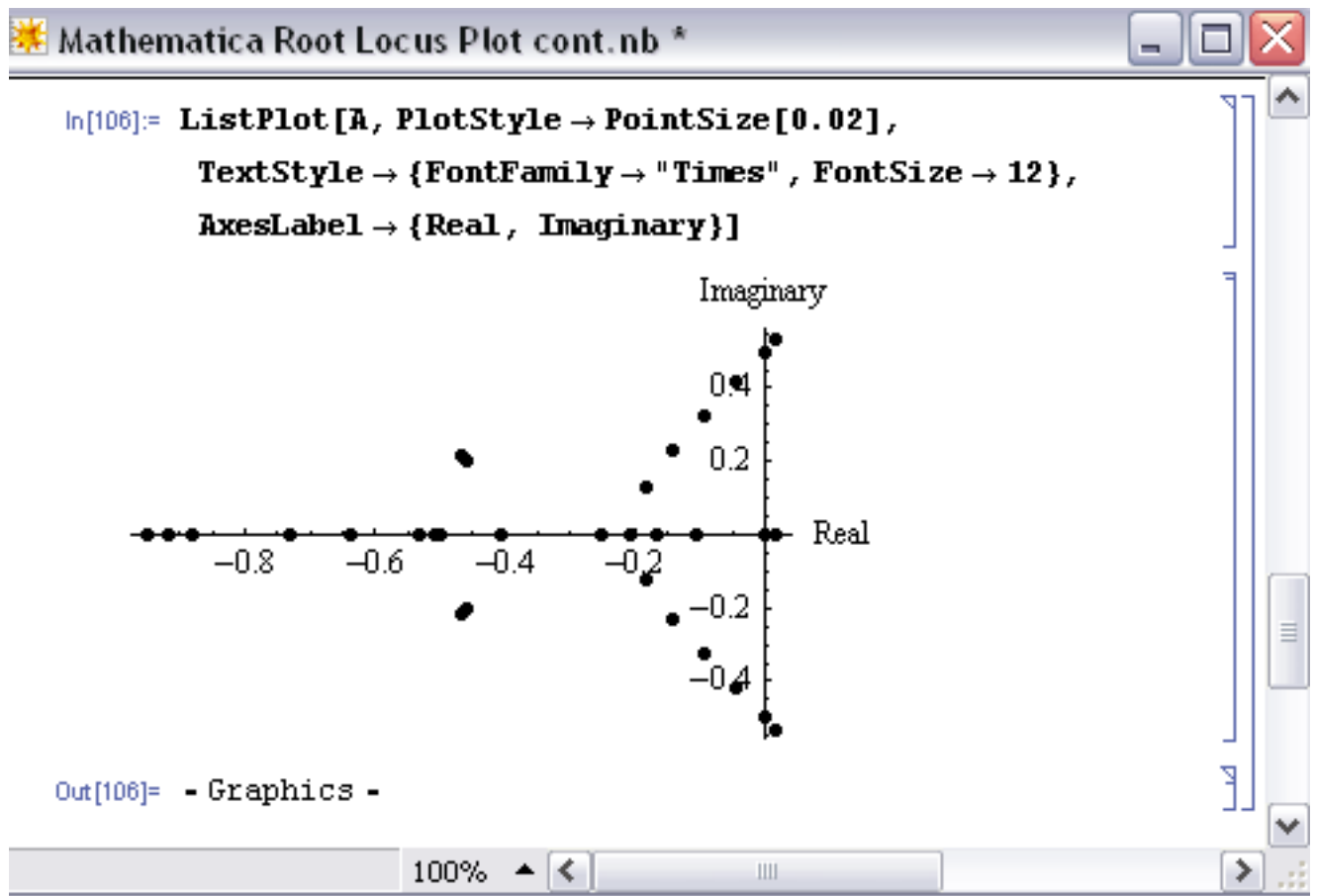
Out[107]//TableForm=

	Real	Imaginary
1	-0.466	0.217
2	-0.466	-0.217
3	0.016	0
4	-0.458	0.2
5	-0.458	-0.2
6	0	0
7	-0.406	0
8	-0.406	0
9	-0.105	0
10	-0.167	0
11	-0.25	0
12	-0.5	0
13	-0.205	0
14	-0.205	0
15	-0.506	0
16	-0.182	0.126
17	-0.182	-0.126
18	-0.533	0
19	-0.14	0.229
20	-0.14	-0.229
21	-0.637	0
22	-0.093	0.325
23	-0.093	-0.325
24	-0.731	0
25	-0.045	0.417
26	-0.045	-0.417
27	-0.88	0
28	0	0.5
29	0	-0.5
30	-0.917	0
31	0.018	0.532
32	0.018	-0.532
33	-0.952	0

100% ◀ ◂ ◃ ▶ ▸ ▹ ▸

In order to produce the table shown above, you only need **TableForm[A]** and nothing else. The other descriptions (ie. **TableAlignments** and **TableHeadings**) are just used for formatting purposes.

Once the real (x) and imaginary (y) roots have been determined and put into table format for your equation, the **ListPlot[]** function can be used to develop your root locus diagram by calling **A**.



As you can see, the **ListPlot[]** function returned the same plot as shown in the “Complex Coordinate System to make Root Locus Plot” section (this plot was created in Excel). The arrows are not shown in this Mathematica plot; however the Excel plot shows the direction of increasing K_c values to show how the roots of the system vary by changing the K_c values.

The Mathematica Help Browser is a very useful tool for understanding the syntax. For example, when using the **ListPlot[]** function you can search how to label the axes and

how to make the points larger (more visible) on the plot. The following examples are used to illustrate the use of root locus plots. Click the following link if you would like to access the actual Mathematica file: [Media:RLPFinalaa.nb](#)

6.5 Second Plot Method Using Arrays

The goal here is to be able to understand exactly what is happening with these Mathematica inputs in order to get a better grasp on the outputs. Basically, once you have found the Eigenvalues of the system, which examples can be found for in other areas of the wiki, we then want to solve explicitly for them. After we solve for the Eigenvalue in terms of the variables, we can create an array by varying this value and solving for the real and imaginary terms of the Eigenvalues.

Eigenvalue Outputs in Mathematica

The Eigenvalues can either be returned as a function of 'l', which is the designation of the Eigenvalue or simply as a complex function in terms of variables. When returned as a function of 'l' there will be a polynomial input that has to be simplified to find 'l' as a function of the variable. In this case: Kc.

```
Eigenvalues[Jac /. param]
{{{-1/2, 0, -Kc/2}, {1/4, -1/4, 0}, {0, 1/6, -1/6}}
{Root[1 + Kc + 12 #1 + 44 #1^2 + 48 #1^3 &, 1],
 Root[1 + Kc + 12 #1 + 44 #1^2 + 48 #1^3 &, 2],
 Root[1 + Kc + 12 #1 + 44 #1^2 + 48 #1^3 &, 3]}
Kc = .
ss = N[Simplify[Solve[48 * l^3 + 44 * l^2 + 12 * l + (1 + Kc) == 0, l]]];
```

This example is taken directly from lecture 17 and its supplementary Mathematica file. What is happening here is that the Jacobian was inputted, and there were multiple eigenvalue arrays that were found. The last array has three complex polynomial functions that equal to 0. The last line is simplifying them, solving for 'l'. This is putting the simplified Eigenvalues into the array 'ss'.

Another output of Eigenvalues is simply in the form of complex numbers themselves. Rather than worry about the simplification steps, these Eigenvalues can be directly inputted as a complex number into an array, again termed 'ss':

$$ss = \left\{ \left\{ 1 \rightarrow \left(-5 - 10 * Kc - \sqrt{150 - 1590 * Kc + 1240 * Kc} \right) \right\}, \right. \\ \left. \left\{ 1 \rightarrow \left(-5 - 10 * Kc + \sqrt{150 - 1590 * Kc + 1240 * Kc} \right) \right\} \right\}$$

This is a variation of the sample in lecture 17.

Plot Array Creation

Now that we have seen the two ways of Eigenvalue array creation, we can use these to create another array that will be the points for the plot. Here we will be substituting in values of the variable Kc to find different values of the Eigenvalues, which will give us information on stability changes as Kc changes.

```
Kc = .
ss = N[Simplify[Solve[48 * l^3 + 44 * l^2 + 12 * l + (1 + Kc) == 0, l]]];
a = {};
Kc = 0;
a = Append[a, {Re[l /. ss[[2]]], Im[l /. ss[[2]]]}];
a = Append[a, {Re[l /. ss[[1]]], Im[l /. ss[[1]]]}];
a = Append[a, {Re[l /. ss[[3]]], Im[l /. ss[[3]]]}];
Kc = 0.5;
a = Append[a, {Re[l /. ss[[2]]], Im[l /. ss[[2]]]}];
a = Append[a, {Re[l /. ss[[1]]], Im[l /. ss[[1]]]}];
a = Append[a, {Re[l /. ss[[3]]], Im[l /. ss[[3]]]}];
...
```

This example is also taken directly from lecture 17 and its supplementary Mathematica file.

In the example above, 'ss' is in the form : {{solution1} , {solution2}, {solution3}} Each solution in this array is in the form l -> a+bi. For example, ss[[2]] refers to solution2, which is the object in the second position in ss. Re[l/.ss[[2]]] applies solution2 to the variable l and then returns only the real part. Im[l/.ss[[2]]] applies solution2 to the variable l and then returns only the imaginary part. The effect of the Append function above is that the ordered pair {a,b} (from a solution of the form a+bi) is added to the array called 'a'.

However, not all Eigenvalue arrays will have the same number of Eigenvalues. For example, as mentioned in the above paragraph, 'ss' is in the form : {{solution1}, {solution2}, {solution3}} There could be 2, or 3, or more separate 'solution' values in the

array. Depending on the number of the 'solution' values, there will be a different format for your 'append' function in Mathematica. For example, in the image below, there are only two eigenvalues in our array that we want to solve for. Thus, there should only be two rows of the addition to the array for the this method:

```
a = {};
F = 0;
a = Append[a, {Re[1 /. ss[[2]]], Im[1 /. ss[[2]]]}];
a = Append[a, {Re[1 /. ss[[1]]], Im[1 /. ss[[1]]]}];
```

These different methods both output arrays of numbers that act essentially as 'x' and 'y' values, or in this case Real and Imaginary, for the plot. The array 'a' is plotted as such:

ListPlot[a, PlotStyle -> PointSize[0.02]]

This is inputted directly to Mathematica, which creates the Root Locus Plot.

6.6 Differential Equation Example of Root Locus Plots in Mathematica

An example problem pulled from the Fall 2008 second exam:

"You have just been put in charge of designing a large-scale bioreactor for the production of a blockbuster protein based drug. After some research, you have come up with the following model to describe the reactor system:"

$$dX / dt = -2X + (10 * X * S) / (S + 2)$$

$$dS / dt = 4 * Fin - S - (3 * X * S) / (S + 2)$$

$$dP / dt = 9 * X - 2 * P$$

X is the cell concentration, S is the nutrient concentration, and P is the protein product. Fin is the flow rate of nutrient into the system.

In this system there are two fixed points found by setting all the differential equations equal to zero and solving in Mathematica.

```
eqn = {0 == -2 * X + (10 * X * S) / (S + 2), 0 == 4 * Fin - S - (3 * X * S) / (S + 2), 0 == 9 * X - 2 * P};
eqns = {-2 * X + (10 * X * S) / (S + 2), 4 * Fin - S - (3 * X * S) / (S + 2), 9 * X - 2 * P};
Solve[eqn, {X, S, P}]
```

$$\text{Out[4]} = \left\{ \{P \rightarrow 0, X \rightarrow 0, S \rightarrow 4 \text{ Fin}\}, \left\{ P \rightarrow \frac{15}{4} (-1 + 8 \text{ Fin}), X \rightarrow \frac{5}{6} (-1 + 8 \text{ Fin}), S \rightarrow \frac{1}{2} \right\} \right\}$$

The two fixed points depend on the value of Fin and with that varying values of Fin will change eventual eigenvalues. Since this problem will eventually want root locus plots for both fixed points it is easier to save both points as parameters to be applied to general equations later. Overall it will help save the need for redundant code. The entire mathematica file being referenced in this example is available here:

[Media:Exam2Probl.nb](#)

From this point a Jacobian matrix should be created to linearize the system around the fixed points (as applied to the Jacobian). Once created the stored fixed point values for X, S, and P can be applied. Once applied, the eigenvalues for each fixed point can be solved for. These will still contain a variable 'Fin' since Fin has not been defined yet.

```
In[192]:= Clear[Fin]
eqn = {0 == -2 * X + (10 * X * S) / (S + 2), 0 == 4 * Fin - S - (3 * X * S) / (S + 2), 0 == 9 * X - 2 * P};
eqns = {-2 * X + (10 * X * S) / (S + 2), 4 * Fin - S - (3 * X * S) / (S + 2), 9 * X - 2 * P};
Solve[eqn, {X, S, P}]
par1 = {P -> 0, X -> 0, S -> 4 * Fin};
par2 = {P -> 15/4 (-1 + 8 Fin), X -> 5/6 (-1 + 8 Fin), S -> 1/2};
Jac = {{D[eqns[[1]], X], D[eqns[[1]], S], D[eqns[[1]], P]},
       {D[eqns[[2]], X], D[eqns[[2]], S], D[eqns[[2]], P]},
       {D[eqns[[3]], X], D[eqns[[3]], S], D[eqns[[3]], P]}};
a = Jac /. par1;
b = Jac /. par2;
MatrixForm[a]
MatrixForm[b]
c = N[Eigenvalues[a]];
d = N[Eigenvalues[b]];
```

Out[201]//MatrixForm=

$$\begin{pmatrix} -2 + \frac{40 \text{ Fin}}{2 + 4 \text{ Fin}} & 0 & 0 \\ -\frac{12 \text{ Fin}}{2 + 4 \text{ Fin}} & -1 & 0 \\ 9 & 0 & -2 \end{pmatrix}$$

Out[202]//MatrixForm=

$$\begin{pmatrix} 0 & \frac{8}{3} (-1 + 8 \text{ Fin}) & 0 \\ -\frac{3}{5} & -8 \text{ Fin} + \frac{1}{5} (-1 + 8 \text{ Fin}) & 0 \\ 9 & 0 & -2 \end{pmatrix}$$

From here the Table[] function can be used to tabulate eigenvalues for various Fin values for visual sake of inspection. This is not necessary since the eigenvalue results have

already been solved for in terms of Fin . To create the root locus plots, values of Fin need to be defined and applied to the eigenvalue equations with the results stored. That step is next. In this table step it is for the user's sake to see with increasing Fin values what the eigenvalues look like. The tabulated eigenvalues are stored as a matrix and displayed as such with the function 'MatrixForm[

```
a = Jac /. par1;  
b = Jac /. par2;  
MatrixForm[a]  
MatrixForm[b]  
c = N[Eigenvalues[a]];  
d = N[Eigenvalues[b]];  
e = Table[c, {Fin, 0, 2, 0.1}];  
MatrixForm[e]  
f = Table[d, {Fin, 0, 2, 0.1}];  
MatrixForm[f]
```

Out[206]//MatrixForm=

-2.	-1.	-2.
-2.	-1.	-0.333333
-2.	-1.	0.857143
-2.	-1.	1.75
-2.	-1.	2.44444
-2.	-1.	3.
-2.	-1.	3.45455
-2.	-1.	3.83333
-2.	-1.	4.15385
-2.	-1.	4.42857
-2.	-1.	4.66667
-2.	-1.	4.875
-2.	-1.	5.05882
-2.	-1.	5.22222
-2.	-1.	5.36842
-2.	-1.	5.5
-2.	-1.	5.61905
-2.	-1.	5.72727
-2.	-1.	5.82609
-2.	-1.	5.91667
-2.	-1.	6.

Out[208]//MatrixForm=

-2.	-1.36886	1.16886
-2.	-1.12456	0.284557
-2.	-0.74 - 0.642184 i	-0.74 + 0.642184 i
-2.	-1.06 - 1.0566 i	-1.06 + 1.0566 i
-2.	-1.38 - 1.27106 i	-1.38 + 1.27106 i
-2.	-1.7 - 1.38203 i	-1.7 + 1.38203 i
-2.	-2.02 - 1.41407 i	-2.02 + 1.41407 i
-2.	-2.34 - 1.37273 i	-2.34 + 1.37273 i
-2.	-2.66 - 1.25076 i	-2.66 + 1.25076 i
-2.	-2.98 - 1.01961 i	-2.98 + 1.01961 i
-2.	-3.3 - 0.556776 i	-3.3 + 0.556776 i
-2.	-4.41019	-2.82981
-2.	-5.26801	-2.61199
-2.	-6.02284	-2.49716
-2.	-6.73787	-2.42213
-2.	-7.4318	-2.3682
-2.	-8.11282	-2.32718
-2.	-8.78524	-2.29476
-2.	-9.4516	-2.2684
-2.	-10.1135	-2.2465
-2.	-10.772	-2.228

These tables make it easy to see with increasing F_{in} (goes from 0 to 2 down the table) what the changes are in the stability of each fixed point. The first table is the first fixed point, the second table the second FP.

Now, to make the root locus plots, a really long string of values needs to be created in order for the real and imaginary roots to be plotted. This is a long string of code that is basically brute force. The overall action occurring here is setting F_{in} to a value, evaluating that F_{in} through the eigenvalues, and saving the real portion separate from the imaginary portion by different columns. This is repeated for as many F_{in} values as you

desire. It is extremely repetitive, but works. After evaluating as many Fin values as you desired you can display the two columns through the ListPlot[] function. Example snippets of the code look like such:

```

Fin = .
rootc = {}
Fin = 0;
rootc = Append[rootc, {Re[c[[2]]], Im[c[[2]]]}];
rootc = Append[rootc, {Re[c[[1]]], Im[c[[1]]]}];
rootc = Append[rootc, {Re[c[[3]]], Im[c[[3]]]}];
Fin = 0.1;
rootc = Append[rootc, {Re[c[[2]]], Im[c[[2]]]}];
rootc = Append[rootc, {Re[c[[1]]], Im[c[[1]]]}];
rootc = Append[rootc, {Re[c[[3]]], Im[c[[3]]]}];
Fin = 0.2;
rootc = Append[rootc, {Re[c[[2]]], Im[c[[2]]]}];
rootc = Append[rootc, {Re[c[[1]]], Im[c[[1]]]}];
rootc = Append[rootc, {Re[c[[3]]], Im[c[[3]]]}];
Fin = 0.3;
rootc = Append[rootc, {Re[c[[2]]], Im[c[[2]]]}];
rootc = Append[rootc, {Re[c[[1]]], Im[c[[1]]]}];
rootc = Append[rootc, {Re[c[[3]]], Im[c[[3]]]}];
Fin = 0.4;
rootc = Append[rootc, {Re[c[[2]]], Im[c[[2]]]}];
rootc = Append[rootc, {Re[c[[1]]], Im[c[[1]]]}];
rootc = Append[rootc, {Re[c[[3]]], Im[c[[3]]]}];
Fin = 0.5;
rootc = Append[rootc, {Re[c[[2]]], Im[c[[2]]]}];
rootc = Append[rootc, {Re[c[[1]]], Im[c[[1]]]}];
rootc = Append[rootc, {Re[c[[3]]], Im[c[[3]]]}];

```

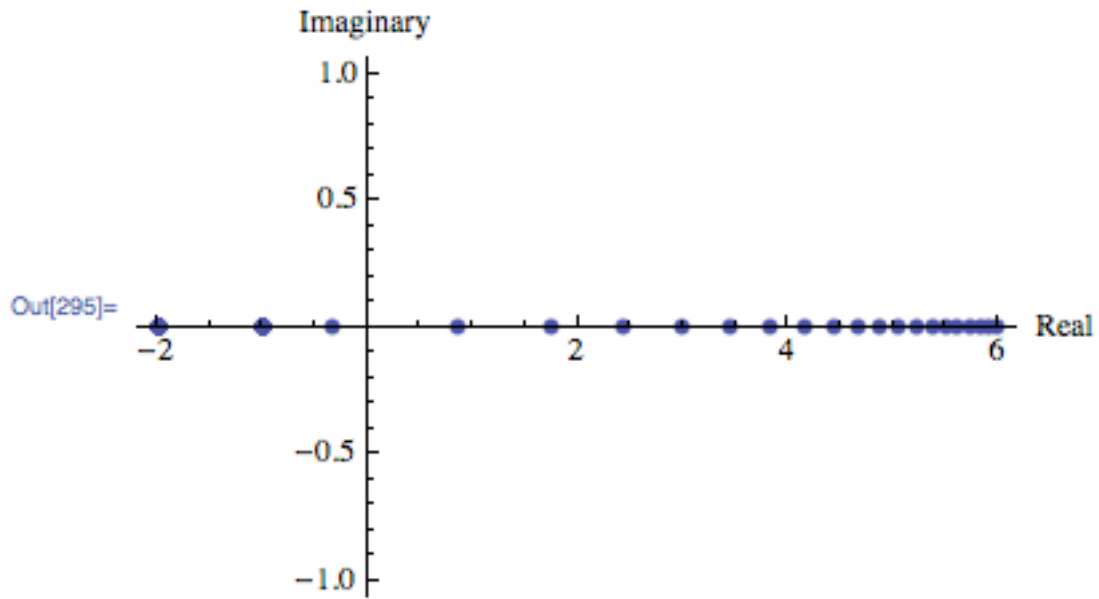
And the ListPlot[] function can look like this:

```

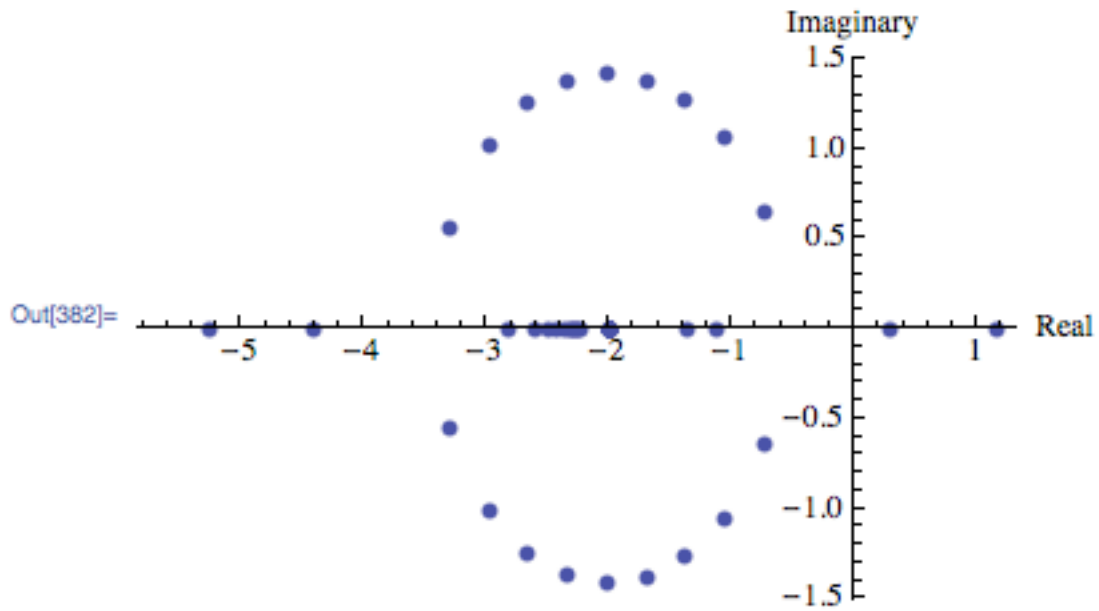
ListPlot[rootc, PlotStyle -> PointSize[0.02],
TextStyl -> {FontFamily -> "Times", FontSize -> 12}, AxesLabel -> {Real, Imaginary}]

```

And would make graphs like these (Fixed Point 1 on top and FP2 on bottom in this example):



Out[297]= {}



Looking back at the tables of eigenvalues the plots can be interpreted. For FP1 the values start real negative and increase to real positive. There are no imaginary values. For FP2, increasing Fin values go from real positive to negative with imaginary values occurring in the transition from low to high Fin values.

6.7 Alternative Mathematica Method

Some Mathematica 6 programs have an add-on or supplementary application known as **ANALOG INSYDES** which contains special options to create Root Locus Plots with ease. The Function is called *RootLocusPlot*. Enter the function that is to be analyzed, into Mathematica with the following format:

```
RootLocusPlot[tfunc,{k,k_0,k_1}]
```

tfunc is the transfer function in the frequency variable *s* and one real parameter *k*. *k_0* and *k_1* are the range for the real parameter *k* that is to be varied in the Root Locus Plot. Follow an example below.

Example: Equation to make a Root Locus Plot with:

$$H(s) = (a + 2 * s + s^2) / (10 + 3 * a * s + 4 * s^2 + s^3)$$

To make a Root Locus Plot follow the example code below:

```
H4[s_, a_] := (a + 2*s + s^2)/(10 + 3*a*s + 4*s^2 + s^3)
```

```
RootLocusPlot[H4[s, a], {a, 3, 5}]
```

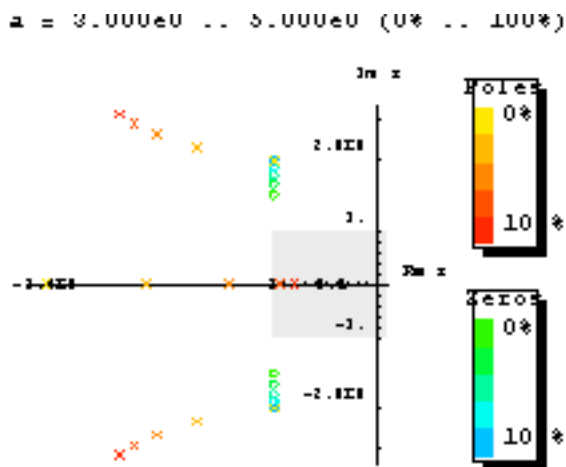


Image: Wolfram.com

Other Mathematica forms for using RootLocusPlot[]:

RootLocusPlot[*func*] This form displays the a pole/zero diagram of a function i.e. *func* without parameters *k* and *k_I*.

RootLocusPlot[*rootloc*] This form displays a root locus calculated with function RootLocusByQZ[[]].

Refer to Mathematica link for further discuss about [RootLocusByQZ](#)

Many options for the plot can be varied including the number of points, plot style, and plot color. All of these options and more can be viewed online with a [Mathematica Tutorial](#)

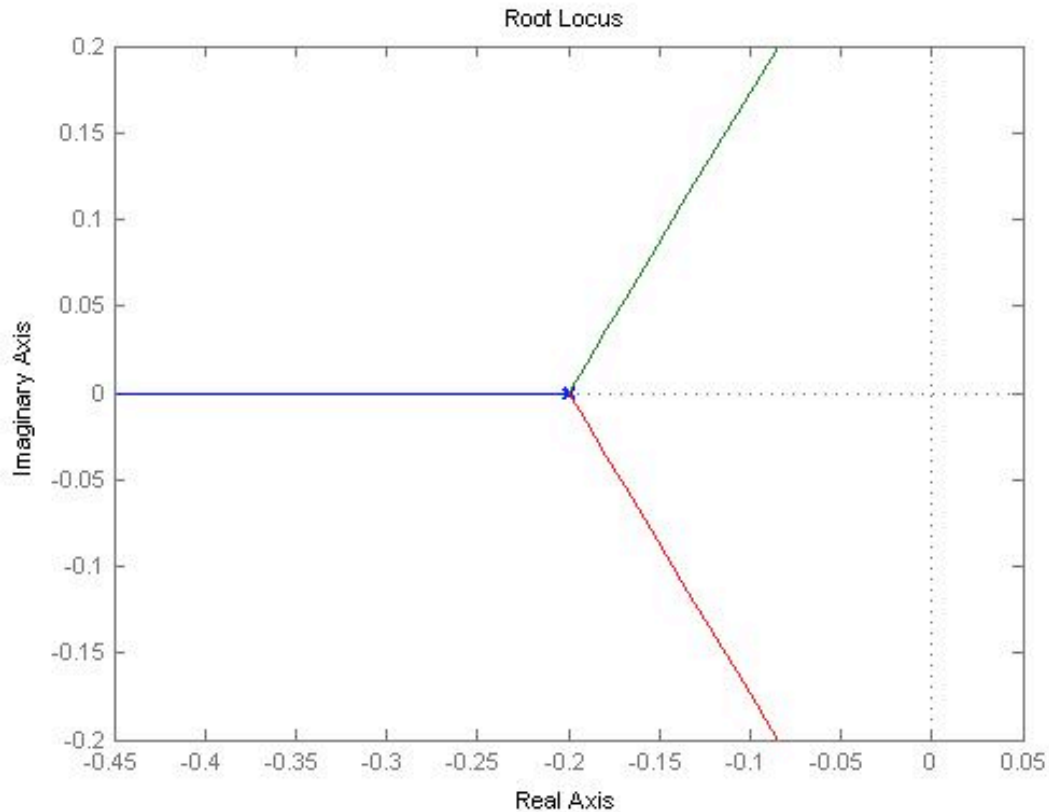
6.8 Creating Root Locus Plots with Matlab

Root Locus Generation in Matlab Three matlab files have been given to obtain the root locus plot and poles of the root locus plot at specified Kc values for a specific transfer function with relative ease. These three files are polesfunction.m, transferfunction.m, and Locusplotpoles.m [1]. The transferfunction file is where the specific transfer function should be input. As written the only line needing variation is line 4 (Gs). The polesfunction file finds the poles of the given transfer function using built in matlab utilities and needs no variation, even after changing the transfer function. The Locusplotpoles file is what is called in matlab to generate the root locus plot as well as the value of the poles and integrates the two previous files. To use this file you type in the values of the specific Kc you require the pole values for as well as a single value of Kc for which you would like to see the root locus plot. An example of the inputs to and outputs of this file are given below.

```
>> Locusplotpoles([0 50 100 200],0)
```

```
ans =
```

```
1.0e+002 *
Columns 1 through 3
      0      -0.0020      -0.0020 + 0.0000i
0.5000      -0.0045      -0.0008 + 0.0022i
1.0000      -0.0051      -0.0004 + 0.0027i
2.0000      -0.0060      -0.0000 + 0.0034i
Columns 4 through 6
-0.0020 - 0.0000i      0      0
-0.0008 - 0.0022i      -0.0020      -0.0020 +
0.0000i -0.0004 - 0.0027i      -0.0020 + 0.0000i      -
0.0020 - 0.0000i -0.0000 - 0.0034i      -0.0020
      -0.0020 + 0.0000i
Column 7
      0      -0.0020 - 0.0000i      -0.0020
-0.0020 - 0.0000i
```



The values inside the brackets are the specific K_c values for which poles are desired. The last value is the K_c which the root locus plot will be plotted for. Notice that the value of K_c for the root locus plot to be generated in this example is zero. This is so that the entire range of K_c can be examined using the interactive graph produced by matlab. If other specific K_c plots would like to be observed this value can be changed to generate these as well. The column lines give the values of K_c input and then value of the poles for each K_c . Note that the actual values are the values matlab gives multiplied by 100.

Now that a basic understanding of root locus plots has been obtained here are a few websites which go further in depth into the underlying principles and generation of these plots.

<http://www.facstaff.bucknell.edu/mastascu/eControlHTML/RootLocus/RLocus1A.html>

This site gives animated examples which progress the value of the control variable through a root locus plot to better explain the fundamental function of these plots. It would be beneficial to go through a few of these examples to observe patterns of fluctuation of the control variable. The parameters for each animation are given to the left of the frame.

<http://www.engin.umich.edu/group/ctm/rlocus/rlocus.html>

This page gives examples of how you generate a root locus plot of a given transfer function using matlab. While you go through the content on this page take special notice of the fact that none of the given transfer functions have an integrated Kc variable for which to generate a locus plot. To see how these plots can be generated when a value of Kc is specified see the code of Locusplotpoles.m. For clarification on the application of root locus plots see the given examples.

6.9 Creating Root Locus plots with Excel and PPLANE

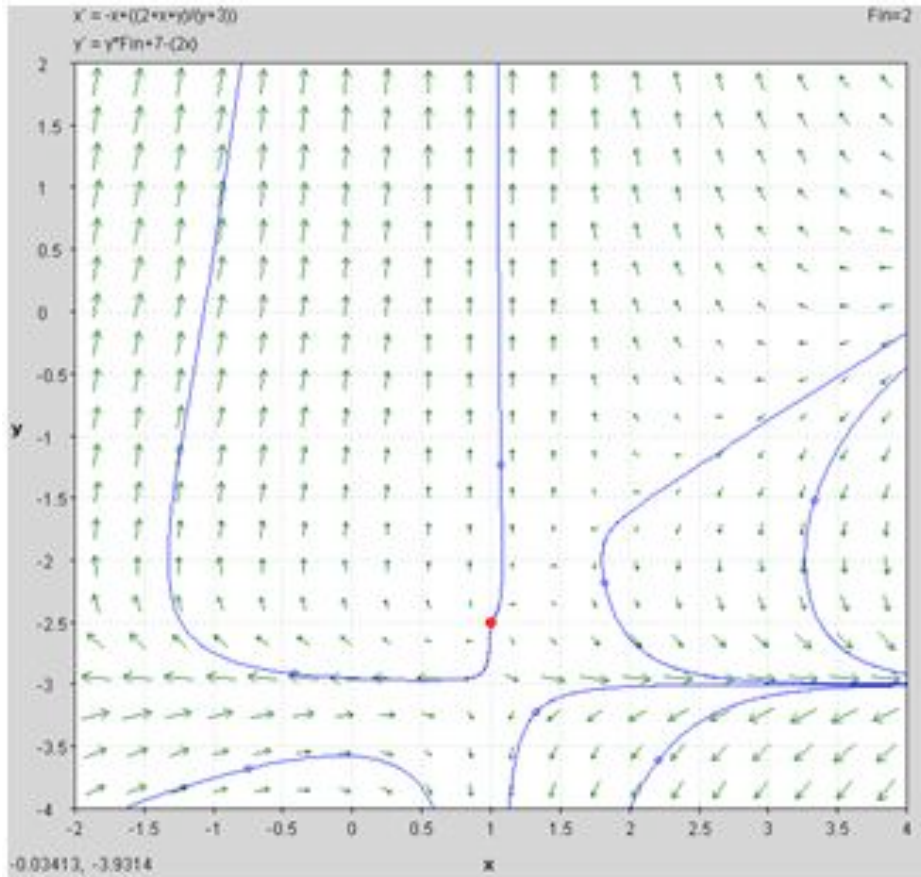
Though this tactic may remain slightly more time consuming and work involved, there is a method in computing the Root Locus plot using PPLANE and Excel. This particular model really aids in better understanding of how to read and acknowledge a Root Locus Plot, and is also useful if alternative options for making a Root Locus Plot are not currently available.

This method involves using PPLANE in order to find the eigenvalues for each equilibrium value, and then plotting these points with Excel software. In order to do this, suppose that you have the following differential equations that represent a reactor:

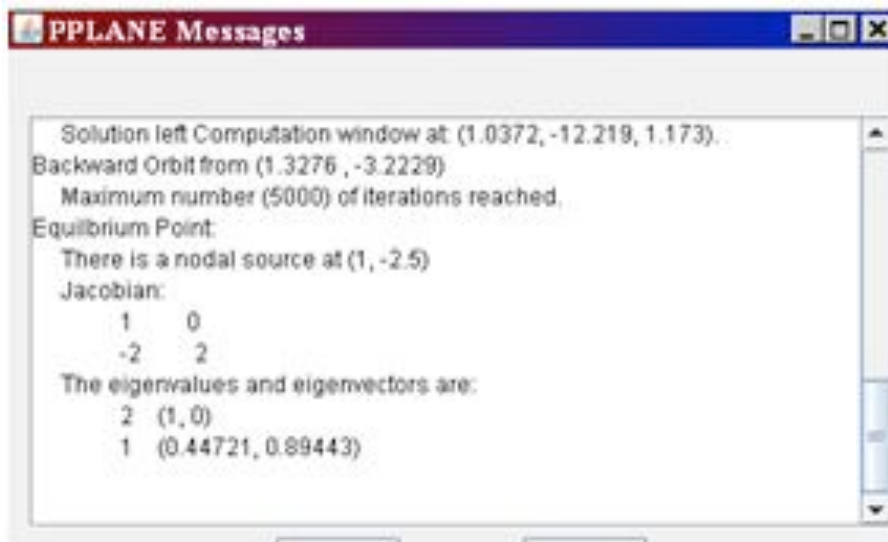
$$(dX/dt) = -X + ((2+X+Y)/(Y+3))$$

$$(dY/dt) = Y * Fin + 7 - (2X)$$

Graphing the following differential equations provides something similar to the following chart (a few lines were drawn, just to better show the graphs flow):



Using the ability to “Find an Equilibrium Point” in PPLANE (if you need help with PPLANE, click [PhasePlaneAnalysis](#)), one can select a particular equilibrium point on the field, and be able to provide the following results:



This window “pops up” in the higher left corner of the screen, when the equilibrium point is found. This window provides the eigenvalues for this equilibrium point.

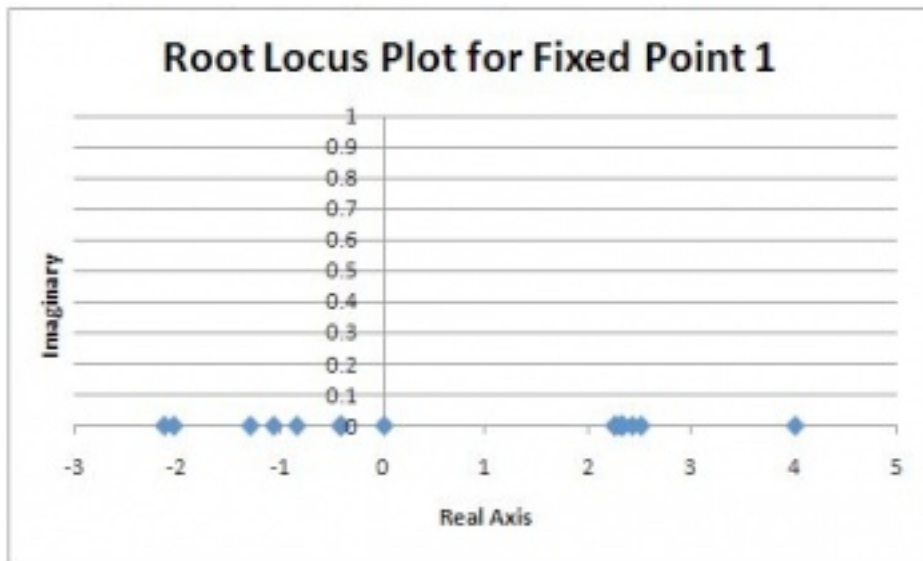
Depending what you are varying (in this case, F_{in}), all you would have to do is enter various values of this F_{in} into PPLANE, and plot the new set of differential formulas. After this is done, just find the same equilibrium point, and record the new given eigenvalues in excel. These values should be entered with an x-component (in one column) and a y-component (in another column) into excel, with the following rules:

- Assuming the example $3+3i$, $3-3i$ were given as eigenvalues.
- For any given eigenvalue, the x-value of a particular eigenvalue is the real part of that number (ie: the “3” part).
- For any given point, the y-value of a particular eigenvalue is the imaginary part of that number (ie: the “3i” part). If there is an imaginary component, ignore the “i,” though the number should be recorded in the y-component. If there is no imaginary number, the y component is zero.
- For both cases, a positive is a positive, and a negative is a negative. Remember: imaginary numbers have 2 parts, a positive and negative “i” value.

These points are simply recorded according to these rules, then the points are plotted against each other, with x components on the x-axis, and the y in the y-axis. Here is an example of an excel diagram, taken from the proposed diagram:

X-axis	Y-axis (imaginary)
2.3028	0
-1.3028	0
2.2415	0
-2.1415	0
2.2471	0
-2.0471	0
4	0
-0.42857	0
2.3058	0
-0.85078	0
2.3252	0
-1.0752	0
2.4142	0
-0.41421	0
2.5	0
0	0

And, the excel data is then plotted, x against y, and is shown below:



As you can see, this particular model did not have any imaginary data. The root locus plot has been formed, and for all accounts of F_{in} , the eigenvalues are along the x-axis for the root locus plot.

6.10 Practical Application

In the past, it was necessary for engineers to master the techniques required to efficiently construct root locus diagrams. In today's engineering world, this is not the case for one of two reasons. In many instances, root locus diagrams are not used industrially because they require models of the system which are generally not available. If a model is available to develop a root locus diagram, there are computer applications that can develop the diagrams much faster than a person. Thus, energy and effort should be placed on understanding and interpreting a root locus diagram and understanding the general rules of stability for a root of the characteristic equation.

6.11 Problems

6.11.1 Example 1

Given the following table of roots to the characteristic equation for a system:

K_c	r_1	r_2	r_3
0	-0.45	-0.60	-0.78
0.33	-0.51	-0.51	-0.83
0.66	$-0.50 + 0.40i$	$-0.50 - 0.40i$	-0.90
1.33	$-0.41 + 0.50i$	$-0.41 - 0.50i$	-0.95
1.67	$-0.35 + 0.57i$	$-0.35 - 0.57i$	-1.01
2.00	$-0.10 + 0.65i$	$-0.10 - 0.65i$	-1.32
2.33	$0.02 + 0.71i$	$0.02 - 0.71i$	-1.50
2.67	$0.23 + 0.76i$	$0.23 - 0.76i$	-1.69
3.00	$0.31 + 0.78i$	$0.31 - 0.78i$	-1.85

1) Construct a root locus plot (Making the plot by hand initially may give some a better understanding of what is going on as you will see the changes in the plot as you add each set of roots).

2) Determine the ranges of K_c that would lead to the following system responses: no oscillations, dampened oscillations, stable oscillations & unstable oscillations. Also, sketch what the output response would look like for a given step change in input for each range of K_c .

3) How would the roots to the characteristic equation be different if this were PI control?

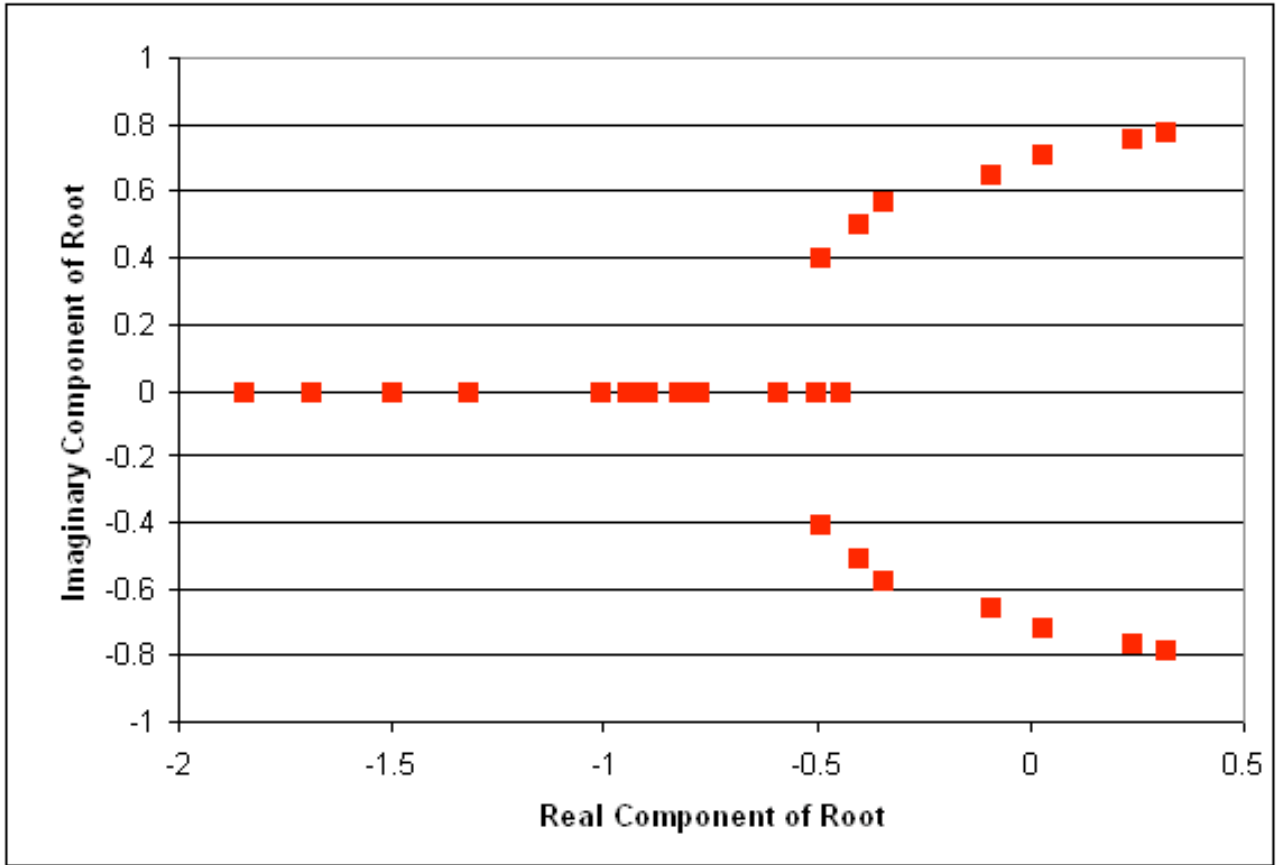
Solution

1) Root locus plot:

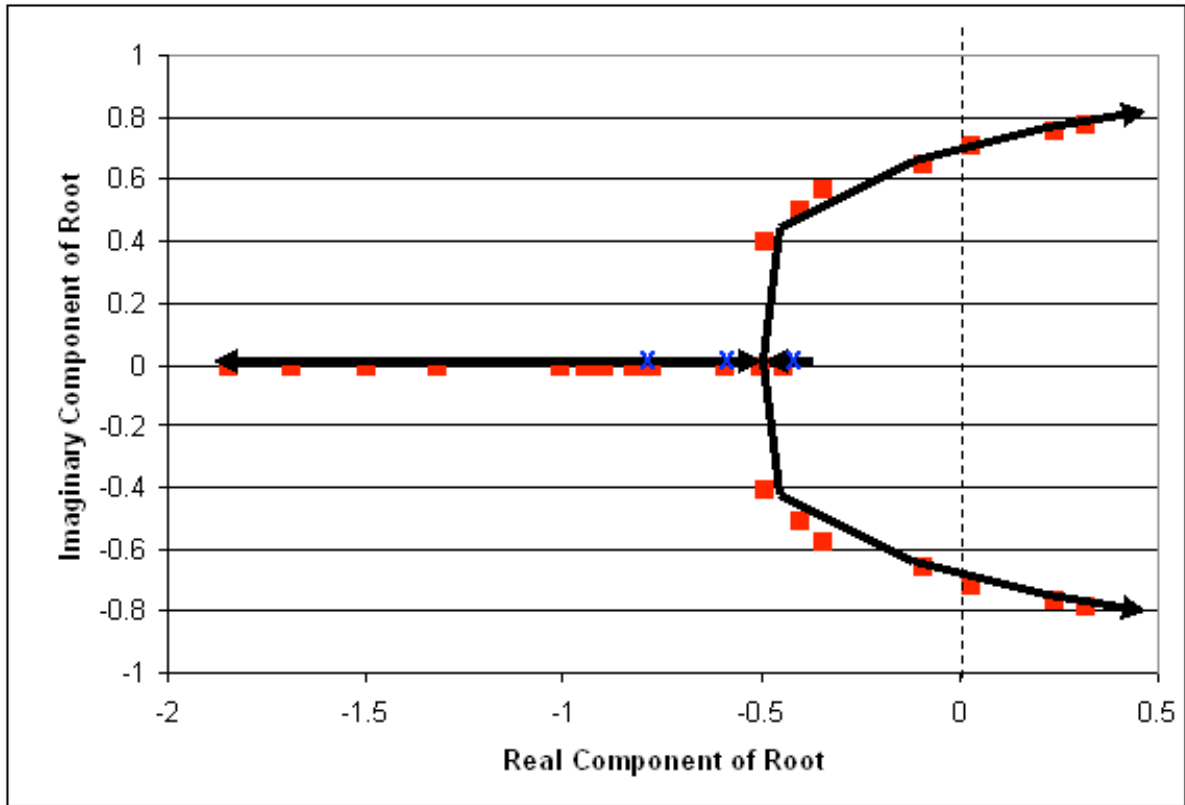
First, we break the roots into their imaginary and real components:

K_c	r1 real	r1 imaginary	r2 real	r2 imaginary	r3 real	r3 imaginary
0	-0.45	0	-0.6	0	-0.78	0
0.33	-0.51	0	-0.51	0	-0.83	0
0.66	-0.5	0.4	-0.5	-0.4	-0.9	0
1.33	-0.41	0.5	-0.41	-0.5	-0.95	0
1.67	-0.35	0.57	-0.35	-0.57	-1.01	0
2	-0.1	0.65	-0.1	-0.65	-1.32	0
2.33	0.02	0.71	0.02	-0.71	-1.5	0
2.67	0.23	0.76	0.23	-0.76	-1.69	0
3	0.31	0.78	0.31	-0.78	-1.85	0

Then, we plot each point on a complex coordinate system (x-axis = real component, y-axis = imaginary component).



Also, it is useful to add lines tracing the path of increasing K_c . These lines are added below. Also, the points where $K_c = 0$ are generally labeled with an x . This has also been done in the figure below.



2) Ranges of K_c with explanations:

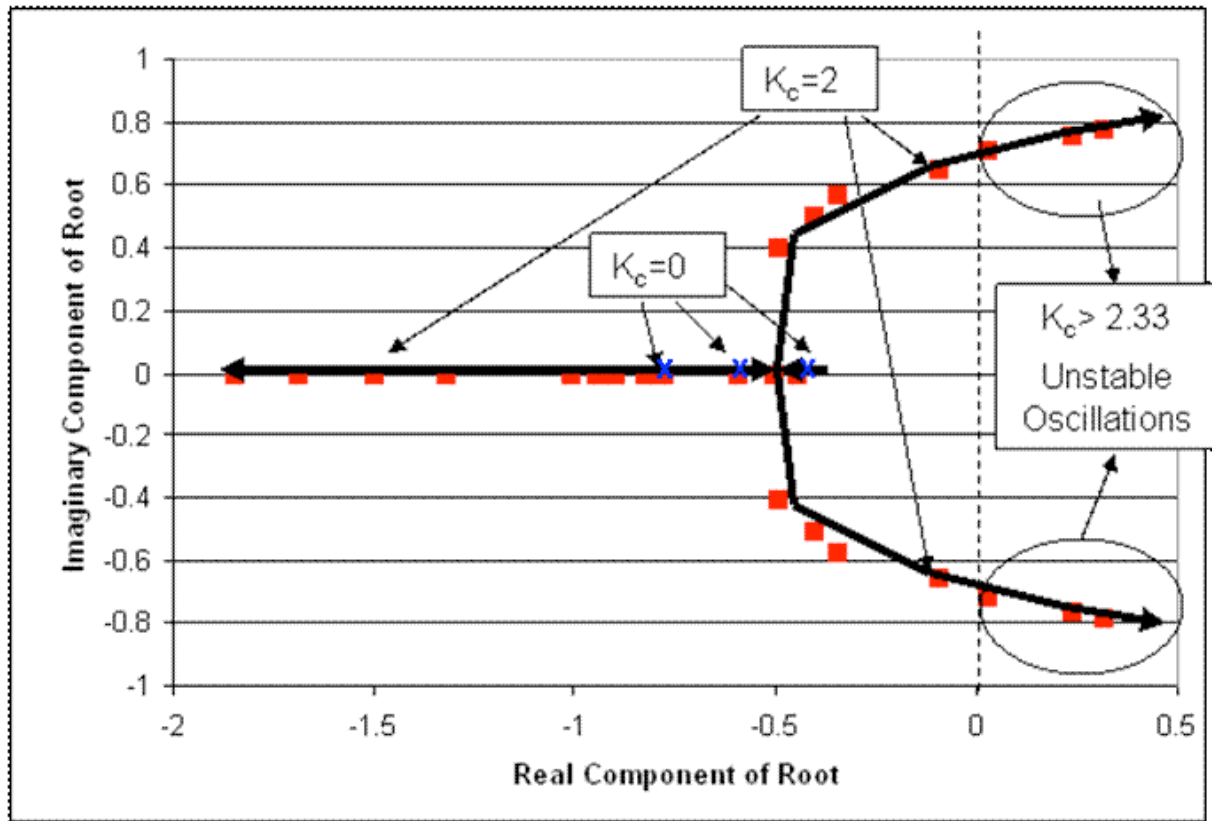
We know that the range where there will be no oscillatory response is when K_c provides all real roots. This occurs when K_c is between 0 and 0.66. (Sketch will look like figure a in the "interpreting a root locus diagram" section above).

Also, K_c yields dampened oscillations when the two of the roots of the characteristic equation are complex with negative real components. This occurs when K_c is greater than 0.66 but less than 2.33. (Sketch will look like figure b in the "interpreting a root locus diagram" section above).

Unstable oscillations are achieved when two of the roots yield complex numbers with positive real components. This occurs when K_c is greater than 2.33. Graphically, we see that when the points move past the dashed line, we will have unstable oscillations. This is represented in the figure below. (Sketch will look like figure c in the "interpreting a root locus diagram" section above).

Based on the data provided, our best assumption is that at a K_c just below 2.33, we will be able to achieve stable oscillations. When $K_c = 2.33$ the real component of the complex root is 0.02 (slightly greater than zero). Ideally, we will achieve stable oscillations when the real component of the complex number is zero. (Oscillations should be consistent in magnitude).

Lastly, it is a good idea to label some values of K_c on the root locus plot. This will help orient the reader when they are trying to determine which point correspond to different values of K_c .



3) If this were PI control, each root to the characteristic equation would be accompanied by not only a K_c value but also a value for integral control parameter, K_I .

6.11.2 Example 2

You've been recently hired at MichChem Controls. In your first week at the company, a virus spreads through the computer network, effectively disabling most of the computational programs. Fortunately, the virus was halted before it was able to disable Mathematica. Shortly after the chaos from the virus subsides, your boss needs to know how to use Mathematica to create a root locus plot for several new Proportional only level control systems that are being tested. Being the highly skilled engineer that you are, he doesn't want you to waste time developing the root locus plots, rather, he wants you to write out example code, with a brief description that someone else could use to develop the root locus plot.

The general characteristic equation for the new level control systems is:

$$f(s) = Ax^3 + Bx^2 - Cx + D + EKc$$

Please, provide your boss with an example of the exact script that would need to be entered into Mathematica in order to develop the root locus plot. You should also brief descriptions explaining what the code does and what steps would need to be repeated to develop the plot.

SOLUTION

First, the user should develop a table of roots for the characteristic equation. This can be done using the solve function in Mathematica. The code would appear like this for $Kc = 0$.

(note: the In[#] appears for each new line of code. This will not be typed in by the user.)

```
In[1]:= Solve[Ax^3 +Bx^2-Cx+D+E*(0)==0,x]
```

This should be repeated for $Kc = 0.1, 0.15, 0.225, 0.5, 0.75, 1.5$, etc. (until the roots of the equation begin to yield two complex solutions whose real components are positive). After a sufficient number of roots have been obtained for the characteristic equation at different values of Kc , these will need to be tabulated. To develop a table of data in Mathematica input the following code:

```
In[2]:= A = {{real component 1, imaginary component 1}, {real component 2,imaginary component 2}},...,{real component n, imaginary component n}}
```

This tabulates the real components and the imaginary components at each value of Kc . Once all of the values are tabulated, the root locus plot can be developed using the ListPlot function.

```
In[3]:= ListPlot[A, PlotStyle -> PointSize[0.02]
```

This will plot all of the tabulated data in In[2] which is the root locus plot.

6.11.3 Multiple Choice 1

1. A root locus plot is used to:

A) Identify the solutions to the characteristic transfer function.

- B) Show the response time of the feedback system to a disturbance.
- C) Graphically illustrate the effect of K_c on the dynamic characteristics of the feedback system.
- D) Choose the optimal K_c for the feedback system.

Ans: C

6.11.4 Multiple Choice 2

2. When a root is complex with positive real parts, the oscillations are:

- A) Decreasing
- B) Increasing
- C) Unstable
- D) A & C
- E) B & C

Ans: E

6.12 Sage's Corner

A brief narration for a better understanding of root locus plots.

<http://video.google.com/googleplayer.swf?docId=384325950654949015>

To view slides [[12](#)]

A narration about the basics of root locus plots and an example for a P-only control system.

<http://video.google.com/googleplayer.swf?docId=1650144670328879934>


If you have problems viewing the google version of the video, you can also view it on Youtube by [clicking here](#).

For the unnarrated version of the powerpoint, please [click here](#).

6.13 References

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- Marlin, Thomas E. "Process Control: Designing Processes and Control Systems for Dynamic Performace 2nd Edition". McGraw-Hill: New York, 2000.
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Section 7. Routh stability: ranges of parameter values that are stable

Note:  [Video lecture](#) available for this section!

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- [First round reviews for this page](#)
- [Rebuttal for this page](#)

7.1 Introduction

The stability of a process control system is extremely important to the overall control process. System stability serves as a key safety issue in most engineering processes. If a control system becomes unstable, it can lead to unsafe conditions. For example, instability in reaction processes or reactors can lead to runaway reactions, resulting in negative economic and environmental consequences.

The absolute stability of a control process can be defined by its response to an external disturbance to the system. The system may be considered stable if it exists at a consistent state or setpoint and returns to this state immediately after a system disturbance. In order to determine the stability of a system, one often must determine the [eigenvalues](#) of the matrix representing the system's governing set of differential equations. Unfortunately, sometimes the characteristic equation of the matrix (the polynomial representing its eigenvalues) can be difficult to solve; it may be too large or contain unknown variables. In this situation, a method developed by British mathematician Edward Routh can yield the desired stability information without explicitly solving the equation.

Recall that in order to determine system stability one need only know the signs of the real components of the eigenvalues. Because of this, a method that can reveal the signs without actual computation of the eigenvalues will often be adequate to determine system stability.

To quickly review, negative real eigenvalue components cause a system to return to a steady state point (where all partial derivatives equal zero) when it experiences disturbances. Positive real components cause the system to move away from a stable point, and a zero real component indicates the system will not adjust after a disturbance. Imaginary components simply indicate oscillation with a general trend in accordance with the real part. Using the method of Routh stability, one can determine the number of each type of root and thus see whether or not a system is stable. When unknown variables

exist in the equation, Routh stability can reveal the boundaries on these variables that keep the roots negative.

7.2 The Routh Array

The Routh array is a shortcut to determine the stability of the system. The number of positive (unstable) roots can be determined without factoring out any complex polynomial.

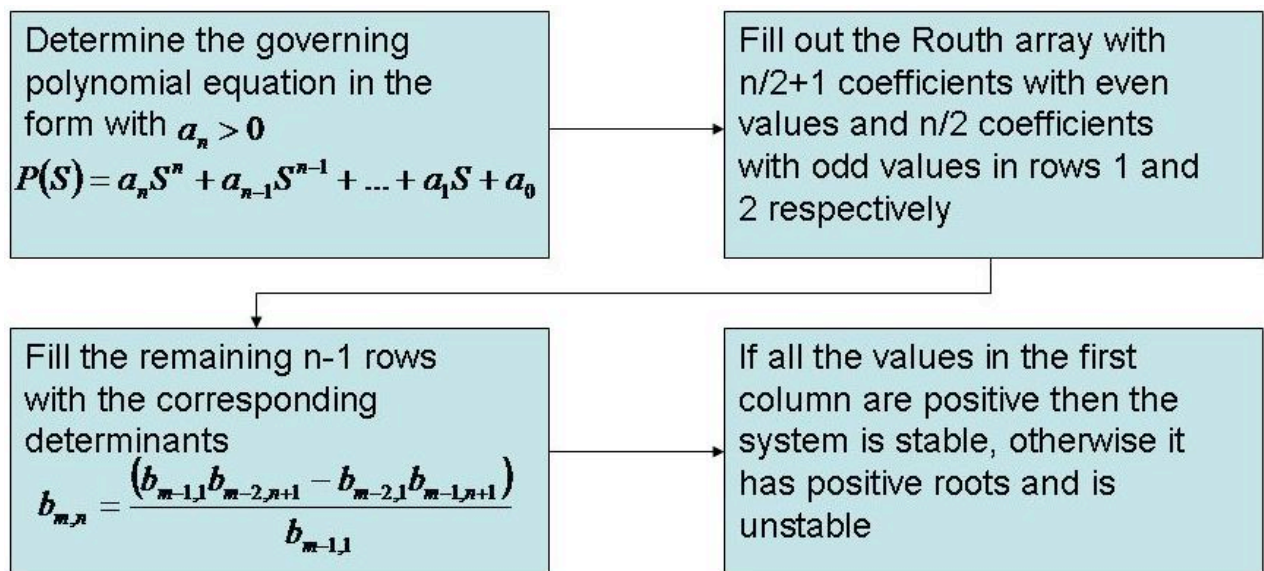
7.2.1 Generating the Array

The system in question must have a characteristic equation of a polynomial nature, as shown below:

$$P(S) = a_n S^n + a_{n-1} S^{n-1} + \dots + a_1 S + a_0$$

In order to examine the roots, set $P(S)=0$, which will allow you to tell how many roots are in the left-hand plane, right hand plane, and on the j -omega axis. If the system involves trigonometric functions it needs to be fit to a polynomial via a Taylor series expansion.

One necessary condition for stability is that $a_n > 0$. (If $a_n < 0$, all coefficients may be multiplied by -1 before checking). The other condition is that all values in column 1 of the Routh array must be positive for the system to be stable.



This flow diagram shows the generation of a Routh array for an idealized case with m,n representing the location in the matrix.

The coefficients of the polynomial are placed into an array as seen below. The number of

rows is one more than the order of the equation. The number of sign changes in the first column indicate the number of positive roots for the equation.

Row 1 :	a_n	a_{n-2}	a_{n-4}	\dots
Row 2 :	a_{n-1}	a_{n-3}	a_{n-5}	\dots
Row 3 :	b_1	b_2	b_3	\dots
Row 4 :	c_1	c_2	c_3	\dots
\vdots	\vdots	\vdots	\vdots	\vdots
Row 5 :	p_1	p_2		
Row 6 :	q_1			
Row 7 :	v_1			

In the array, the variables b_1, b_2, c_1, c_2 , etc. are determined by calculating a determinant using elements from the previous two rows as shown below:

$$b_1 = \frac{a_{n-1}a_{n-2} - a_n a_{n-3}}{a_{n-1}}, b_2 = \frac{a_{n-1}a_{n-4} - a_n a_{n-5}}{a_{n-1}}, b_3 = \frac{a_{n-1}a_{n-6} - a_n a_{n-7}}{a_{n-1}}, \dots$$

$$c_1 = \frac{b_1 a_{n-3} - a_{n-1} b_2}{b_1}, c_2 = \frac{b_1 a_{n-5} - a_{n-1} b_3}{b_1}, c_3 = \frac{b_1 a_{n-7} - a_{n-1} b_4}{b_1}, \dots$$

The general expression for any element x after the first two rows with index (m,n) is as follows:

$$A = \begin{bmatrix} x_{m-2,1} & x_{m-2,n+1} \\ x_{m-1,1} & x_{m-1,n+1} \end{bmatrix}$$

For

$$x_{m,n} = \frac{-\det(A)}{x_{m-1,1}}$$

Note, that if the Routh array starts with a zero, it may still be solved (assuming that all the other values in the row are not zero), by replacing the zero with a constant, and letting that constant equal a very small positive number. Subsequent rows within that column that have this constant will be calculated based on the constant chosen.

Once the array is complete, apply the following theorems to determine stability:

- 1) If all of the values in the first column of the Routh array are >0 , then $P(S)$ has all negative real roots and the system is stable.
- 2) If some of the values in the first column of the Routh array are <0 , then the number of times the sign changes down the first column will = the number of positive real roots in the $P(S)$ equation.
- 3) If there is 1 pair of roots on the imaginary axis, both the same distance from the origin (meaning equidistant), then check to see if all the other roots are in the left hand plane. If so, then the imaginary roots location may be found using $AS^2 + B = 0$, where A and B are the elements in the Routh array for the 2nd to last row.

To clarify even further, an example with real numbers is analyzed.

7.2.2 Example Array

The following polynomial was generated from a sample system.

$$P(S) = 5S^3 - 10S^2 + 7S + 20$$

The preceding polynomial must be investigated in order to determine the stability of the system. This is done by generating a Routh array in the manner described above. The array as a result of this polynomial is,

Row 1 :	5	7
Row 2 :	-10	20
Row 3 :	17	
Row 4 :	20	

In the array shown above, the value found in the third row is calculated as follows.

$$b_1 = \frac{-10 * 7 - 5 * 20}{-10}$$

The array can now be analyzed. When looking down the first column, it can be seen that 5 is positive in magnitude, then the sign changes in the -10 entry, and the sign changes a second time to positive 17. This counts as two changes in sign, which corresponds to two positive roots, making the system unstable.

7.3 Finding Stable Control Parameter Values

Often, for a unit operation, a PID parameter such as controller gain (K_c), the integral time constant (T_i), or the derivative time constant (T_d) creates an additional variable in the characteristic equation. This can be carried through the computations of the Routh array to indicate which values of the variable will provide stability to the system through by preventing positive roots from occurring in the equation. For example, if a controller output is governed by the function:

$$10s^3 + 5s^2 + 8s + (T_d + 2)$$

The stable values of T_d can be found via a Routh array:

$$\begin{array}{l} \text{Row 1 :} \quad 10 \quad \quad 8 \\ \text{Row 2 :} \quad 5 \quad \quad (T_d + 2) \\ \text{Row 3 :} \quad 4 - 2T_d \\ \text{Row 4 :} \quad (T_d + 2) \end{array}$$

We reveal $-2 < T_d < 2$ in order to keep the first column elements positive, so this is the stable range of values for this parameter.

If multiple parameters were in the equation, they would simply be solved for as a group, yielding constraints along the lines of " $T_i + K_c > 2$ " etc, so any value chosen for one parameter would give a different stable range for the other.

7.4 Special Cases

There are a few special cases that one should be aware of when using the Routh Test. These variances can arise during stability analysis of different control systems. When a special case is encountered, the traditional Routh stability solution methods are altered as presented below.

7.4.1 One of the coefficients in the characteristic equation equals zero

If the power of the $0 \cdot S^n$ is ≥ 1 , replace the zero with a quantity, ϵ , which would be positive and will approach zero. Then continue with your analysis as normal. Essentially this gives the limit of the roots as that coefficient approaches zero. (If the power = 0, see Case 3). For example,

$$\text{Equation: } 2S^3 - 24S + 32 = 0$$

Working Equation: $2S^3 + \epsilon S^2 - 24S + 32 = 0$

Row 1 :	2	-	24
Row 2 :	ϵ		32
Row 3 :	$\frac{-24\epsilon - 64}{\epsilon}$		0
Row 4 :	32		

Since ϵ is positive we know that in the first column row 2 will be positive, row 4 will be positive, and row 3 will be negative. This means we will have a sign change from 2 to 3 and again from 3 to 4. Because of this, we know that two roots will have positive real components. If you actually factor out the equation you see that

$(S - 2)^2(2S + 8) = 0$, showing that we do have 2 positive roots. Both of these roots are equal to 2, so there is technically only one root, but in any case we know the system is unstable and must be redesigned.

7.4.2 One of the roots is zero

This case should be obvious simply from looking at the polynomial. The constant term will be missing, meaning the variable can be factored from every term. If you added an ϵ to the end as in case 1, the last row would be ϵ and falsely indicate another sign change. Carry out Routh analysis with the last zero in place.

Equation: $S^3 - S^2 - 2S = 0$

Row 1 :	1	-	2
Row 2 :	-1		0
Row 3 :	-2		
Row 4 :	0		

As you can see in column one we have row 1 positive, row 2 and 3 negative, and row 4 zero. This is interpreted as one sign change, giving us one positive real root. Looking at this equation in factored form,

$$(S + 1)(S - 2)S = 0$$

we can see that indeed we have only one positive root equal which equals 2. The zero in the last row indicates an additional unstable root of zero. Alternatively, you may find it easier to just factor out the variable and find the signs of the remaining eigenvalues. Just remember there is an extra root of zero.

7.4.3 A row full of zeros

When this happens you know you have either a pair of imaginary roots, or symmetric real roots. The row of zeros must be replaced. The following example illustrates this procedure.

Equation: $S^4 - 6S^3 + 10S^2 - 6S + 9 = 0$

Row 1 :	1	10	9
Row 2 :	-6	-6	
Row 3 :	9	9	
Row 4 :	0	0	

Row 4 contains all zeros. To determine its replacement values, we first write an auxiliary polynomial A determined by the entries in Row 3 above.

$$A(S) = 9S^2 + 9$$

Notice that the order decreases by 1 as we go down the table, but decreases by 2 as we go across.

We then take the derivative of this auxiliary polynomial.

$$A'(S) = 18S$$

The coefficients obtained after taking the derivative give us the values used to replace the zeros. From there, we can proceed the table calculations normally. The new table is

Row 1 :	1	10	9
Row 2 :	-6	-6	

Row 3 : 9 9
 Row 4 : 18 0
 Row 5 : 9

In fact, the purely imaginary or symmetric real roots of the original polynomial are the same as the roots of the auxiliary polynomial. Thus, we can find these roots.

$$9S^2 + 9 = 0$$

$$S = \pm i$$

Because we have two sign changes, we know the other two roots of the original polynomial are positive.

In fact, after factoring this polynomial, we obtain

$$(S^2 + 1)(S - 3)^2 = 0$$

Therefore, the roots are $S = \pm i, 3$, where in this case, the root 3 has multiplicity 2.

7.5 Limitations

Routh arrays are useful for classifying a system as stable or unstable based on the signs of its eigenvalues, and do not require complex computation. However, simply determining the stability is not usually sufficient for the design of process control systems. It is important to develop the extent of stability as well as how close the system is to instability. Further stability analysis not accounted for in the Routh analysis technique include finding the degree of stability, the steady state performance of the control system, and the transient response of the system to disturbances.

More involved techniques, such as those discussed in [Eigenvalues and Eigenvectors](#), must be used to further characterize the system stability (with the exception of system polynomials resulting in pure imaginary roots). Another limitation of the Routh method occurs when the polynomial in question becomes so large that Routh stability is too computationally time consuming (a personal judgment). For this situation another method, such as [a root locus plot](#) must be used.

Note that for defining stability, we will always start out with a polynomial. This polynomial arises from finding the eigenvalues of the linearized model. Thus we will never encounter other functions, say exponential functions or sin or cos functions in general for stability analysis in control theory.

7.6 Advantages Over Root Locus Plots

Routh stability evaluates the signs of the real parts of the roots of a polynomial without solving for the roots themselves. The system is stable if all real parts are negative. Therefore unlike root locus plots, the actual eigenvalues do not need to be calculated for a Routh stability analysis. Furthermore, sometimes the system has too many unknowns to easily construct and interpret a root locus plot (e.g. with two PID controllers there are the variables $Kc1$, $Kc2$, $\tau i1$, $\tau i2$, $\tau d1$, and $\tau d2$).

7.7 Example 1

Assume the following polynomial describes the eigenvalues of a linearized model of your process. For this polynomial, complete a Routh array and determine the system's stability?

$$P(x) = x^4 + 10x^3 + 35x^2 + 50x + 24$$

Answer

Since $P(X)$ is a fourth-order polynomial, the Routh array contains five rows.

$$\begin{array}{l} \text{Row 1:} \\ \text{Row 2:} \\ \text{Row 3:} \\ \text{Row 4:} \\ \text{Row 5:} \end{array} \begin{array}{ccc} a_n & a_{n-2} & a_{n-4} \\ a_{n-1} & a_{n-3} & a_{n-5} \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \\ d_1 & d_2 & d_3 \end{array}$$

Rows 1 and 2 correspond to the coefficients of the polynomial terms:

$$\begin{array}{l} \text{Row 1:} \\ \text{Row 2:} \end{array} \begin{array}{ccc} 1 & 35 & 24 \\ 10 & 50 & \end{array}$$

Rows 3, 4, and 5 contain the determinants using elements from the previous two rows.

$$\begin{array}{l} \text{Row 3} \\ \text{:} \end{array} \quad b_1 = \frac{a_{n-1}a_{n-2} - a_n a_{n-3}}{a_{n-1}} \quad b_2 = \frac{a_{n-1}a_{n-4} - a_n a_{n-5}}{a_{n-1}} \quad b_3 = \frac{a_{n-1}a_{n-5}}{a_{n-1}}$$

Row 4

$$: c_1 = \frac{b_1 a_{n-3} - a_{n-1} b_2}{b_1} \quad c_2 = \frac{b_1 a_{n-5} - a_{n-3} b_2}{b_1}$$

$$: d_1 = \frac{c_1 b_2 - b_1 c_2}{c_1}$$

Row 5

Therefore,

$$\text{Row 3: } b_1 = \frac{10(35) - 1(50)}{10} = 30 \quad b_2 = \frac{10(24) - 1(0)}{10} = 24 \quad b_3 = \frac{10(0) - 1(0)}{10} = 0$$

$$\text{Row 4: } c_1 = \frac{30(50) - 10(24)}{30} = 42 \quad c_2 = \frac{30(0) - 10(0)}{30} = 0$$

$$\text{Row 5: } d_1 = \frac{42(24) - 30(0)}{42} = 24$$

The complete Routh array:

$$\text{Row 1: } \quad 1 \quad 35 \quad 24$$

$$\text{Row 2: } \quad 10 \quad 50$$

$$\text{Row 3: } \quad 30 \quad 24$$

$$\text{Row 4: } \quad 42$$

$$\text{Row 5: } \quad 24$$

Since all the values in the first column are positive, the equation $P(x)$ has all negative roots and the system is stable.

7.8 Example 2

Consider a system with the following characteristic equation:

$$20s^3 + 59s^2 + 46s + (4 + K_c) = 0$$

Using a P-only controller, find the range of controller gain that will yield a stable system.

Answer

Since the equation is a third-order polynomial, the Routh array has four rows. Routh Array:

Row 1 :	20	46
Row 2 :	59	$(4 + K_c)$
Row 3 :	$46 - \frac{20}{59}(4 + K_c)$	0
Row 4 :	$(4 + K_c)$	0

For the system to be stable, all the elements of the first column of the Routh array have to be positive.

The first column will contain only positive elements if:

$$\bullet \quad 46 - \frac{20}{59}(4 + K_c) > 0$$

$$K_c < \frac{2634}{20}$$

$$\bullet \quad 4 + K_c > 0$$

$$K_c > -4$$

$$-4 < K_c < \frac{2634}{20}$$

Acceptable stable range

7.9 Example 3

Consider a system with the following characteristic equation:

$$s^5 - 3s^4 + s^3 + s^2 + 4 = 0$$

Determine the stability of this system.

Answer

One of the coefficients in the characteristic equation equals 0. We replace the zero with a quantity which would be positive (approach zero from the right-hand side) and continue with the analysis as normal.

Working equation: $s^5 - 3s^4 + s^3 + s^2 + \epsilon s + 4 = 0$

Row 1 :	1	1	ϵ
Row 2 :	-3	1	4
Row 3 :	$\frac{4}{3}$	$\epsilon + \frac{4}{3}$	
Row 4 :	$4 + \frac{9\epsilon}{4}$	4	
Row 5 :	$\epsilon + \frac{4}{3} - \frac{64}{27\epsilon + 48}$	0	
Row 6 :	4		

Since ϵ is positive, in the first column, there are two sign changes, from row 1 to row 2 and from row 2 to row 3. Thus, we know that the roots will have two positive real components. If you actually factor out the equation you will see that,

$(s^2 + 1)(s - 2)^2(s + 1) = 0$, showing that we do have two positive roots, both equal to 2.

Additional complication exists because at row 5, as ϵ goes to zero, the term also goes to zero, which means that for row 5, we are getting a row full of zeros. This means that we have a pair of imaginary roots, and this situation can be solved using the equation,

$a_2 S^2 + a_0 = 0$.

In this case, the working equation is, $S^2 + 4 = 0$

The imaginary roots are, $S = \pm 2i$

7.10 Example 4

You are an engineer at an icecream factory. There is a storage vat with a cooling system that has a PI controller scheme. It has the following characteristic equation:

$$10s^4 + 3s^3 - K_c s^2 + 3s + (T_i + 6) = 0$$

Your job is to determine the constraints on the values K_c and T_i such that the system is stable.

Answer

The goal is to make the matrix such that the first column has no sign changes. Since the first two entries in the first column are numbers and positive, therefore all other values in this column must be positive.

Working equation: $10s^4 + 3s^3 - K_c s^2 + 3s + (T_i + 6) = 0$

Row 1 :	10	$-K_c$	$T_i + 6$
Row 2 :	3	3	
Row 3 :	$10 - K_c$	$T_i + 6$	
Row 4 :	$3 - \frac{3(T_i + 6)}{(10 - K_c)}$	0	
Row 5 :	$T_i + 6$		

Since $10 - K_c$ is in the first column, it gives the constraint $K_c < 10$.

Likewise, $T_i + 6$ must be positive, giving the constraint $T_i > -6$. Which

brings the final entry of $3 - \frac{3(T_i + 6)}{(10 - K_c)}$. By dividing by three and

rearrangement of the terms, it is seen that $\frac{(T_i + 6)}{(10 - K_c)} < 1$. The terms are then rearranged to arrive at the inequality: $T_i + K_c < 4$.

Thus the stable conditions for the constants are:

$$K_c < 10$$

$$T_i > -6$$

$$T_i + K_c < 4$$

7.11 Sage's Corner

Routh Stability Analysis Example

<http://video.google.com/googleplayer.swf?docId=-2205168127672510812>

[Routh Stability Analysis Example Slides without narration](#)

<http://video.google.com/googleplayer.swf?docId=2535630044259965045>


[Routh Stability Slides](#)

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Chapter 11. Control Architectures

Section 1. Feedback control: What is it? When useful? When not? Common usage.

Note:  [Video lecture](#) available for this section!

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1.1 Introduction

There are many different control mechanisms that can be used, both in everyday life and in chemical engineering applications. Two broad control schemes, both of which encompass each other are *feedback control* and [feed-forward control](#). *Feedback control* is a control mechanism that uses information from **measurements** to manipulate a variable to achieve the desired result. *Feed-forward control*, also called anticipative control, is a control mechanism that predicts the effects of measured **disturbances** and takes corrective action to achieve the desired result. The focus of this article is to explain application, advantages, and disadvantages of feedback control.

Feedback control is employed in a wide variety of situations in everyday life, from simple home thermostats that maintain a specified temperature, to complex devices that maintain the position of communication satellites. Feedback control also occurs in natural situations, such as the regulation of blood-sugar levels in the body. Feedback control was even used more than 2,000 years ago by the Greeks, who manufactured such systems as the [float valve](#) which regulated water level. Today, this same idea is used to control water levels in boilers and reservoirs.

1.2 Feedback Control

In feedback control, the variable being controlled is measured and compared with a target value. This difference between the actual and desired value is called the error. Feedback control manipulates an input to the system to minimize this error. **Figure 1** shows an overview of a basic feedback control loop. The error in the system would be the *Output - Desired Output*. Feedback control reacts to the system and works to minimize this error. The desired output is generally entered into the system through a user interface. The output of the system is measured (by a flow meter, thermometer or similar instrument) and the difference is calculated. This difference is used to control the system inputs to reduce the error in the system.

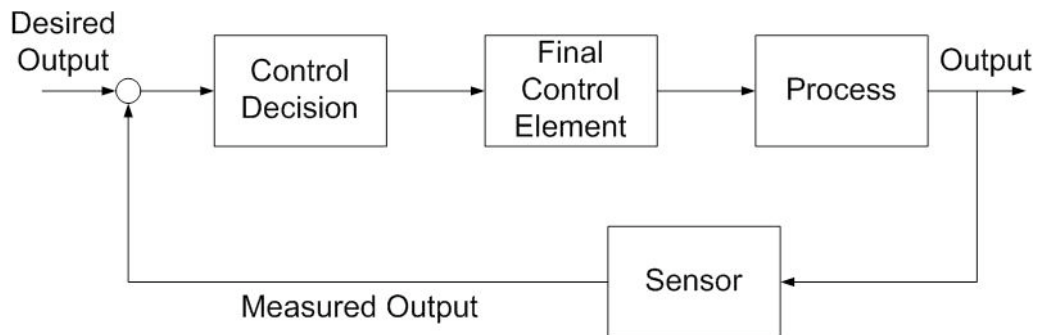


Figure 1. Feedback control loop (Adapted from Lee, Newell, and Cameron 1998: 6)



cookies

To understand the principle of feedback control, consider **Figure 2**. In order to bake cookies, one has to preheat an electric oven to 350°F. After setting the desired temperature, a [sensor](#) takes a reading inside the oven. If the oven is below the set temperature, a signal is sent to the heater to power on until the oven heats to the desired temperature. In this example, the variable to be controlled (oven temperature) is measured and determines how the input variable (heat into oven) should be manipulated to reach the desired value.

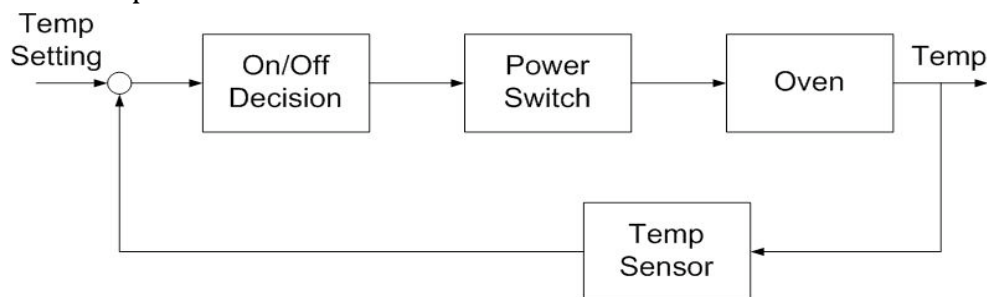
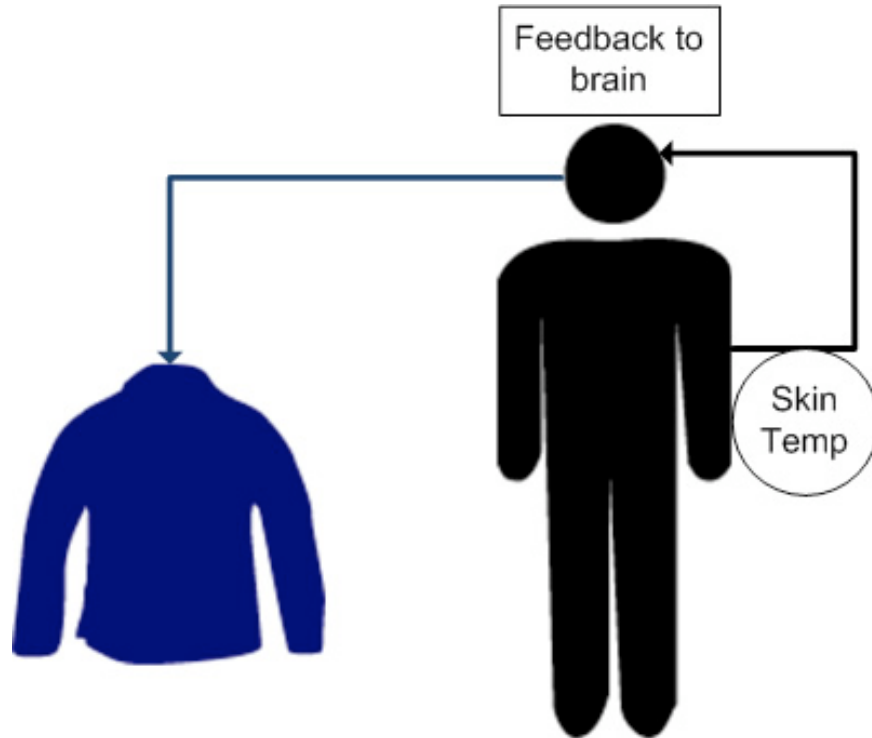


Figure 2. Feedback control in an electric oven (Adapted from Lee, Newell, and Cameron 1998: 6)

Feedback control can also be demonstrated with human behavior. For example, if a person goes outside in Michigan winter, he or she will experience a temperature drop in the skin. The brain (controller) receives this signal and generates a motor action to put on a jacket. This minimizes the discrepancy between the skin temperature and the physiological set point in the person. The example is illustrated below:



There are two types of feedback control: negative and positive. Negative feedback is the most useful control type since it typically helps a system converge toward an equilibrium state. On the other hand, positive feedback can lead a system away from an equilibrium state thus rendering it unstable, even potentially producing unexpected results. Unless stated explicitly, the term feedback control most often refers to negative feedback.

1.2.1 Negative Feedback

By definition, negative feedback is when a change (increase/decrease) in some variable results in an opposite change (decrease/increase) in a second variable. This is demonstrated in **Figure 3** where a loop represents a variation toward a plus that triggers a correction toward the minus, and vice versa. Negative feedback leads to a tight control situation whereby the corrective action taken by the controller forces the controlled variable toward the set point, thus leading the system to oscillate around equilibrium.

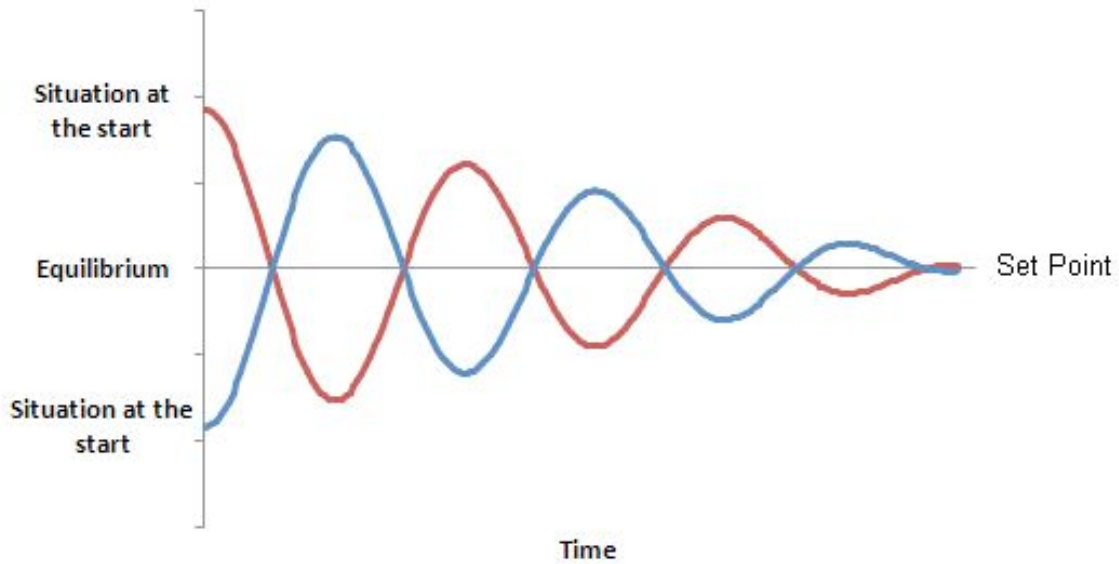


Figure 3. Negative Feedback: Maintenance of equilibrium and convergence

Figure 4 shows the negative feedback mechanism between Duck Population and Duck Death Rate. For a given flock, we say that if the death rate increases, the duck flock will decrease. On the contrary, if the duck flock increases, the death rate of the flock will decrease.

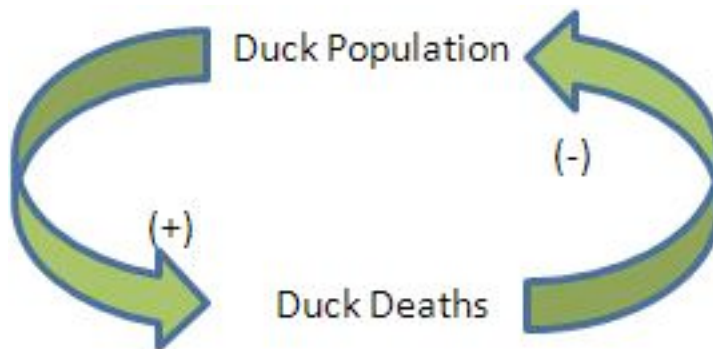


Figure 4. Duck population negative feedback loop

1.2.2 Positive Feedback

As opposed to negative feedback, positive feedback is when a change (increase/decrease) in some variable results in a subsequently similar change (increase/decrease) in a second variable. In some cases, positive feedback leads to an undesirable behavior whereby the system diverges away from equilibrium. This can cause the system to either run away

toward infinity, risking an expansion or even an explosion, or run away toward zero, which leads to a total blocking of activities (**Figure 5**).

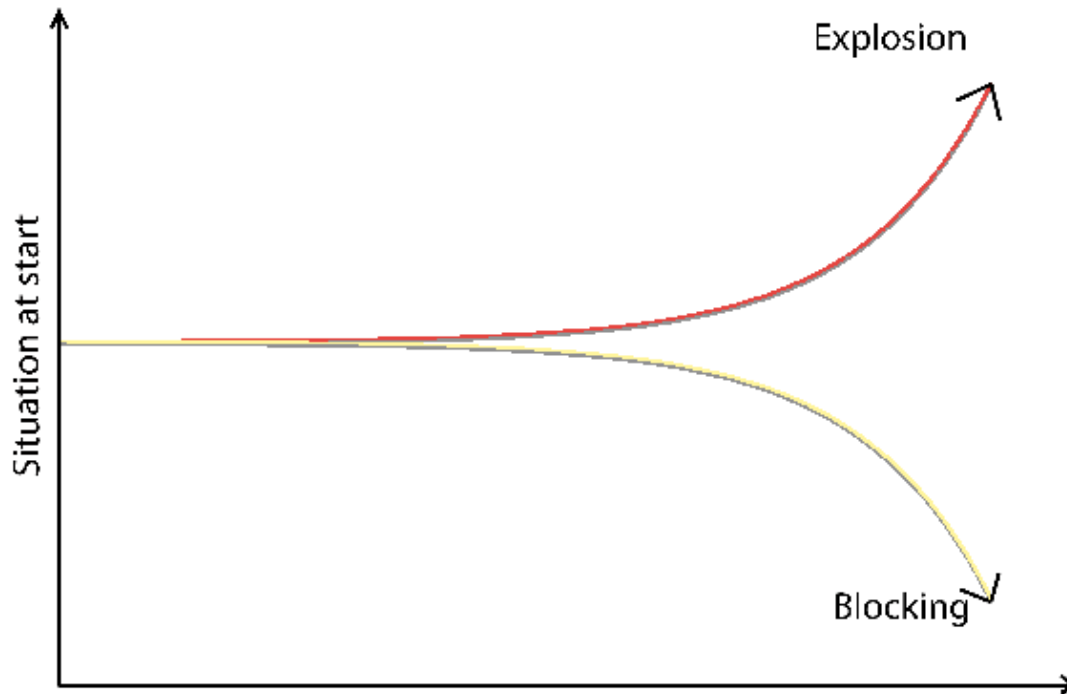


Figure 5. Positive Feedback: Exponential Growth and divergent behavior, no intermediate situation

Figure 6 shows the feedback mechanism responsible for the growth of a duck flock via births. In this example, we consider two system variables: Duck Births and Ducks Population. For a given flock, we state that if the birth rate increases, the duck flock will increase. Similarly, if the duck flock increases, the birth rate of the flock will increase.

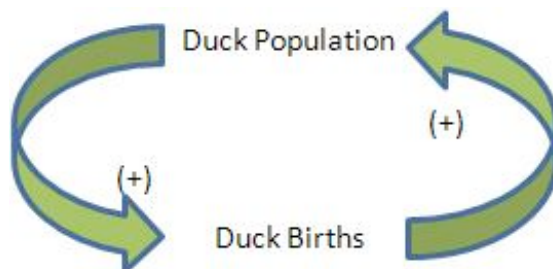


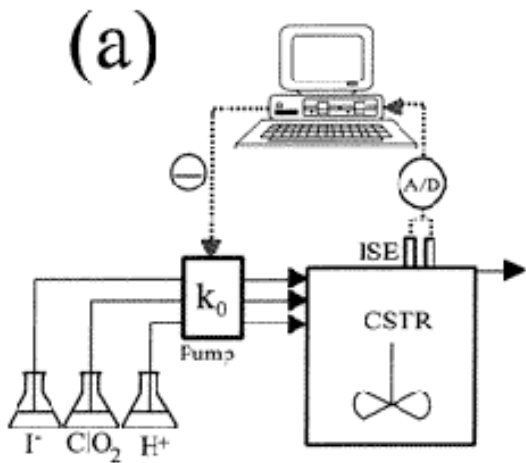
Figure 6. Duck population positive feedback loop

1.3 Applications

Control mechanisms are used to achieve a desired output or operating condition. More specifically, feedback control is a useful mechanism in numerous applications across many engineering fields. In chemical engineering, feedback control is commonly used to manipulate and stabilize the conditions of a CSTR. **Figure 7** shows how feedback control can be effectively used to stabilize the concentrations of reactants in a CSTR by adjusting the flow rates.

1.3.1 CSTR with Feedback Control

Several types of feedback control can be used to manipulate the conditions in a [CSTR](#): [positive feedback](#), [negative feedback](#), or a combination of both. **Figure 7** illustrates each of these possible situations. As depicted below, each CSTR is equipped with two electrodes that measure the voltage of the solution contained inside the reactor. A computer adjusts the flow rates of the pump(s) in response to any changes in the voltage.



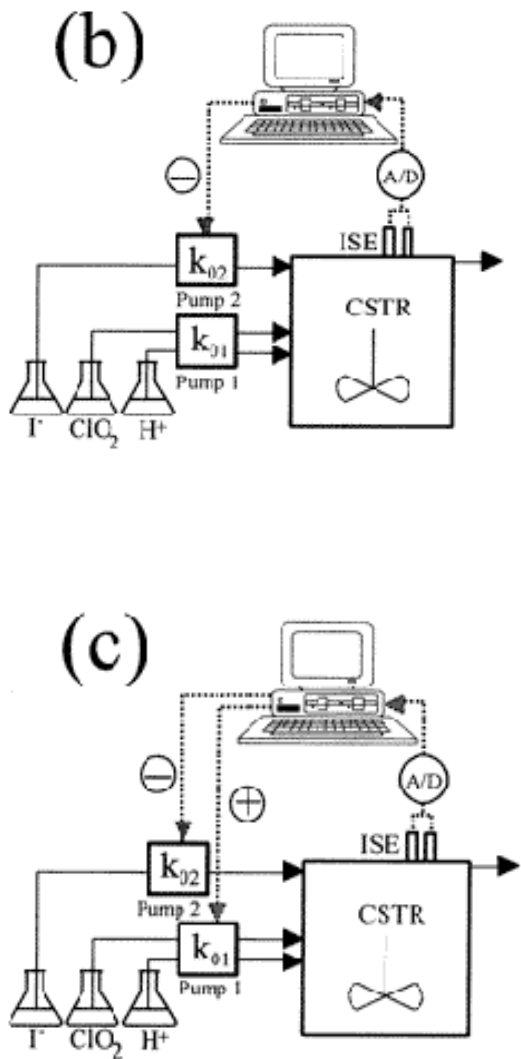


Figure 7. CSTR with feedback control: equipment and control configuration (Dolnik et al. 1997)

- **(a)** All of the reagents are pumped into the reactor by the same pump. The flow rate through the pump is adjusted constantly by a negative feedback mechanism; when level of the iodide solution is low, the computer detects the insufficiency and increases the flow rate of all the reactants.
- **(b)** The iodide solution is pumped into the reactor by one pump, while the other two reactants are pumped in at a constant flow rate. The flow rate of the iodine solution is controlled by a negative feedback mechanism; when the computer detects an insufficient amount of iodine in the CSTR, it signals the pump. The flow rate of iodine into the CSTR is therefore increased.

- **(c)** Two pumps are used to feed the reactor: one pump for the iodine solution and one for the ClO_2 and H^+ solutions. The flow of the iodine solution is controlled by a negative feedback mechanism; if the computer detects an iodine deficiency, it signals Pump 2 to increase the flow rate of the iodide solution. The flow rate of the ClO_2 and H^+ solutions is controlled by a positive feedback mechanism; if the computer detects an iodide deficiency, it will signal Pump 1 to decrease the flow rates of ClO_2 and H^+ , thereby increasing the concentration of iodide.

It is easy to see that by combining feedback controls, such as in **Figure 7 (c)**, output concentrations and operating conditions can be maintained at the desired state much more effectively than by only using one type of feedback control.

1.4 Advantages and Disadvantages

The unique architecture of the feedback control provides for many advantages and disadvantages. It is important to look at the exact application the control will be used for before determining which type of control will be the best choice (see [Cascade Control Systems](#) and [Feed Forward Control](#)).

Advantages

The advantages of feedback control lie in the fact that the feedback control obtains data at the process output. Because of this, the control takes into account unforeseen disturbances such as frictional and pressure losses. Feedback control architecture ensures the desired performance by altering the inputs immediately once deviations are observed regardless of what caused the disturbance. An additional advantage of feedback control is that by analyzing the output of a system, unstable processes may be stabilized. Feedback controls do not require detailed knowledge of the system and, in particular, do not require a mathematical model of the process. Feedback controls can be easily duplicated from one system to another. A feedback control system consists of five basic components: (1) input, (2) process being controlled, (3) output, (4) sensing elements, and (5) controller and actuating devices. A final advantage of feedback control stems from the ability to track the process output and, thus, track the system's overall performance.

Disadvantages

Time lag in a system causes the main disadvantage of feedback control. With feedback control, a process deviation occurring near the beginning of the process will not be recognized until the process output. The feedback control will then have to adjust the process inputs in order to correct this deviation. This results in the possibility of substantial deviation throughout the entire process. The system could possibly miss process output disturbance and the error could continue without adjustment. Generally, feedback controllers only take input from one sensor. This may be inefficient if there is a more direct way to control a system using multiple sensors. Operator intervention is generally required when a feedback controller proves unable to maintain stable closed-

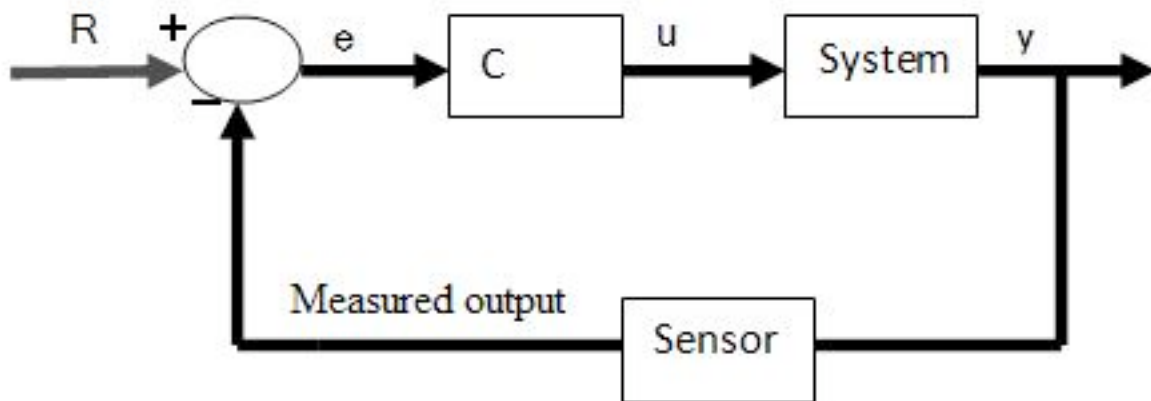
loop control. Because the control responds to the perturbation after its occurrence, perfect control of the system is theoretically impossible. Finally, feedback control does not take predictive control action towards the effects of known disturbances.

1.5 Closed Loop Control versus Open Loop Control

Although there are various types of controllers, most of them can be grouped into one of the two broad categories: closed loop and [open loop](#) controllers. The subsections below summarize the differentiation.

Closed Loop System

In a closed loop control system, the input variable is adjusted by the controller in order to minimize the error between the measured output variable and its set point. This control design is synonymous to feedback control, in which the deviations between the measured variable and a set point are fed back to the controller to generate appropriate control actions. The controller C takes the difference e between the reference r and the output to change the inputs u to the system. This is shown in figure below. The output of the system y is fed back to the sensor, and the measured outputs go to the reference value



Open Loop System

On the other hand, any control system that does not use feedback information to adjust the process is classified as open loop control. In open loop control, the controller takes in one or several measured variables to generate control actions based on existing equations or models. Consider a CSTR reactor that needs to maintain a set reaction temperature by means of steam flow (**Figure 8**): A temperature sensor measures the product temperature, and this information is sent to a computer for processing. But instead of outputting a valve setting by using the error in temperature, the computer (controller) simply plugs the

information into a predetermined equation to reach output valve setting. In other words, the valve setting is simply a function of product temperature.

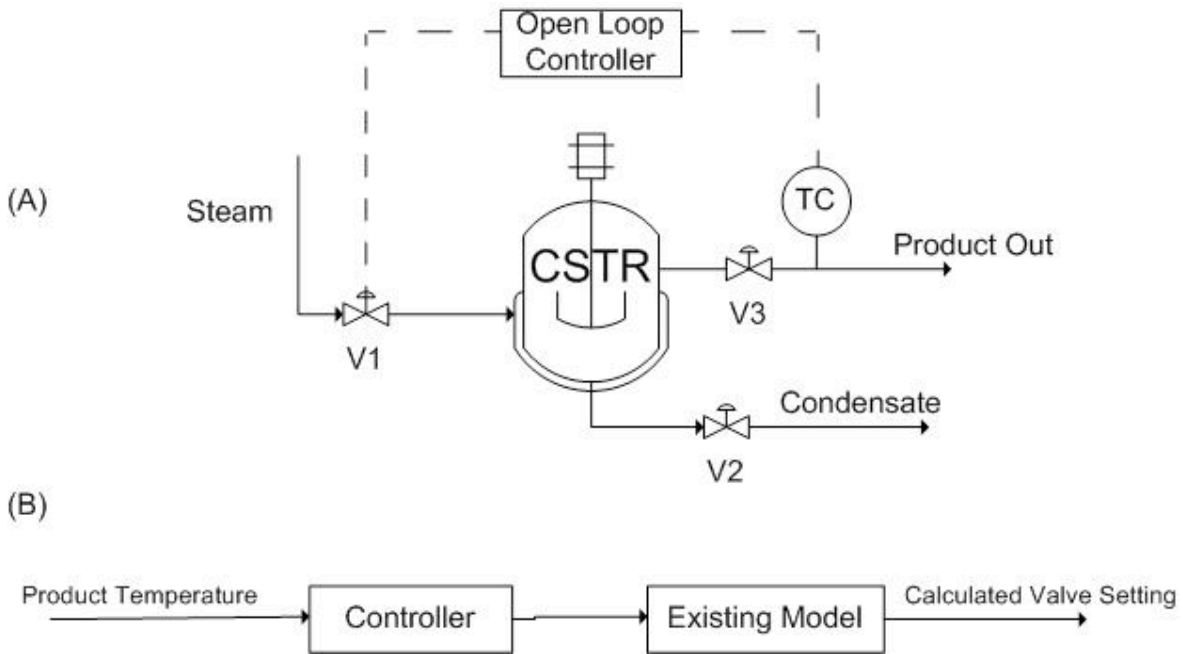


Figure 8. Example of CSTR open loop controller. (A) System diagram. (B) Open control loop.

Note that the open loop controller only uses the **current state** of the measured variable (product temperature) and a model to generate its control output (valve setting), as opposed to monitoring errors that have already taken place. As the result, the quality of the control system depends entirely upon the accuracy of the implemented model, which is challenging to develop. For this reason, feedback, or closed loop, controllers are generally recognized as the more reliable control system.

Short Summary on Closed and Open Loop Controllers

Feedback Controller = Closed Loop Controller

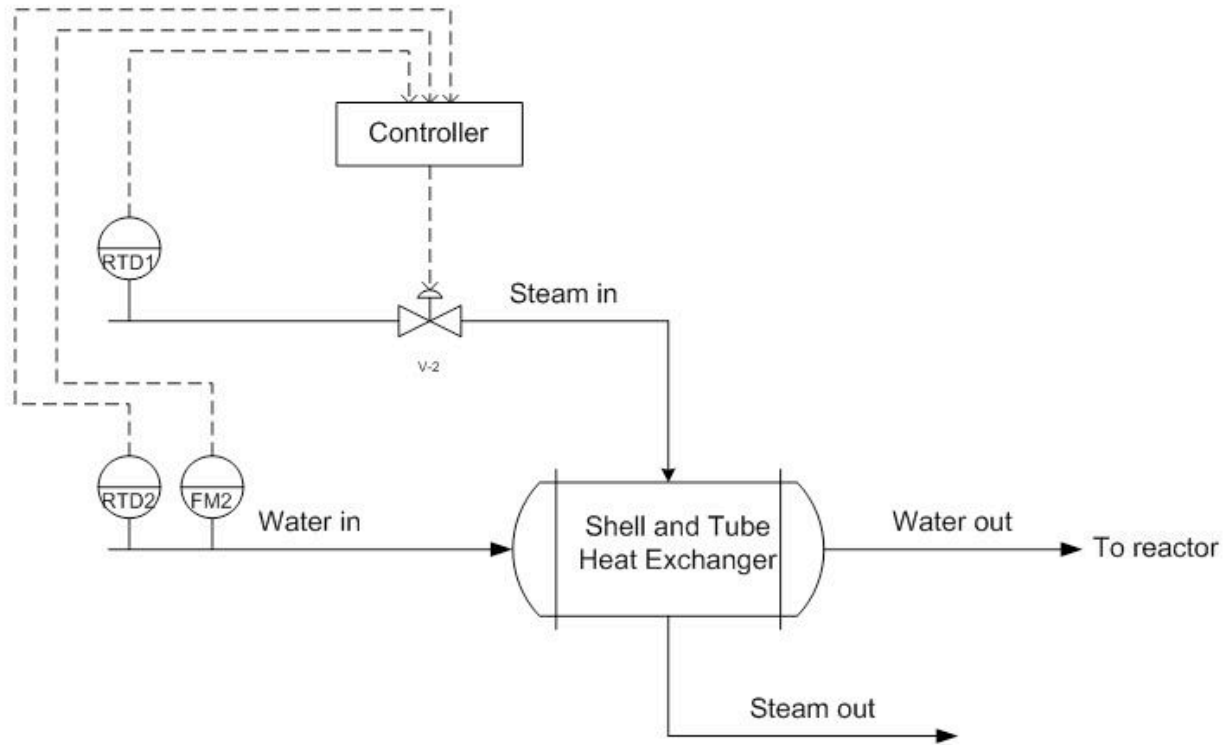
Non-Feedback Controller = Open Loop Controller

1.6 Worked Out Example 1

Your company is designing a plant to produce biodiesel. Several of the unit processes require heated water that is under tight temperature control. The desired temperature of the water is $65^{\circ}\text{C} \pm 1^{\circ}\text{C}$. To accomplish this, steam will be used in a shell and tube heat exchanger to heat the incoming water.

A member on the project team suggests the following feed forward control system to regulate the temperature of the water stream. Temperature and flow rate data for the

incoming steam and water streams will be used along with energy balance calculations to determine the flow rate of steam required to keep the exiting water stream at the appropriate temperature.

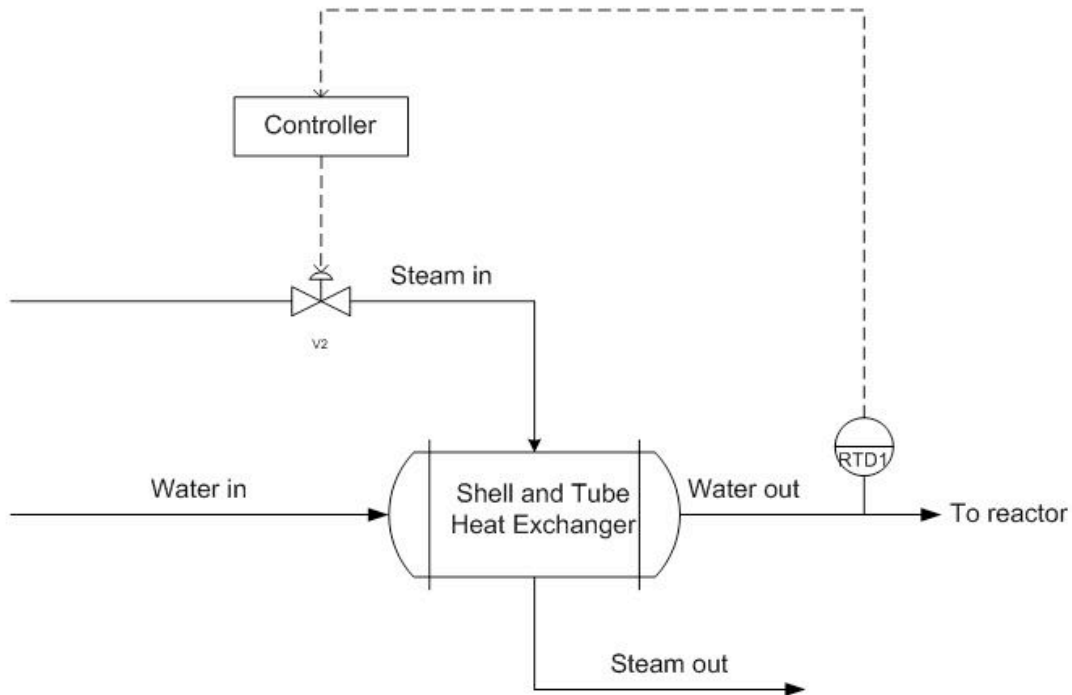


You on the other hand suggest a feedback control system. Place the appropriate sensors, actuators, and controllers to implement a feedback control system that will allow for the control of the exiting water temperature.

What are some of the advantages and disadvantages of using a feedback control system over a feed forward control system?

Solution

In the feedback control system, the temperature of the variable to be controlled is measured directly. If the exiting water temperature is too high, the controller will decrease the amount of steam entering the shell side of the heat exchanger. Likewise, if the exiting water temperature is too low, the controller will increase the amount of steam entering the shell side of the heat exchanger. This is an example of negative feedback at work to keep the exiting temperature at the setpoint.



Advantages

- Effective regardless of the origin of the disturbance.
- Relatively simple to implement. A mathematical model of the exiting water temperature is not needed.

Disadvantages

- Corrective action taken only after there is a deviation in the output from the set point.
- Can cause instability if incorrectly tuned

1.7 Worked Out Example 2

Of the following two scenarios, which would be the best to use a feedback control?

- An aqueous acidic waste stream from a process must be neutralized before it is discharged from the plant. If the stream goes below pH 6.0, your company will be assessed a minimum \$10,000 fine by the EPA for Clean Water Act violations. A relatively inexpensive source of lime slurry, suitable for acid neutralization purposes, is available. The pH of the acidic waste stream and the concentration of the lime slurry are both subject to fluctuations. It is desirable to maintain the pH of the waste stream as close to pH 6.0 as

reasonably possible (neutralizing the waste stream to a higher pH will use more lime and therefore be more expensive).

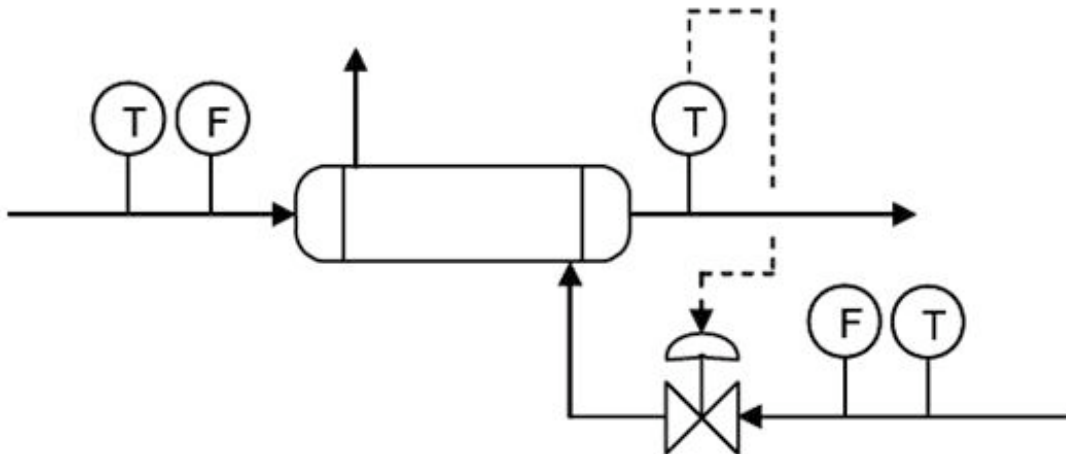
- You work for a company that uses concentrated red wine to make a steak sauce. The wine is concentrated by passing it through an evaporator, which evaporates some of the water and alcohol present in the wine. The amount of steam delivered to the evaporator can be controlled. Your objective is to obtain a set concentration (quantified as density) of the concentrated wine effluent from the evaporator. Different wines may be used so the initial concentration is not always known. Small fluctuations in the concentration of the reduced wine are acceptable, as these will not cause perceptible effects on the flavor or consistency of the steak sauce.

Solution

- A [feed-forward control](#) or feed-forward/feedback system would most appropriate for the first scenario. In this situation, it is critical that the pH of the waste stream not drop below the setpoint of pH 6. It is also desirable to minimize the use of lime, since this reduces the cost of the waste treatment. Therefore very tight process controls are desired, for which a feed-forward or feed forward/feedback system would be most appropriate. A feed-forward system can adjust to changes in inputs before they cause deviations in the output stream. Additionally, since there are important fluctuations two process inputs (pH variations in both the lime slurry and the acidic waste), feed-forward controls would be favored over feedback control.
- A feedback control would be most useful for the second scenario. There is only one monitored variable (concentration of reduced wine) and only one manipulated variable (steam). Since minor fluctuations about the wine concentration set point are not critical, the performance of a typical feedback control system would be acceptable. It would be hard to implement a feed-forward control system since the concentration of the wine feed to the evaporator may fluctuate and is not monitored.

1.8 Worked Out Example 3

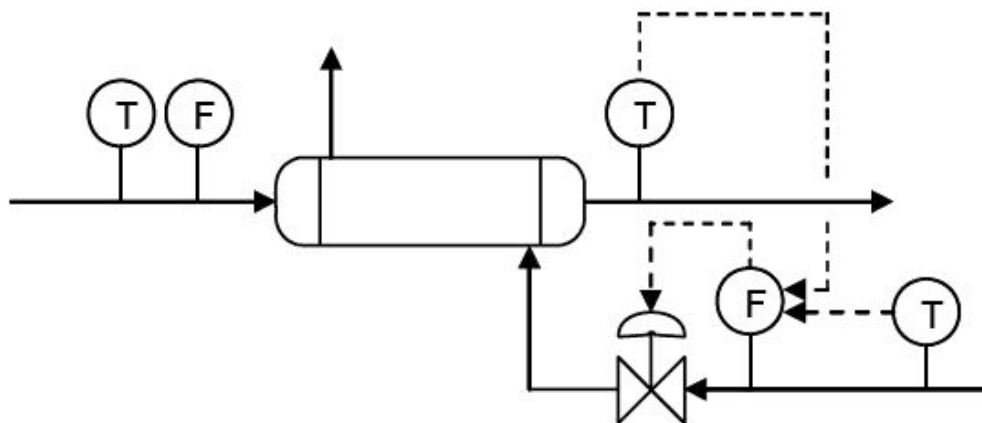
Using a shell and tube heat exchanger, a fuel stream is pre-heated using a steam stream from the utilities part of the plant. The plant is located in Ann Arbor, Michigan. Originally, a feedback controller is implemented to control the amount of steam coming into the shell and tube exchanger based on the temperature of the flow out of the exchanger. This is depicted below.



Upon implementation in the process, it was found that the feed temperature was not the only factor in the variance of the outlet stream. Because the plant is operated in Michigan, the steam temperature varies between seasons, colder in the winter and warmer in the summer. Propose a control scheme to account for both of these variances.

Solution

Here a cascade control scheme would be optimal to control the outlet temperature of the stream to a desired temperature, not just a feedback controller. The scheme is depicted below.



The feedback control previously used to control the system is still implemented, however it is now reporting to the flow controller before the steam control valve. Also, there is a temperature controller now incorporated in the control scheme. This is a feed forward controller that also controls the flow controller for the steam control valve. Thus the

primary control loops, the feed forward and feedback control loops, comprise the secondary control loop in the cascade control. This incorporates both the temperature of the incoming feed stream, which is controlled by feedback control via the temperature sensor after the exchanger. This is because the temperature of the outlet stream would vary with the temperature of the inlet stream if the steam stream were not accounted for. But accounting for the temperature of the steam stream, via a feed forward controller that is based on a temperature sensor before the control valve, will give a better approximation and more control over the temperature of the outlet stream. This is also a very good example of combining several control architectures and how they function in a real-world application, and why a feedback controller is not necessarily the most accurate control.

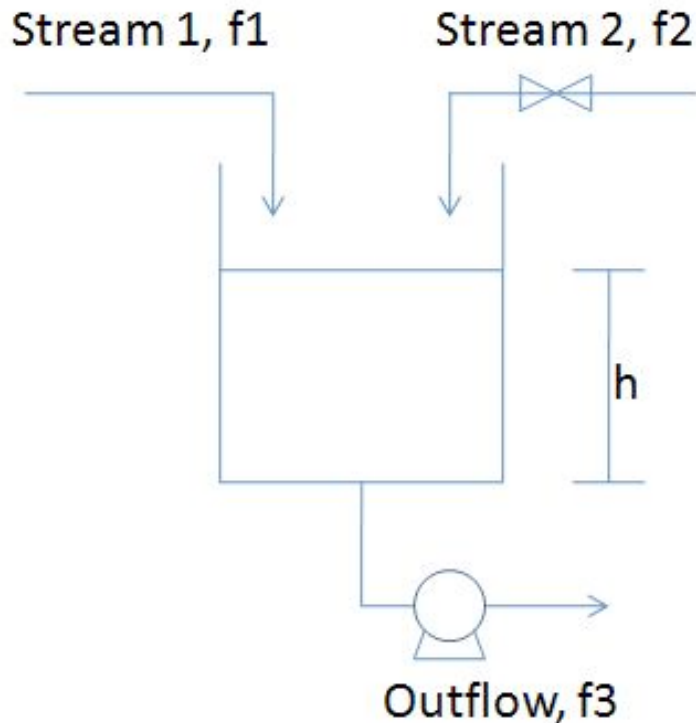
1.9 Worked Out Example 4

A blending system is used to mix a process stream (Stream 1, pure A) with liquid catalyst (Stream 2, pure B). The mixture then flows into a reactor. The flowrate of stream 1 (f_1) can vary but it is possible to manipulate the flowrate of stream 2 (f_2). The outflow rate from the reactor (f_3) also can be manipulated via a pump. The level in the tank is measured by a level transmitter that sends its signal to a level controller. All three flow rates can be measured, but measuring the composition of the streams is impossible. In order to control the level of the tank, an engineer has two options:

- (i) manipulate f_2 while holding f_3 constant
- (ii) manipulate f_3 while holding f_2 constant

Could method (i) utilize feedforward or feedback control of the level? If so, explain how it can be done.

Could method (ii) utilize feedforward or feedback control of the level? If so, explain how it can be done.



Answer For configuration (i)

- Feedback: If you measure h , when it goes up, you can reduce f_2 , and when it goes down, you can increase f_2
- Feedforward: If you measure f_1 , when it goes up, you can reduce f_2 , and when it goes down, you can increase f_2 . You are indirectly controlling h due to the mass balance.

For configuration (ii)

- Feedback: If you measure h , when it goes up, you can increase f_3 , and when it goes down, you can decrease f_3 .
- Feedforward: If you measure f_1 , when it goes up, you can reduce f_3 , and when it goes down, you can increase f_3 .

This problem was meant to explore different strategies for both feedback and feedforward control configurations. Additionally, it demonstrates how controlling the manipulated variables (either f_2 for configuration (i) or f_3 for configuration (ii)) affects the desired outcome (maintaining consistent tank height).

1.10 Sage's Corner

[Powerpoint Slides from the example](#)

you must click on this link below to view the video:


- <http://video.google.com/videoplay?docid=-8096439316697651765>

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Section 2. Feed forward control: What is it? When useful? When not? Common usage.

See also [ECOSSE](#)

Note:  [Video lecture](#) available for this section!

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Date Revised: 09/25/2007

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

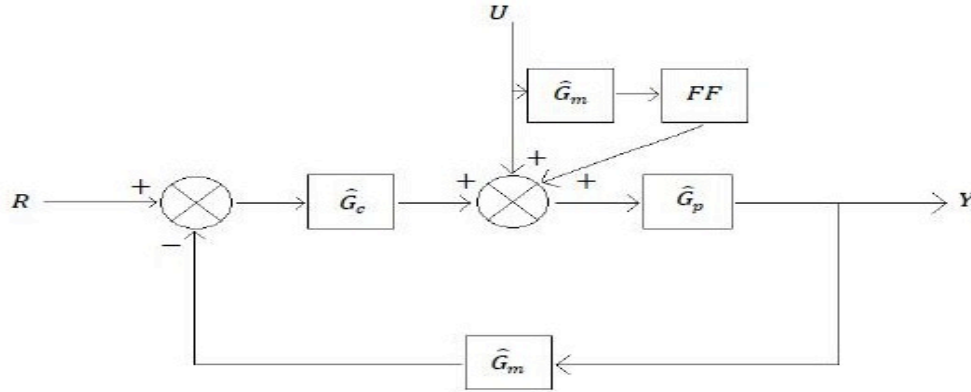
2.1 Introduction

Feed-forward control is a useful tool in the field of chemical engineering when there is a known set of deviations occurring upstream of the system. This would allow engineers to account for that particular deviation within the controller and reduce the effects of the deviation on the system. An example would be a car's cruise-control system. If it has feedback control, when there is a slope and therefore a speed reduction, the feedback controller would compensate by applying additional throttle to the engine. If it uses a feed-forward controller instead, the controller would calculate the slope beforehand and throttle the engine before any speed reduction occurs. In this sense, the controller predicts the incoming deviation and compensates for it.

The following block diagram shows a feed-forward controller implemented on a idealized process with a setpoint R and load U :

Where:

\hat{G}_P represents the process operator, \hat{G}_M represents the measurement operator, \hat{G}_C represents the controller operator, and FF is the feed-forward controller.



The perfect feed-forward controller is the inverse of the process operator, \hat{G}_P^{-1}

$$\hat{G}_P^{-1} = K_P \left(\tau \frac{\delta}{\delta t} + 1 \right) = \hat{G}_{FF}$$

For example:

$$\hat{G}_P^{-1} Y = \left(U + \hat{G}_{FF} U \right) + \hat{G}_C (R - Y)$$

In General:

(in the language of operator or state space).

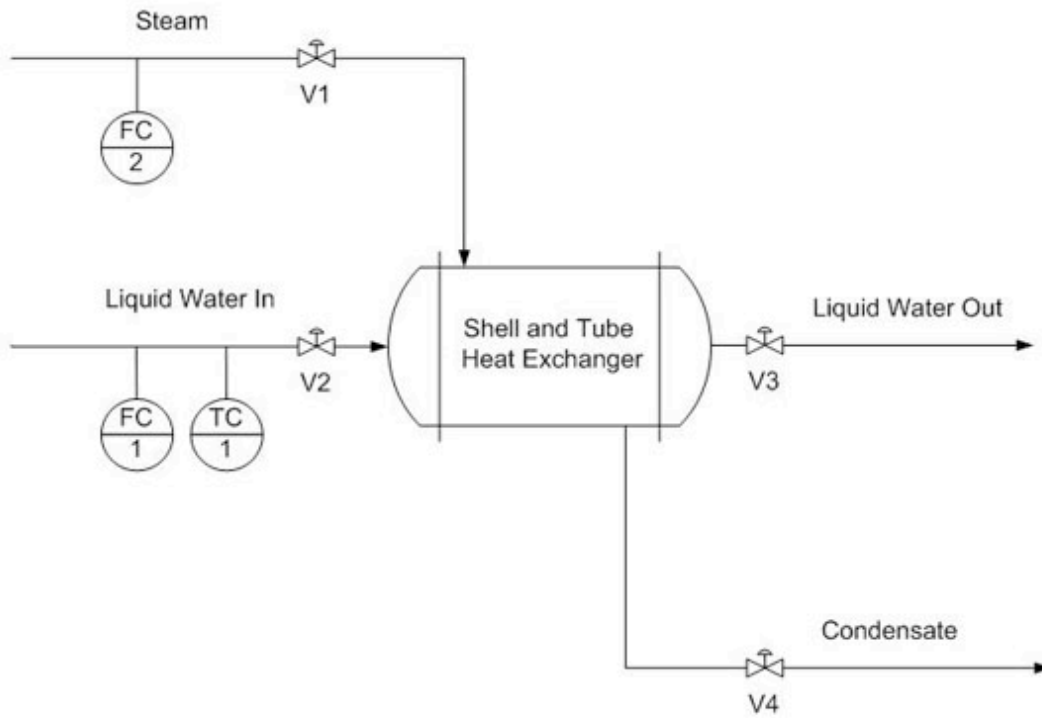
[Note: this needs some expansion and checking == RZ]

2.2 Feed-Forward Control

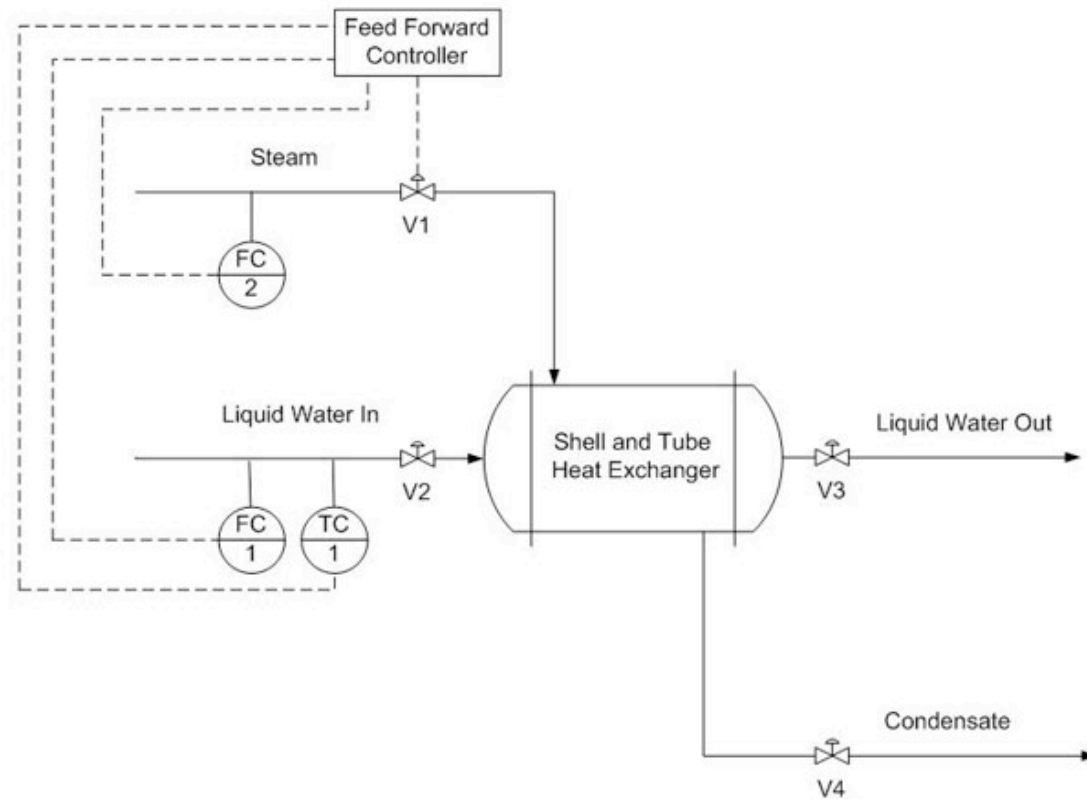
The objective of feed-forward control is to measure disturbances and compensate for them before the controlled variable deviates from the setpoint. Feed-forward control basically involves a control equation which has certain corrective terms which account for predicted disturbances entering the system. The equation is only effective for gains in a steady state process. [Dynamic compensation](#) should be used in the control equation if there are any dynamic deviations with the process response to the control action. This dynamic compensation ability will be discussed further in the next section.

One form of a feed-forward control would be a Derivative (D) control which calculates the change in error and compensates proportionately. But a D-control can't perform by itself and usually requires working in conjunction with a Proportional (P) or Proportional Integral (PI) control. More information can be found in the [PID Intro](#) article.

Simulated below is a typical shell and tube heat exchanger which heats up liquid water using steam.



Adding a feed-forward control into the system manipulates the amount of steam required to compensate for the varying amounts of liquid feed coming in.



Overall heat balance:

Heat into the system is equal to the heat leaving the system.

Heat gained by liquid:

$$q_{out} = m_l C_p (T_2 - T_1) \quad (1)$$

Where:

m_l -- mass flow rate of the liquid

C_p -- the heat capacity of the liquid

T_1 -- the input temperature of the liquid

T_2 -- the desired temperature setpoint for the liquid

Heat lost by steam:

$$q_{in} = m_s \lambda \quad (2)$$

Where:

λ -- heat of vaporization
 m_s -- mass flow rate of the steam

Therefore:

$$m_s = \frac{C_p}{\lambda} m_l (T_2 - T_1) \quad (3)$$

To compensate for a deviation from the desired inlet temperature of the liquid water, the amount of steam must be adjusted. Equation (3) acts as the control equation for the feed-forward controller. This controller actuates the inlet valve of the steam and acquires temperature and flow rate data from the inlet streams. Based on the desired temperature setpoint, T_2 , and the actual input temperature, T_1 , we can use this equation to calculate the mass flow rate of the steam required to compensate for the temperature deviation.

2.2.1 Accounting for System Non-Idealities

Often, one of the most difficult tasks associated with creating a functional feed forward controller is determining the necessary equations that govern the system. Even more complexities arise when the system is not, and cannot be treated as, ideal. This is the case with many real and practical systems. There is simply too much heat lost or too many unforeseen effects to safely assume ideal conditions. The pure math of the example above does not account for these effects.

The equations will output a value to a control valve (often in voltage). That voltage will be derived from some previously determined relationship between voltage, valve %open, and steam flow rate. A very simple way to begin managing the issue of non-ideality is by including a "non-ideality constant". This can be an additive or a multiplicative constant that adjusts the voltage output determined by the equations.

$$V = f(m_s) \quad \text{Voltage output is some function of the calculated required steam flow}$$

$V = c_N * f(m_s)$ or $V = c_N + f(m_s)$ Voltage output is adjusted by some constant

This non-ideality constant c_n often must be determined by trial. One way to accomplish this is to use manual control to determine the output voltage needed at various inlet conditions. Using the data from the manual trials, and the resulting voltage that your unadjusted feed forward controller would output, it is possible to determine by what factor your feed forward voltage needs to be adjusted. For example, if by manual control you determine that for inlet conditions X the required voltage is 300mV and your feed forward controller is only outputting 270mV for conditions X, you need some factor to adjust.

It may also happen that your "non-ideality constant" will not turn out to be constant when you begin to look at the data. In this situation, consider using a linear relationship between the non-ideality factor and some inlet condition or implementing CASE or IF statements covering discrete ranges of inlet conditions and giving different constants.

2.3 Dynamic Compensation

Dynamic compensation is a method to account for factors such as lead and lag times when using feed-forward control. For instance, in the example above, when the feed forward controller monitors a temperature decrease in the liquid feed, it will increase the steam flow rate - the manipulated variable - to compensate and thus maintain the temperature of the exiting liquid flow - the controlled variable. However, the steam may enter the heat exchanger faster than the liquid feed and this will cause a transient increase in the controlled variable from the setpoint. In an ideal case the steam and liquid feed would enter the heat exchanger at the same time and no deviation from the set exiting temperature would be observed. Therefore, dynamic compensation involves predicting non-ideal behavior and accounting for it. While perfect feed-forward control is nearly impossible, dynamic compensation is one step closer.

2.4 Open Loop System

Feed-forward control is an open loop system. In an open loop system, the controller uses current, or live, information of the system to generate appropriate actions by using predetermined models. The sensor providing the reference command to the closed loop actuator is not an error signal generated from a feedback sensor but a command based on measurements. This is the defining characteristic of an open loop system, in which the controller does not manipulate the system by trying to minimize errors in the controlled variable.

Because a feed-forward controller listens to the system and calculates adjustments without directly knowing how well the controlled variable is behaving (if it does, it is

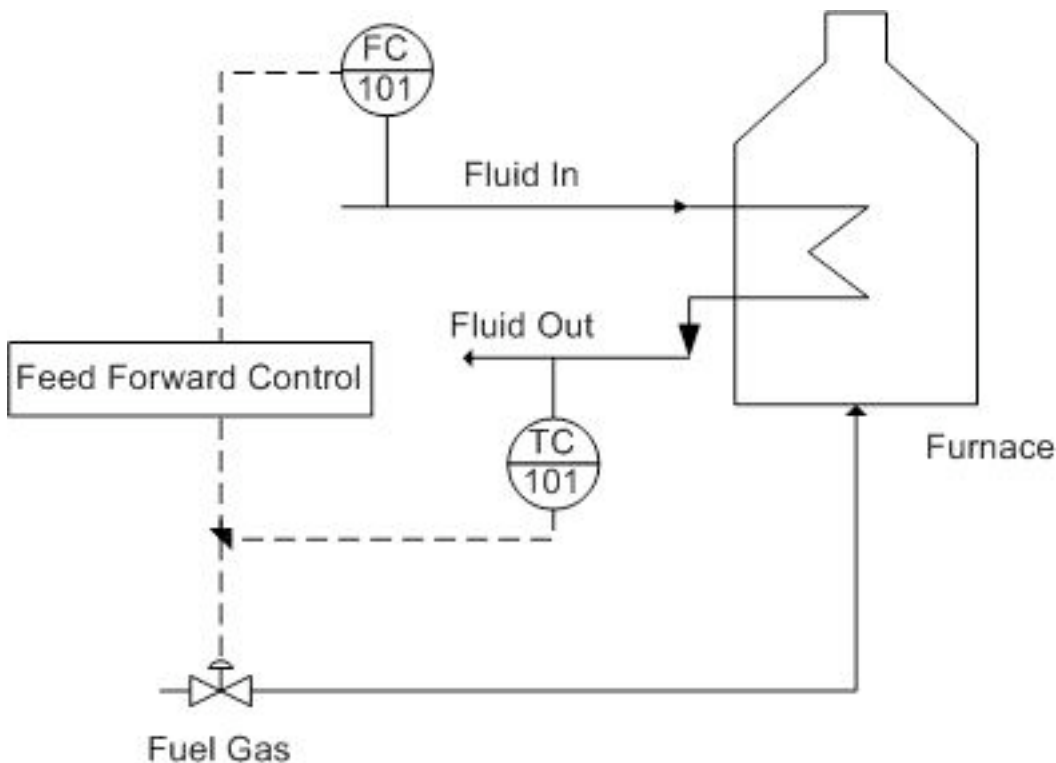
getting feedback), it is open loop in nature. In other words, the controller operates on "faith", that its mathematical models are able to accurately generate responses (valve setting, motor speed, etc.) that lead to expected results. Therefore, it is critical to implement good models in feed-forward systems. This is often the most difficult part of a feed-forward design, as mentioned previously.

However, not all open loop systems are feed-forward. Open loop simply means the system is not getting feedback information, in which the controlled variable tells the controller how well it is doing compared to its set point (i.e. error). Feed-forward control, on the other hand, takes an extra step by using non-feedback information to produce predictive actions.

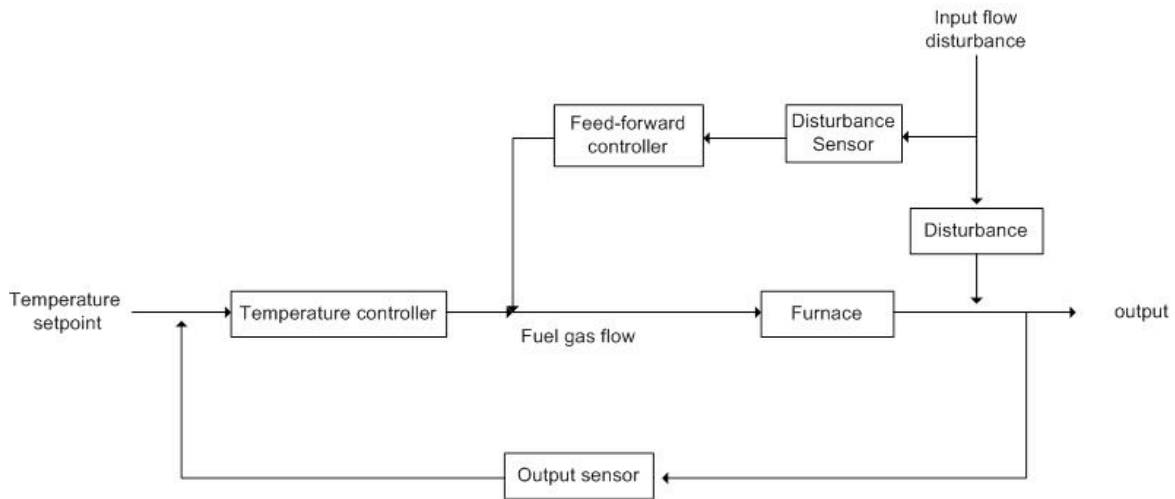
This simple [open loop system](#) is an example of an open loop system that is not feed-forward. The controller simply takes the current state of the controlled variable to generate a valve setting. It is not getting a feedback, because the product temperature is not compared to a set point. It is not feed-forward either, because there is no mechanism that produces actions that may yield expected results in the future.

2.5 Feed-forward applications

Feed-forward control is used in many chemical engineering applications. These include heat exchangers, CSTRs, distillation columns and many other applications. A typical furnace, shown below, is heating up an input fluid using fuel gas.



One possible disturbance is the flow rate of the incoming fluid. For example: If the fluid input rate was increased by 10%, then the required heat duty should also be increased by approximately 10%. This feed-forward control strategy immediately changes the fuel gas flow rate and therefore the heat duty. The performance of feed-forward controls is limited by model uncertainty, and in practice feed-forward control is combined with feedback control in order to ensure better control of the system. Feed-forward control will compensate for fluid input disturbances while feedback control will compensate for other disturbances—such as the fuel gas flow rate or the temperature of the furnace—and model uncertainty. This system can also be represented by the following block diagram.



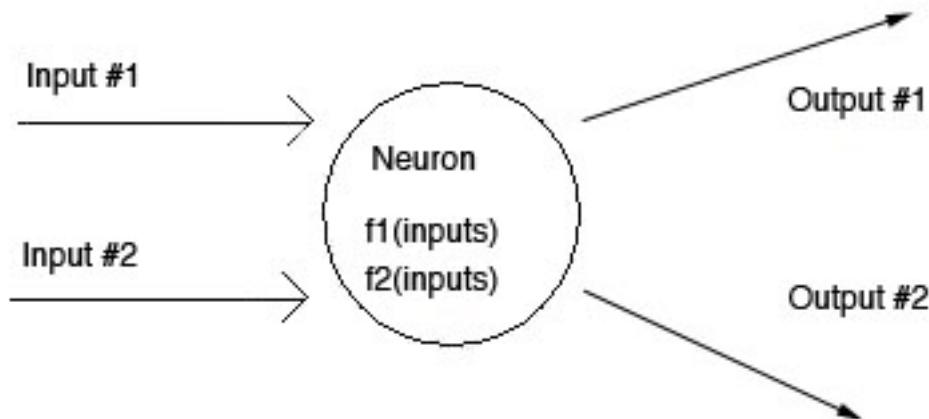
2.5.1 Pros & Cons of Feed-Forward Control

Different applications require different types of control strategies. Sometimes feed-forward solutions are required for proper system control; sometimes only feedback solutions are necessary. Feedback systems don't always maintain the setpoint as well because of the lag that comes with waiting for the disturbance to propagate through the system. As a result, many control systems use a combination of feed-forward and feedback strategies, such as PID controllers. PID controllers use the Proportional-Integral control for feedback and the Derivative control for feed-forward control. This forms a system with multiple loops, otherwise known as a [cascading system](#). A critical advantage of running both forward and backward controls is that the system is still somewhat able to adjust a variable if one mechanism fails since the two loops use different sensors. As a result, PID controllers are great for controlling processes, however, they require a number of equations to determine feed-forward and feedback correction.

Feed-forward systems work by checking the conditions of an incoming stream and adjusting it before the system is adversely affected. If the controller is told the traits of an acceptable incoming stream, then it can compare that standard to whatever is coming

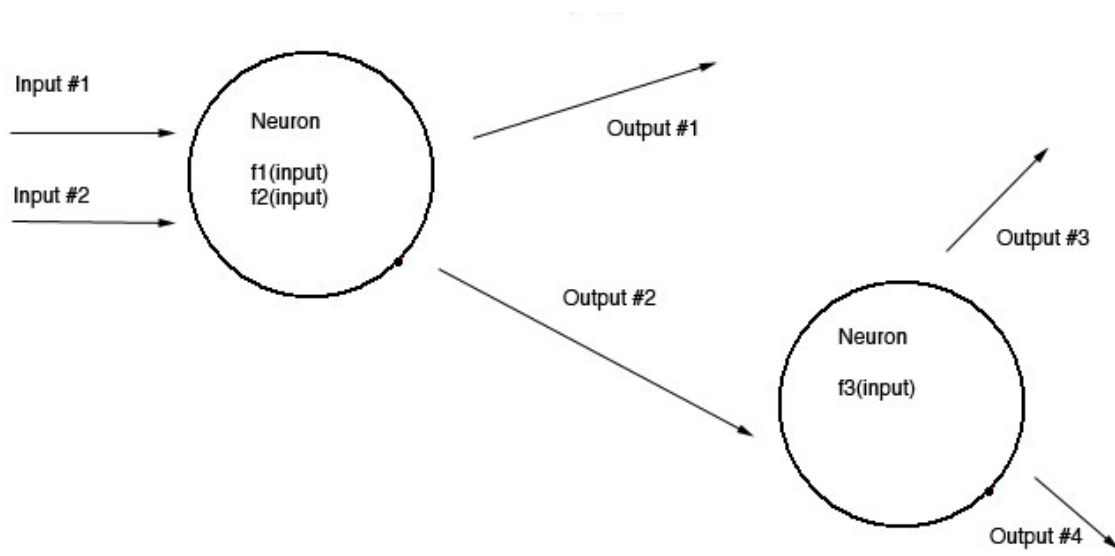
down the pipe. The feed-forward controller can look at this error and send a corrective signal to the automatic valve responsible for that pipe (or any other control device). In order to have this kind of predictive ability, the controller must have explicitly defined equations that account for the effects of a disturbance on the system. In addition, these equations must also then prescribe action to counter-act the disturbance. This can become even more difficult when there are several incoming stream traits that are being observed. When there are multiple inputs, the feed-forward system will require non-linear equations, leading to the development of [neural networks](#).

Neural networks are based on “neurons”, which are representations of non-linear equations. This concept is based on the brain's use of neurons to process and transmit information. The neuron is actually comprised of a set of sigmoidal equations relating inputs to outputs. Sigmoid functions are non-linear equations that take inputs and apply constants, or weights, to transform the value to make an output. Below is a picture that illustrates the function that these neurons serve.



The picture above shows a multiple input-output system. Most feed-forward systems have to deal with more than one input.

Neurons can be “connected” in ways that allow the inputs to be transformed any number of times. Neurons that are connected indicate that one sigmoidal function's output becomes the input of another one. Although the concept of neurons is easily understandable, the difficulty lies in the potential complexity of real systems. For example: the number and type of inputs go to which neurons, the initial weights be, the number of neurons needed, etc. As you can see, there are a lot of design questions that make developing the neural network difficult.

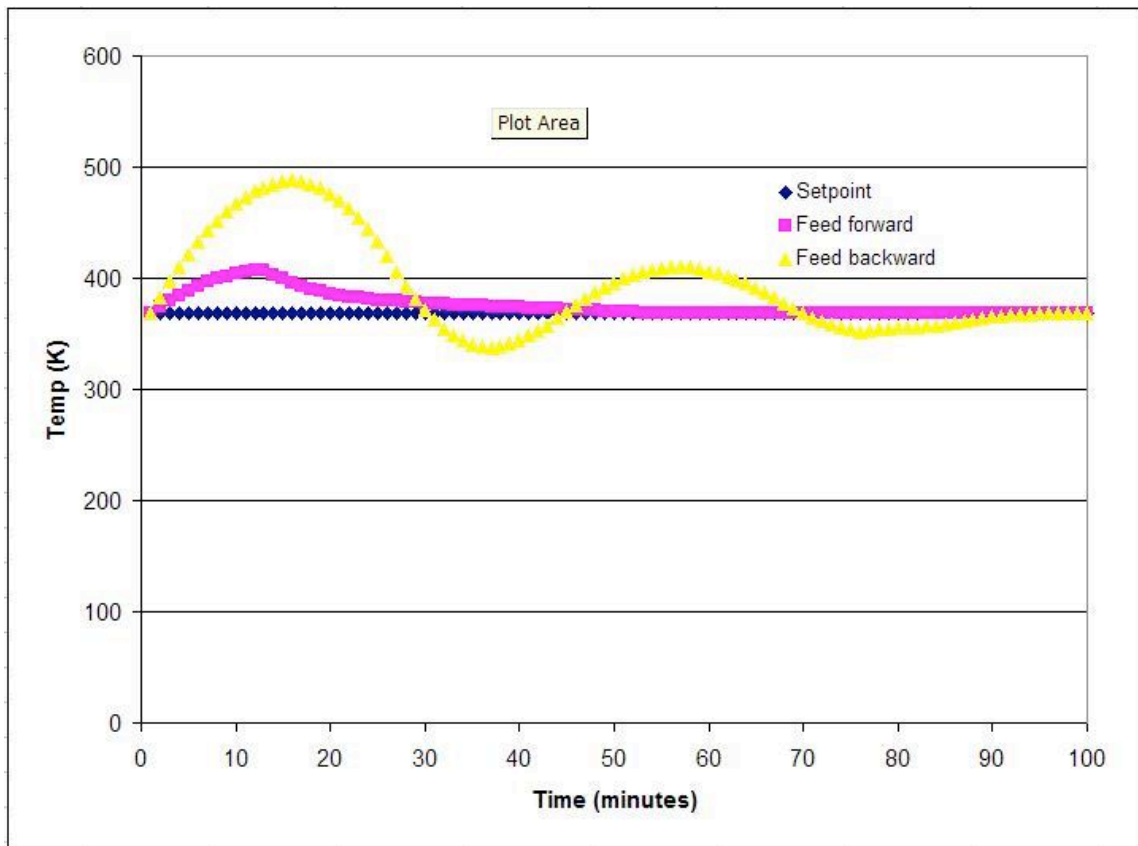


Coupled with an expected set of upstream conditions, the feed-forward system can continually adjust the method it uses to control an output variable. The system is capable of doing this by measuring sensor inputs coming into the controller, using neurons to transform the data, and comparing the resulting output(s) to a set of known or desired outputs. If the actual output is different from the desired output, the weights are altered in some fashion and the process repeats until convergence is achieved. This is how a controller is able to "learn". Learning is just discovering the weighting factors that allow the transformed outputs to match the desired outputs.

The following table shows a list of feed-forward pros and cons:

Feed-Forward Pros	Feed-Forward Cons
<ul style="list-style-type: none"> • Does not require disturbance to propagate through system for detection • Able to predict incoming disturbance before they hit the system • Neural network utilized to familiarize control system with a changing environment • Provides better set point management than feed-backward control • Can be used in conjunction with feed-back control to provide multiple input single output (MISO) control 	<ul style="list-style-type: none"> • Explicit non-linear equation required for adequate disturbance prediction. Much harder to implement as a result • Cannot compensate for any disturbances that occur WITHIN the system • Requires infinitely accurate models • Requires infinitely accurate measurements

A CSTR with a given volume with heat-exchange capability has a coolant water system to maintain a specific system temperature (368K). To maintain this temperature, the flow of coolant water oscillates. Let a temperature disturbance of 100K be introduced over a period of 10 minutes. For this simulation, the Excel spreadsheet from PID-Tuning Optimization was used to create feed-forward and feed-backward data. In the following plot, observe the difference between using feed-forward control versus feed-backward control in an example.



As shown, the feed-forward strategy works more effectively than the feed-backward strategy at nullifying the disturbance (over the time frame). The temperatures reached in feedback mode vary more than the ones seen in feed-forward mode. However, the controller response is solely defined by the parameters used in the Excel spreadsheet. If one assumes that the PID parameters used by the **PID-optimization group** were optimized, then we can say feed-forward would be the best option here.

2.6 Feed-Forward Design Procedure

This section provides an outline of the different steps for designing a feed-forward control strategy. The steps pay close attention to designing a feed-forward controller where there are multiple disturbances. Feed-forward design can be broken down into eight steps (Corripio,1990).

Step 1. State the control objective. This step includes defining which variable needs to be controlled and what the set point is. The setpoint should be adjustable by the operator.

Step 2. List the possible measured disturbances. This step includes identifying which disturbances are easily measured and how fast each disturbance should be expected to vary.

Step 3. State which variable is going to be manipulated by the feed-forward controller.

Step 4. The feed-forward controller consists of two parts: steady-state and dynamic compensators. Develop the steady-state compensator first. The compensator should be an equation where the manipulated variable, identified in step 3, can be calculated from the measured disturbances, identified in step 2, and the control objective (set point), identified in step 1.

Step 5. Reevaluate the list of disturbances. The effect of a disturbance on the controlled variable can be calculated from the equation. Three criteria will be used to determine which disturbance the feed-forward controller will correct: the effect the disturbance has on the controlled variable, the frequency and magnitude of variation, and the capital cost and maintenance of the sensor.

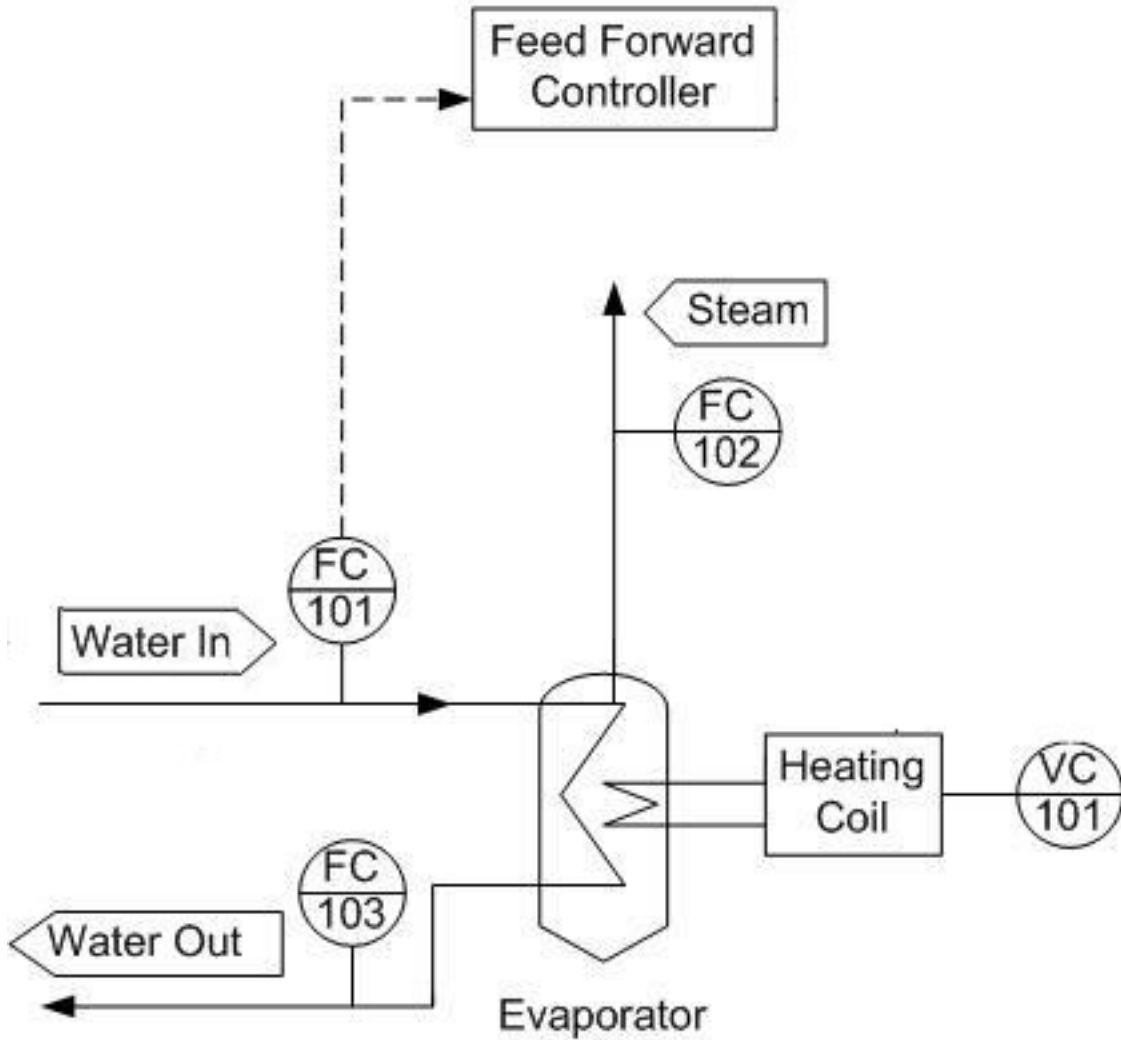
Step 6. Introduce the feedback compensation. This depends on the physical significance assigned to the feedback signal.

Step 7. Decide whether dynamic compensation, lead/lag, and/or dead time is required, and decide how to introduce it to the design.

Step 8. Draw the instrumentation diagram from the feed forward control strategy. The details of the diagram depend largely on the control system being used.

2.7 Worked out Example 1

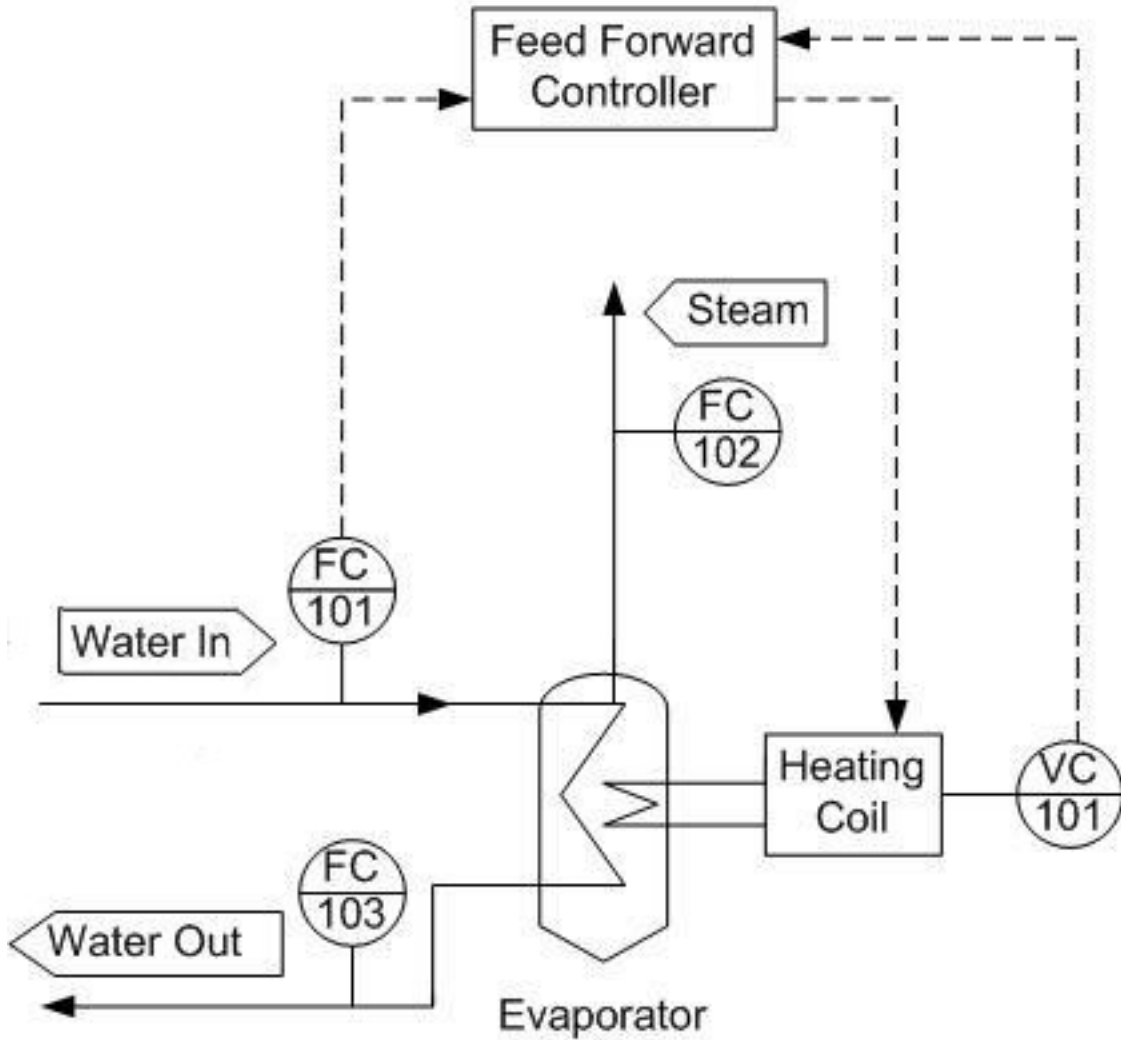
For the first example, a water stream enters an evaporator. A discrete amount of the water stream is to be evaporated. Below is the design diagram for the evaporator. The incoming stream is being used as the input to the feed forward control box.



Determine what additional input will be needed to regulate the amount of steam produced and draw this on the design diagram.

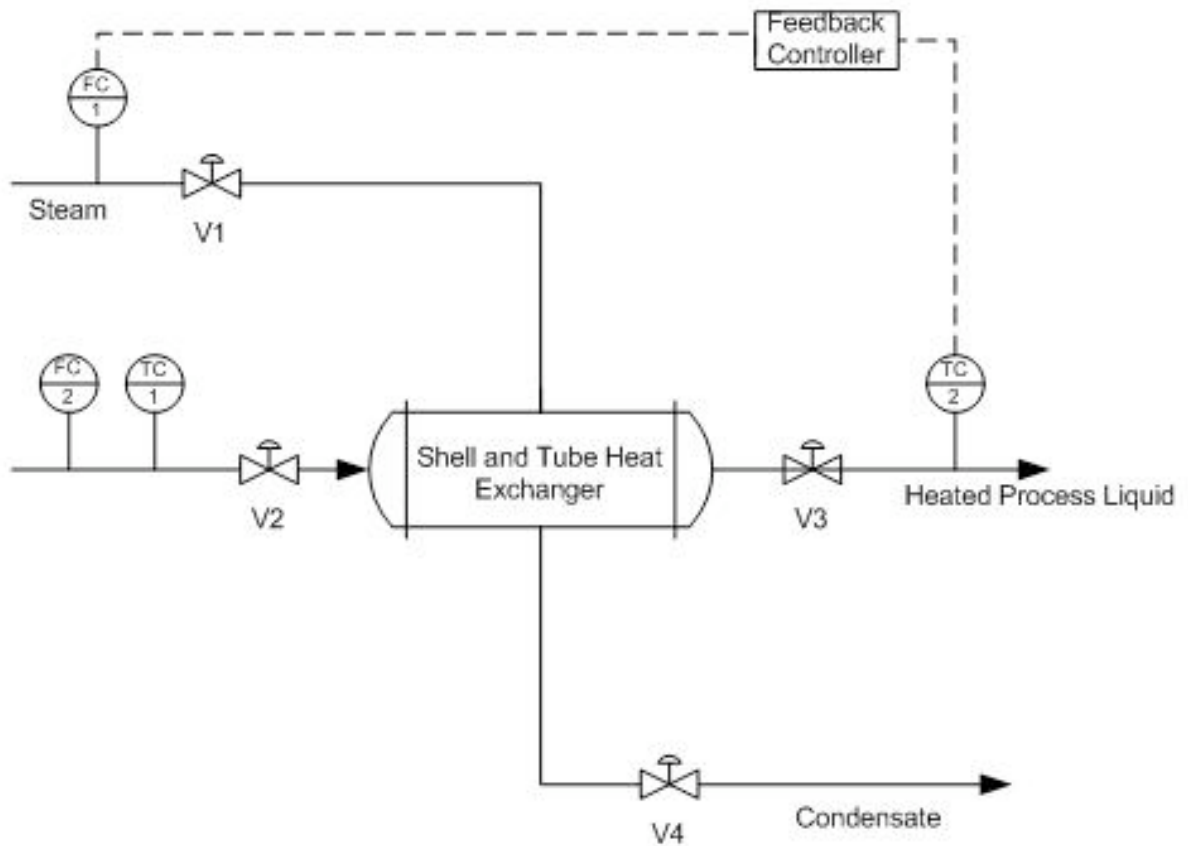
2.7.1 Solution

By regulating the heating coil, we can regulate how much water will boil off in accordance with any change of the feed stream.



2.8 Worked out Example 2

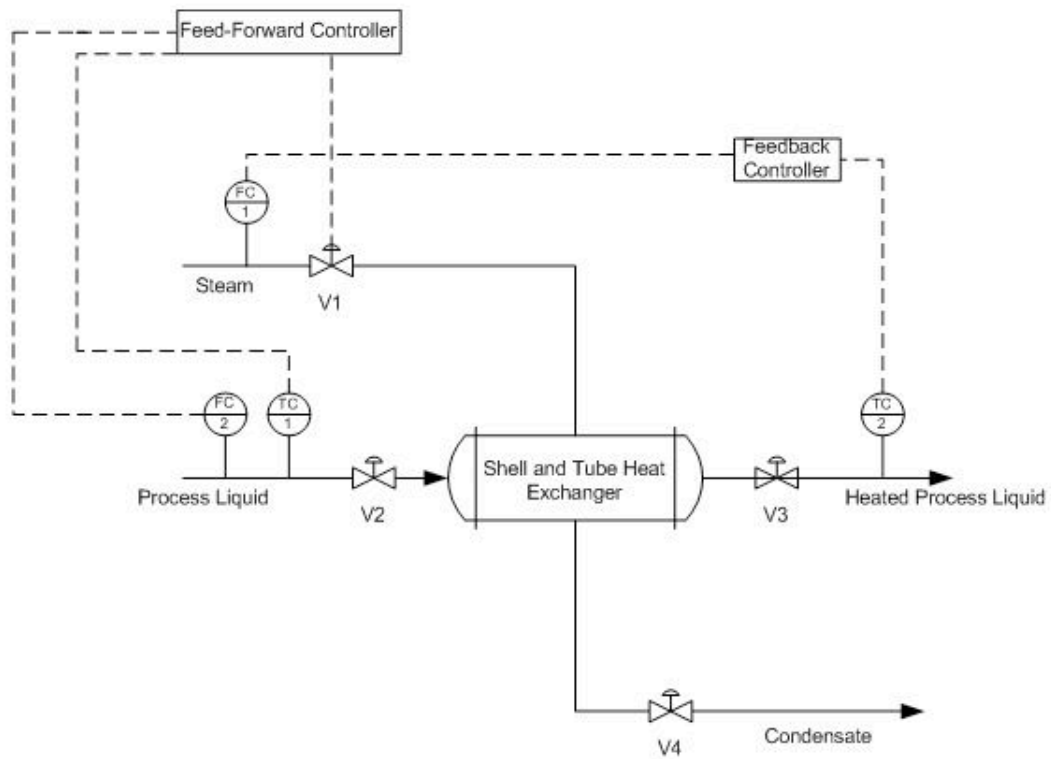
For the second example, a particular process liquid from a previous reaction will be heated before proceeding to the next phase of reactions. A shell and tube heat exchanger has been installed for this purpose with steam providing the heat duty. A feedback controller is used to control the output temperature of the process liquid stream, but the flowrate and the temperature of the input liquid stream vary too much for the feedback controller to be effective.



What sort of controller would be appropriate in addition to the feedback controller to account for the deviations of the input liquid stream? How would this controller be implemented? For simplicity it is assumed that all the steam condenses.

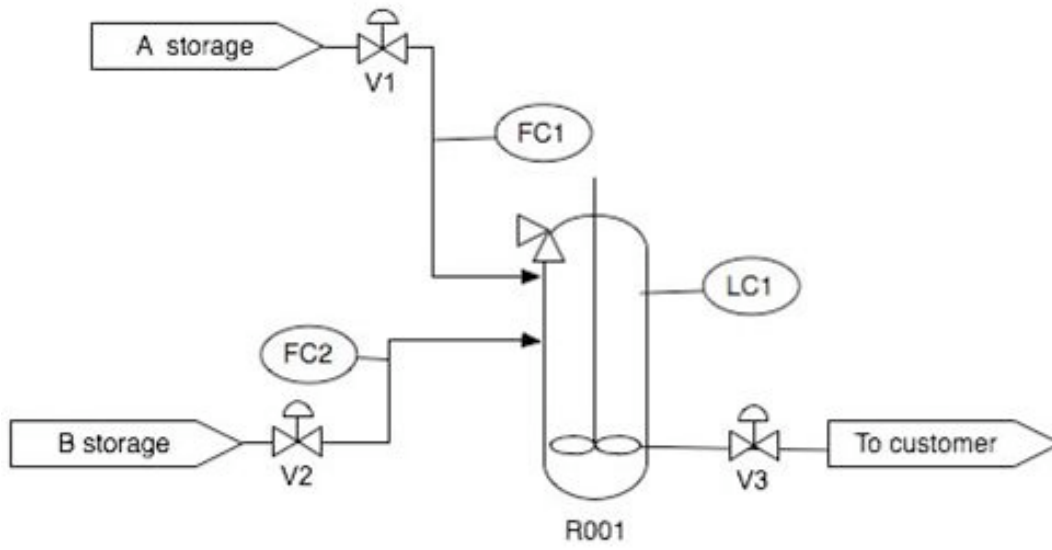
2.8.1 Solution

The solution is to implement a feed-forward controller that gathers the input temperature and flowrate data from TC1 and FC2 and adjusts the steam valve V1 in order to account for any deviation that may occur in the input liquid stream. This sort of feedback feed-forward combination is a typical setup for the majority of control systems. The feed-forward controller accounts for any upstream disturbances while the feedback controller accounts for the disturbances within the system.



2.9 Worked out Example 3

Using the P&ID shown below, write out the feed-forward controller expressions for v3. List any assumptions used in your controller expression.



2.9.1 Solution

To maintain LC1 by measuring FC1 and FC2 and preemptively adjust v3, we must use the controller expression below.

$$v_3 = k_{valves}(FC1 + FC2)$$

The controller expression above assumes that the valve is linear. Also, it assumes that FC1, FC2, and the model are infinitely accurate.

2.10 Sage's Corner

A summary and example of Feed Forward Control:

<http://video.google.com/googleplayer.swf?docId=-2914206783288486300>

A copy of the slides can be found here: [\[1\]](#)

Another summary and example of Feed Forward Control:

<http://video.google.com/googleplayer.swf?docId=6443635005819064435>


A copy of these slides can be found here: [\[2\]](#)

2.11 References

- Svrcek, William Y., Mahoney, Donald P. & Young, Brett R. (2006). *A Real-Time Approach to Process Control*. John Wiley & Sons, Ltd.

- Astrom, Karl J. & Haggund, Tore (1998). *Advanced PID Control*. Automatic Tuning of PID Controllers. The Instrumentation Systems and Automation Society.
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Section 3. Cascade control: What is it? When useful? When not? Common usage.

Note:  [Video lecture](#) available for this section!

Authors: Joseph Casler, Andry Haryanto, Seth Kahle and Weiyin Xu

Stewards: Irene Brockman, Robert Chockley, Scott Dombrowski, Chloe Sweet

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- [First round reviews for this page](#)
- [Rebuttal for this page](#)

3.1 Introduction

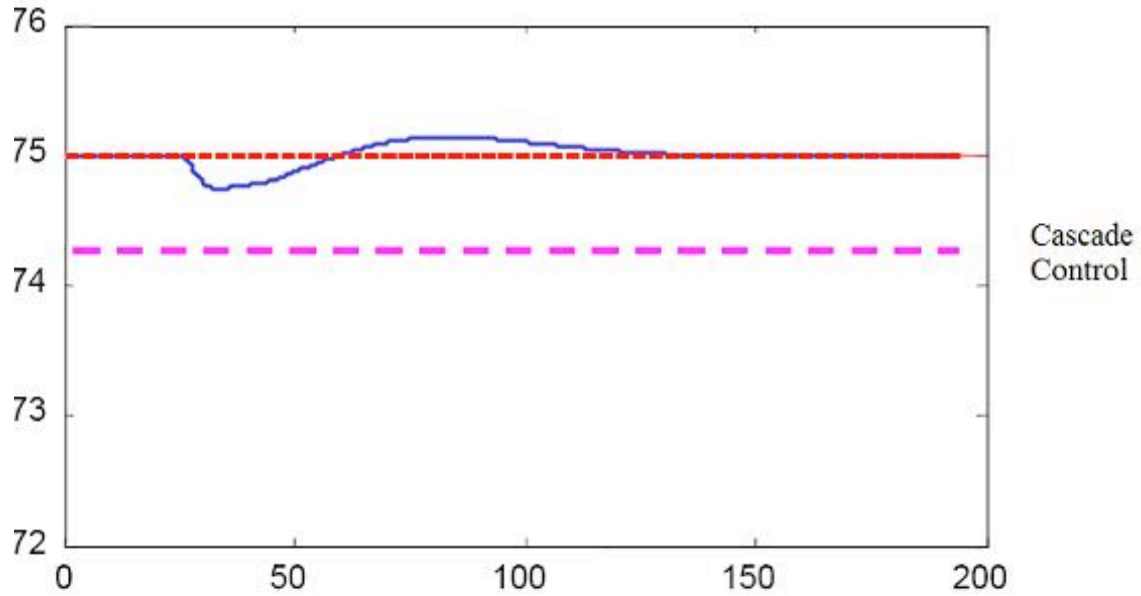
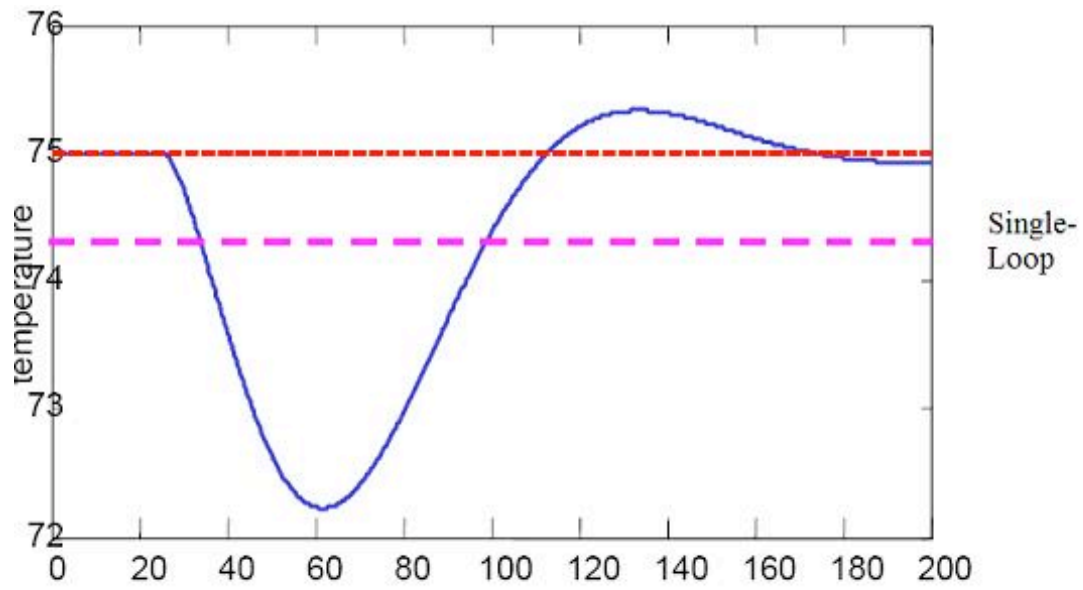
In the previous chapters, only single input, single output (SISO) systems are discussed. SISO involves a single loop control that uses only one measured signal (input). This signal is then compared to a set point of the control variable (output) before being sent to an actuator (i.e. pump or valve) that adjusts accordingly to meet the set point. Cascade controls, in contrast, make use of multiple control loops that involve multiple signals for one manipulated variable. Utilizing cascade controls can allow a system to be more responsive to disturbances.

Before venturing further into the topic of cascade controls, the terms 'manipulated variables', 'measured variables' and 'control variables' should be clarified. The definitions of these terms commonly found in literature are often interchangeable; but, they typically refer to either the input or output signal. For the purpose of this article, 'control variables' will refer to inputs like flow rates, pressure readings, and temperature readings. 'Manipulated variables' and 'measured variables' will refer to the output signals which are sent to the actuator.

The simplest cascade control scheme involves two control loops that use two measurement signals to control one primary variable. In such a control system, the output of the primary controller determines the set point for the secondary controller. The output of the secondary controller is used to adjust the control variable. Generally, the secondary controller changes quickly while the primary controller changes slowly. Once cascade control is implemented, disturbances from rapid changes of the secondary controller will not affect the primary controller.

3.2 Cascade Control

To illustrate how cascade control works and why it is used, a typical control system will be analyzed. This control system is one that is used to adjust the amount of steam used to heat up a fluid stream in a heat exchanger. Then an alternative cascade control system for the same process will be developed and compared to the typical single loop control. The figure below shows the performance of cascade control vs. single-loop control in CST heater



Cascade control gives a much better performance because the disturbance in the flow is quickly corrected

3.2.1 Example of Cascade Control

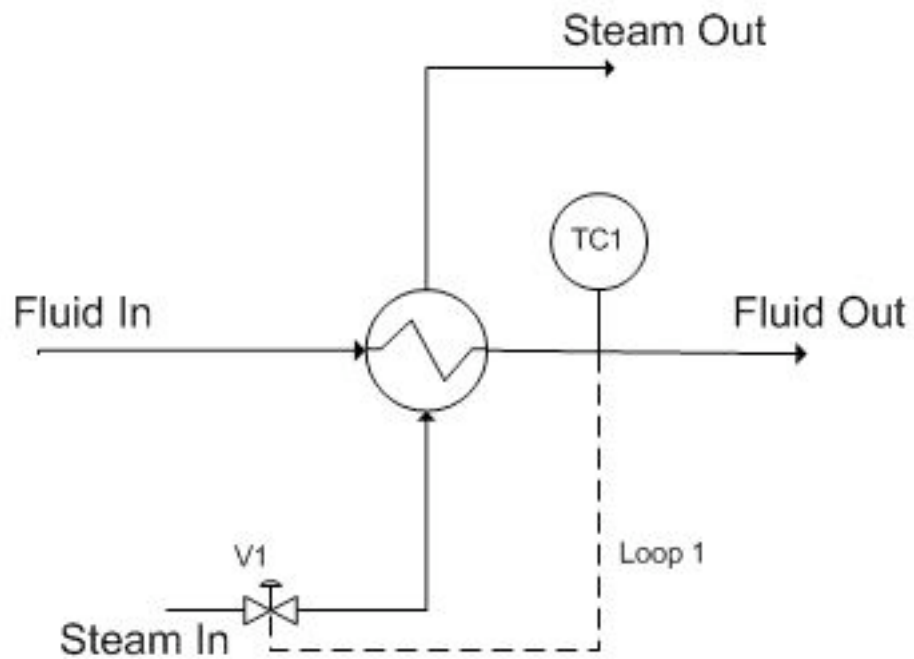


Figure 1. Single loop control for a heat exchanger

In the above process, the fluid is to be heated up to a certain temperature by the steam. This process is controlled by a temperature controller (TC1) which measures the temperature of the exiting fluid and then adjusts the valve (V1) to correct the amount of steam needed by the heat exchanger to maintain the specified temperature. Figure 2 shows the flow of information to and from the temperature controller.

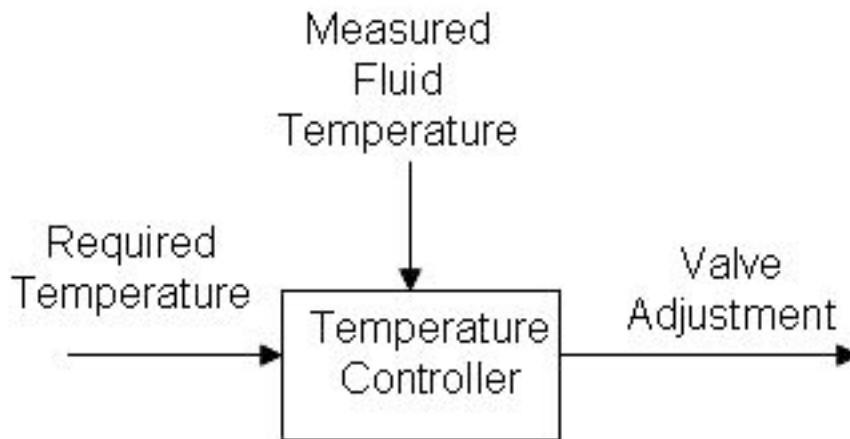


Figure 2. Flow of information when single loop feedback control is used for a heat exchanger

Initially, this process seems sufficient. However, the above control system works on the assumption that a constant flow of steam is available and that the steam to the heat exchanger is solely dependent on opening the valve to varying degrees. If the flow rate of the steam supply changes (i.e. pipeline leakage, clogging, drop in boiler power), the controller will not be aware of it. The controller opens the valve to the same degree expecting to get a certain flow rate of steam but will in fact be getting less than expected. The single loop control system will be unable to effectively maintain the fluid at the required temperature.

Implementing cascade control will allow us to correct for fluctuations in the flow rate of the steam going into the heat exchanger as an inner part of a grander scheme to control the temperature of the process fluid coming out of the heat exchanger. A basic cascade control uses two control loops; in the case presented below (see Figure 3), one loop (the outer loop, or master loop, or primary loop) consists of TC1 reading the fluid out temperature, comparing it to $TC1_{set}$ (which will not change in this example) and changing $FC1_{set}$ accordingly. The other loop (the inner loop, or slave loop, or secondary loop) consists of FC1 reading the steam flow, comparing it to $FC1_{set}$ (which is controlled by the outer loop as explained above), and changing the valve opening as necessary.

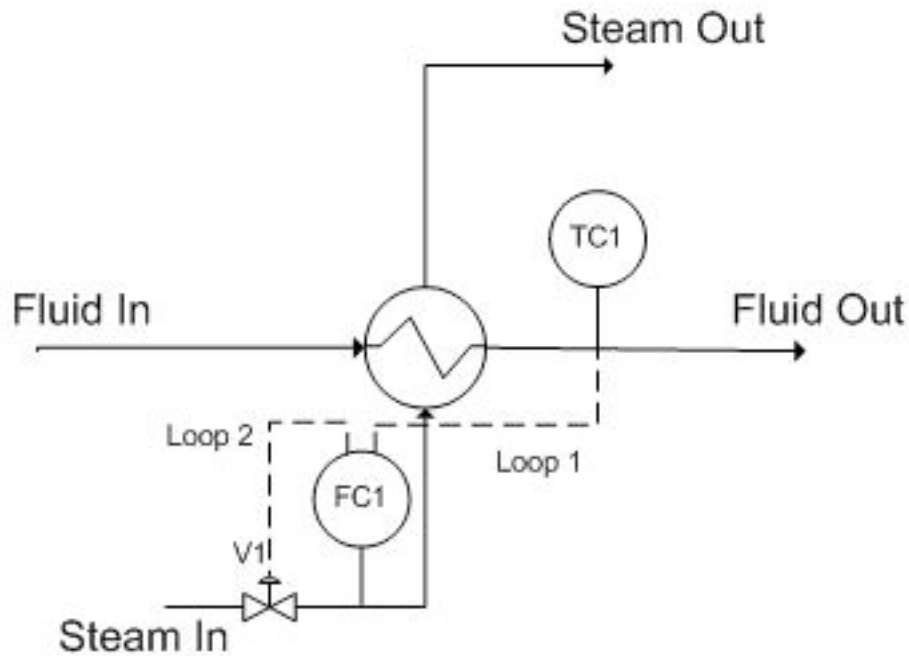


Figure 3. Cascade control for a heat exchanger

The main reason to use cascade control in this system is that the temperature has to be maintained at a specific value. The valve position does not directly affect the temperature (consider an upset in the stream input; the flow rate will be lower at the same valve setting). Thus, the **steam flow rate** is the variable that is required to maintain the process temperature.

The inner loop is chosen to be the inner loop because it is prone to higher frequency variation. The rationale behind this example is that the steam in flow can fluctuate, and if this happens, the flow measured by FC1 will change faster than the temperature measured by TC1, since it will take a finite amount of time for heat transfer to occur through the heat exchanger. Since the steam flow measured by FC1 changes at higher frequency, we chose this to be the inner loop. This way, FC1 can control the fluctuations in flow by opening and closing the valve, and TC1 can control the fluctuations in temperature by increasing or decreasing $FC1_{set}$.

Thus, the cascade control uses two inputs to control the valve and allows the system to adjust to both variable fluid flow and steam flow rates. The flow of information is shown in figure 4.

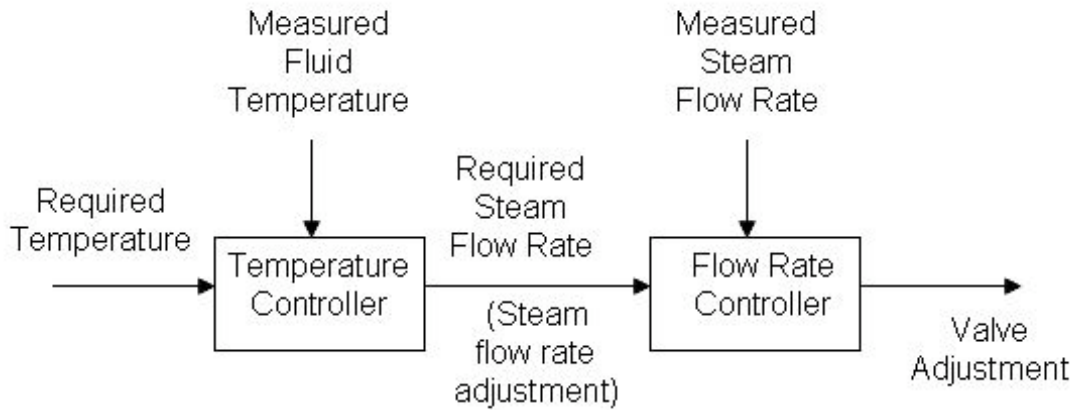


Figure 4. Flow of information when cascade control is used for a heat exchanger

In order to accomplish this, relationships between the primary and secondary loops (see definitions below) must be defined. Generally, the primary loop is a function of the secondary loop. A possible example of such relations is:

$$TC_1 = f(FC_1); \frac{d(TC_1)}{d(FC_1)} = \dots$$

$$FC_1 = f(V_1); \frac{d(FC_1)}{d(V_1)} = \dots$$

$$\frac{d(V_1)}{d(t)} = \dots$$

3.2.2 Primary and Secondary Loops

In Figure 3, there are two separate loops. Loop 1 is known as the primary loop, outer loop, or the master, whereas loop 2 is known as the secondary loop, inner loop, or the slave. To identify the primary and secondary loops, one must identify the control variable and the manipulated variable. In this case, the control variable is the temperature and the reference variable is the steam flow rate. Hence, the primary loop (loop 1) involves the control variable and the secondary loop (loop 2) involves the reference variable. The information flow for a two loop cascade control system will typically be as shown in Figure 5. Please note that the user sets the set point for loop 1 while the primary controller sets the set point for loop 2.

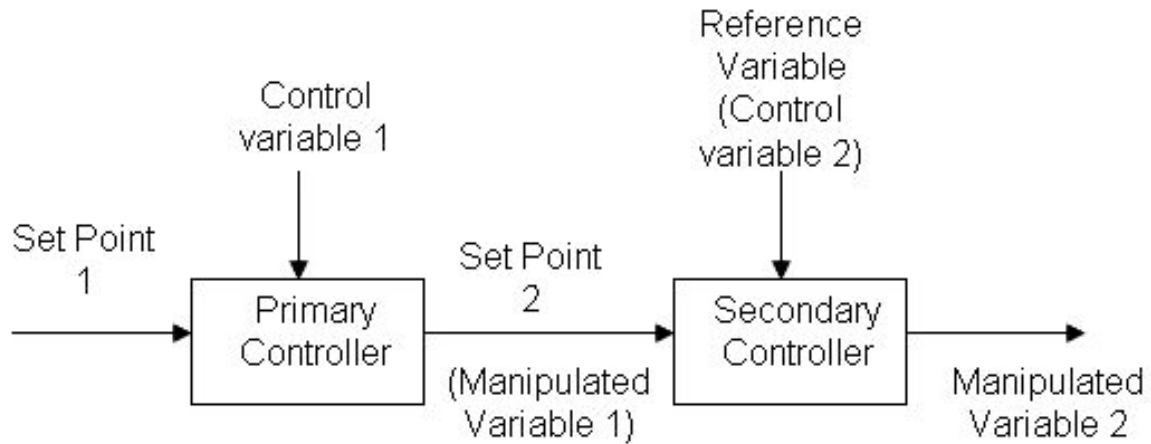
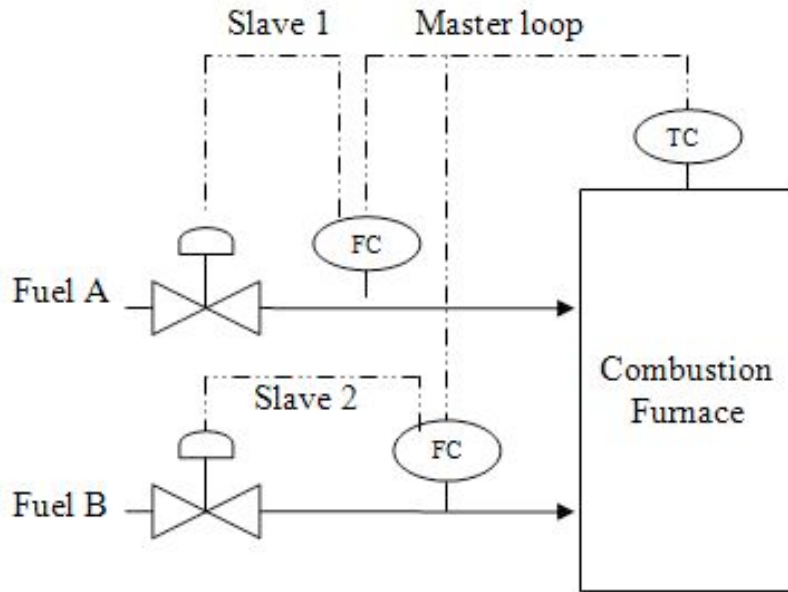


Figure 5: Information flow of a two loop cascade control

In addition to this common architecture, cascade control can have multiple secondary loops; however, there is still one primary loop and a main controlled variable. Unfortunately, with multiple inner loops, tuning the PID becomes even more challenging, making this type of cascade less common. The secondary loops can be either independent of each other, or dependent on each other, in which case each secondary loop affects the set point of the other secondary loop. When tuning such controller, the inner most loop should be tuned first. The loop that manipulates the set point of the inner-most loop should be tuned next and so for. The figure below shows an example of using two secondary loops, independent of each other, in a fuel combustion plant. In this combustion furnace, the master controller controls the temperature in the furnace by changing the set point for the flow of fuels A and B. The secondary loops correspond to the change in the set point for the flow, by opening or closing the valves for each fuel.

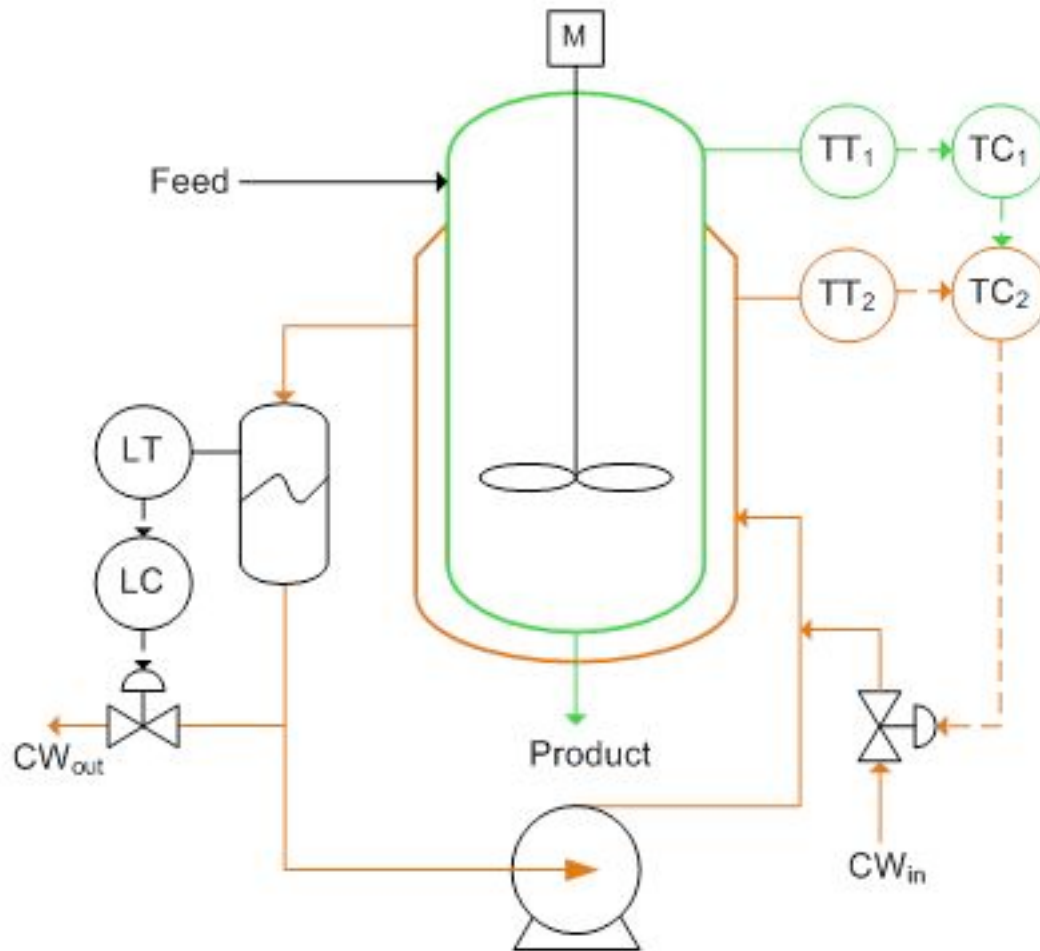


Cascade control is generally useful when

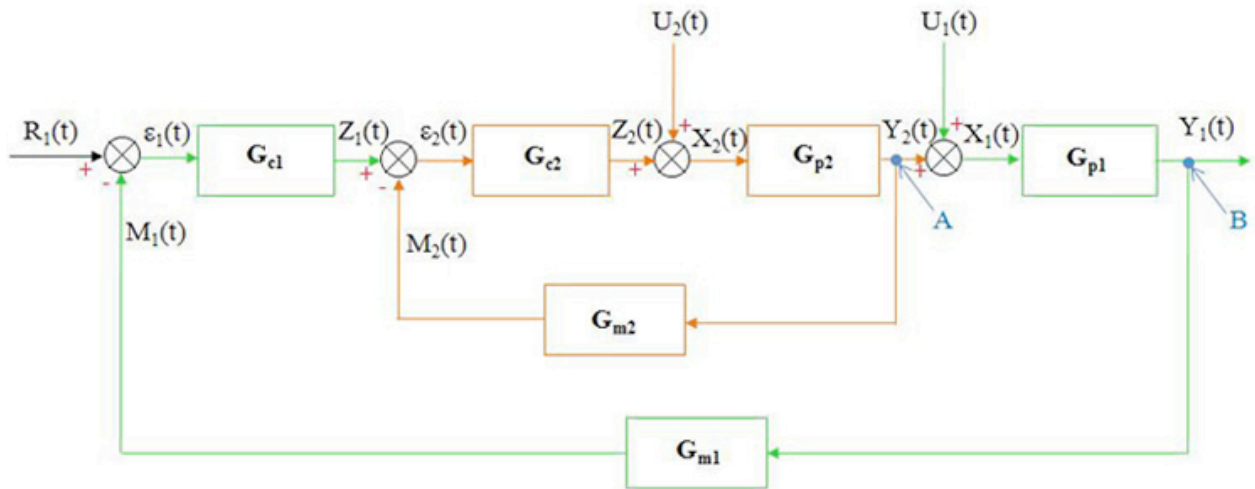
- A system error affects the primary control variable only after a long period of time as it propagates through [dead time](#) and lag time.
- A system has long dead times and long lag times.
- Multiple measurements with only one control variable are required for better response to a disturbance of a system.
- Variance occurs in multiple streams

3.3 General Cascade Control Schematic

The reactor below needs to be cooled during continuous-feed operation of an exothermic reaction. The reactor has been equipped with a cooling water jacket with the water flow rate being controlled by cold water valve. This valve is controlled by two separate temperature controllers. An “inner-loop” or “slave” (highlighted in orange) temperature transmitter communicates to the slave controller the measurement of the temperature of the jacket. The “outer-loop” or “master” (green) temperature controller uses a master temperature transmitter to measure the temperature of the product within the reactor. The output from the slave controller is fed into the master controller and used to adjust the cold water valve accordingly.



The cascade control loop used to control the reactor temperature can be generalized with the schematic below. We will use this main diagram to go through the formal derivation of the equations describing the behavior of the system when there are changes in the loads U_1 and U_2 but with no change in the set point, $R_1(t)$. The general equations derived below can be used to model any type of process (first, second, third order differential equations, ect.) and use any type of control mechanism (proportional-only, PI, PD, or PID control). See wiki pages titled “first-order differential equations” and “P, I, D, PI, PD, PID Control” for more details.



Step 1: Write down all the equations for each stage of the control loop

Master Loop

$$Y_1(t) = \hat{G}_{P1} X_1(t)$$

$$X_1(t) = U_1(t) + Y_2(t)$$

$$Z_1(t) = \hat{G}_{C1} \varepsilon_1(t)$$

$$\varepsilon_1(t) = R_1(t) - M_1(t)$$

$$M_1(t) = \hat{G}_{M1} Y_1(t)$$

Slave Loop

$$Y_2(t) = \hat{G}_{P2}X_2(t)$$

$$X_2(t) = U_2(t) + Z_2(t)$$

$$Z_2(t) = \hat{G}_{C2}\varepsilon_2(t)$$

$$\varepsilon_2(t) = Z_1(t) - M_2(t)$$

$$M_2(t) = \hat{G}_{M2}Y_2(t)$$

Gp1 and Gp2 are the process operators and are usually of the form:

$$\hat{G}_P^{-1} = \left(\tau_P \frac{d}{dt} + 1 \right)^n$$

Where n is a natural number.

Gc1 and Gc2 are the control operators and depend on the type of controller used. For PID controllers, they would be:

$$\hat{G}_C = K_C \left(1 + \frac{1}{\tau_I} \int_0^t dt' + \tau_D \frac{d}{dt} \right)$$

Gm1 and Gm2 are the measurement operators and usually are just equal to 1. Note that there are no equations for the "intersections" A and B shown on the diagram.

Step 2: Simplify the equations for the slave loop

$$Y_2(t) = \hat{G}_{P2}X_2(t)$$

$$Y_2(t) = \hat{G}_{P2}\{U_2(t) - Z_2(t)\}$$

$$Y_2(t) = \hat{G}_{P2}[U_2(t) - \hat{G}_{C2}\varepsilon_2(t)]$$

$$Y_2(t) = \hat{G}_{P2}[U_2(t) - \hat{G}_{C2}(Z_1(t) - M_2(t))]$$

$$Y_2(t) = \hat{G}_{P2}\left[U_2(t) - \hat{G}_{C2}\left(Z_1(t) - \hat{G}_{M2}Y_2(t)\right)\right]$$

Solve for Y2(t)

$$Y_2(t) = \left(\frac{\hat{G}_{P2}}{1 + \hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2}} U_2(t) + \frac{\hat{G}_{P2}\hat{G}_{C2}}{1 + \hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2}} Z_1(t) \right)$$

Step 3: Simplify the equations for the master loop

$$Y_1(t) = \hat{G}_{P1}X_1(t)$$

$$Y_1(t) = \hat{G}_{P1}\{U_1(t) + Y_2(t)\}$$

$$Y_1(t) = \hat{G}_{P1}\left[U_1(t) + \frac{\hat{G}_{P2}}{1 + \hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2}} U_2(t) + \frac{\hat{G}_{P2}\hat{G}_{C2}}{1 + \hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2}} Z_1(t)\right]$$

$$Y_1(t) = \hat{G}_{P1}\left[U_1(t) + \frac{\hat{G}_{P2}}{1 + \hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2}} U_2(t) + \frac{\hat{G}_{P2}\hat{G}_{C2}}{1 + \hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2}} \hat{G}_{C1}\varepsilon_1(t)\right]$$

$$Y_1(t) = \hat{G}_{P1}\left[U_1(t) + \frac{\hat{G}_{P2}}{1 + \hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2}} U_2(t) + \frac{\hat{G}_{P2}\hat{G}_{C2}}{1 + \hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2}} \hat{G}_{C1}(R_1(t) - M_1(t))\right]$$

$$Y_1(t) = \hat{G}_{P1}\left[U_1(t) + \frac{\hat{G}_{P2}}{1 + \hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2}} U_2(t) + \frac{\hat{G}_{P2}\hat{G}_{C2}}{1 + \hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2}} \hat{G}_{C1}(R_1(t) - \hat{G}_{M1}Y_1(t))\right]$$

Solve for $Y_1(t)$

$$Y_1 = \left(\frac{(\hat{G}_{P1} + \hat{G}_{P1}\hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2})U_1(t) + \hat{G}_{P1}\hat{G}_{P2}U_2(t) + \hat{G}_{P1}\hat{G}_{P2}\hat{G}_{C1}\hat{G}_{C2}R_1(t)}{1 + \hat{G}_{P2}\hat{G}_{C2}\hat{G}_{M2} + \hat{G}_{P1}\hat{G}_{P2}\hat{G}_{M1}\hat{G}_{C1}\hat{G}_{C2}} \right)$$

(Note: here the G's are written as operators rather than Laplace transforms, and as such they shouldn't be divided. Thus, expressions in the denominator should be interpreted as inverse operators in the numerator.)

3.4 Conditions for Cascade Control

In order to have a smooth flow of information throughout the control system, a hierarchy of information must be maintained. In a double loop cascade system, the action of the secondary loop on the process should be faster than that of the primary loop. This ensures that the changes made by the primary output will be reflected quickly in the process and observed when the primary control variable is next measured. This hierarchy of information can be preserved by applying the following conditions when setting up the cascade controls.

1. There must be a clear relationship between the measured variables of the primary and secondary loops.
2. The secondary loop must have influence over the primary loop.
3. Response period of the primary loop has to be at least 4 times larger than the response period of the secondary loop.
4. The major disturbance to the system should act in the primary loop.
5. The primary loop should be able to have a large gain, K_c .

Cascade control is best when the inner loop is controlling something that happens at fairly high frequency. Cascade control is designed to allow the master controller to respond to slow changes in the system, while the slave controller controls disturbances that happen quickly. If set up in reverse order, there will be a large propagation of error. Hence, it is important to maintain the hierarchy of information. In summary, the master controller responds to SLOW changes in the system, while the slave controller responds to the high frequency, or FAST changes in the system. This also requires that the inner control scheme be tuned TIGHTLY so error is not allowed to build. Commonly, the inner loops controls a flow controller, which will reduce the effect of changes such as fluctuations in steam pressure.

3.5 Cascade Control Design Considerations

Open Loop and Closed Loop

Although cascade control generally incorporates information from several secondary loops, the system overall does not automatically become a closed loop or an open loop

process. For a cascade control to be open loop, all control loops in the system should be open loop in nature. On the other hand, if any of the control loops in the system is feedback-based, the system overall is considered as closed loop. This is due to the fact that the system is getting some sort of feedback, no matter how little the “feedback” variable influences the system.

Cascade with Feed-Forward and Feedback Controls

Cascade controllers have a distinct advantage over other kinds of controller due to its ability to combine both feedback and feed-forward controls. While feed-forward loops have the potential to adjust the controlled variables to the ideal states, the feedback loops in a mixed system check deviations to make sure the system is on track. The figure below is an example of a mixed cascade control:

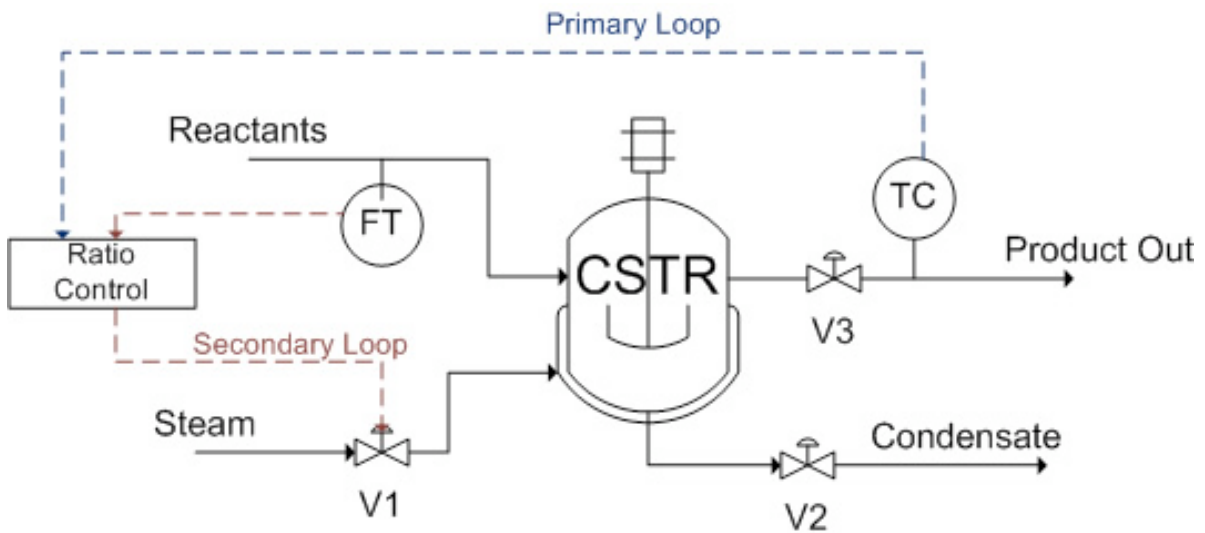


Figure 6. Cascade control with both feed-forward and feedback controls

An endothermic reaction takes place in a jacketed CSTR, in which the reactor is heated by steam. A reactant stream feeds into the CSTR, which serves as the wild stream for the ratio controller to predict a required steam flow rate (feed-forward). On the product stream side, a temperature controller manipulates the ratio setting of the ratio controller in order to minimize the product temperature errors (feedback). The temperature controller is the primary loop, whereas the ratio controller is the secondary loop.

3.6 Advantages and Disadvantages of Cascade Control

The following table shows a list of cascade control pros and cons:

Cascade Control Pros	Cacade control Cons
<ul style="list-style-type: none"> • Accounts for disturbances in the primary vairable more quickly and hence control the primary variable more effectively • Reduces the effects of dead time and phase lag time in the system • Can be combined with feed-forward control or other forms of control • Integrated multiple sensors readings • Improve dynamic performance and provide limits on the secondary variables 	<ul style="list-style-type: none"> • Cascade control makes the system more complex • Cascade control requires more equipment and instrument that will drive up the cost of the process • Tuning cascade controllers is more difficult as the set point changed + more parameters

3.7 Starting up a Cascade System

A cascade system needs to be set up properly in order to function. The inner loop should be tuned before the outer loop. The following are the suggested steps for starting up a cascade system (both controllers start in automatic mode):

1. Place the primary controller in manual mode. This will break the cascade and isolate the secondary controller so that it can be tuned.
2. Tune the secondary controller as if it were the only control loop present.
3. Return the secondary controller to the remote set point and/or place the primary controller in automatic mode. This will isolate the primary controller so that it can be tuned.
4. Tune the primary control loop by manipulating the set point to the secondary controller. If the system begins to oscillate when the primary controller is placed in automatic, reduce the primary controller gain.

Cascade control systems can be tuned using conventional methods. Ziegler-Nichols tuning method can be used to tune the secondary controller. Then the parameters (depending on the system, it can be P, PI, or PID) need to be fine tuned by introducing disturbances to the system and changing the parameters accordingly. The secondary controller must be tuned tightly (no oscillations when disturbance is added), otherwise the primary controller will be responding to oscillations due to the secondary controller as well as from disturbances to the system. This will cause the parameters for the primary controller to be inaccurate, which will cause a high controller effort. This is undesirable because it will wear down the controller. The primary controller often utilizes internal model control (IMC), which allows for improved performance by incorporating the process model into the controller setup. Another way to tune the primary controller is by using trial and error. For example, if the system has a PID primary controller, the integral

and derivative gains should be set at small values. Then a small proportional gain should be introduced. The proportional gain should be tuned first then the integral and derivative gains can be added. For more information about the trial and error method refer to [PID Tuning Classical](#) section.

3.7.1 Startup Example

A simple example of starting up a cascade system is shown using the heat exchange system seen in Figure 3. To begin startup the temperature controller (primary) is set to manual mode. The flow controller (secondary) is then tuned by adjusting the set point of the flow controller. This is shown in Figure 6 below.

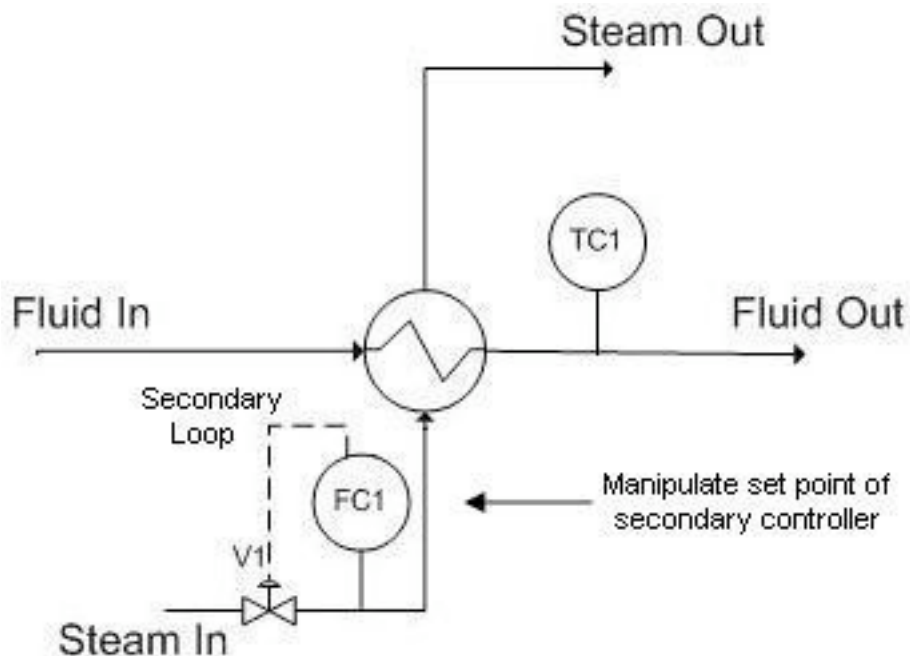


Figure 6: Automatic mode for secondary controller (manual mode for primary controller)

Now the temperature controller is set to automatic mode and the flow controller is set to manual mode. In this system the temperature controller outputs a set point to the flow controller just like it would in regular cascade mode. The temperature controller is then tuned by adjusting the output to the valve. This is shown in Figure 7 below.

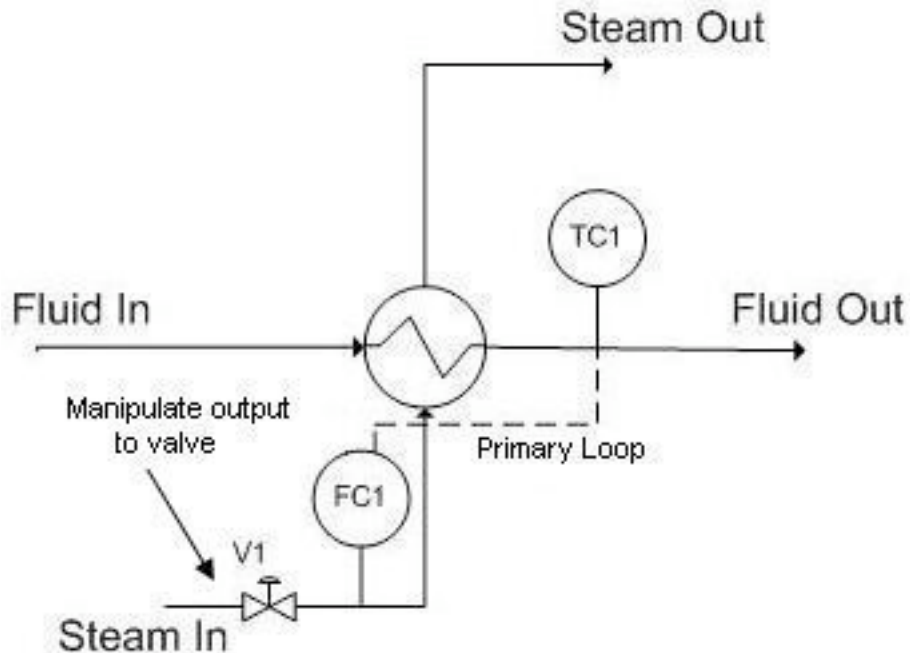


Figure 7: Manual mode for secondary controller (automatic mode for primary controller)

3.7.2 Developing the Structure of a Cascade Algorithm

Below is a step-by-step method through which the basic structure of a Cascade Algorithm can be developed. The examples in each step refer to Figure 3.

1 – **Determine the goal of your algorithm.** That is, which **ultimate output** you would like to ultimately end up changing. Also determine what **“tool”** (or aspect of the system) will most directly and physically allow you to accomplish this desired change.

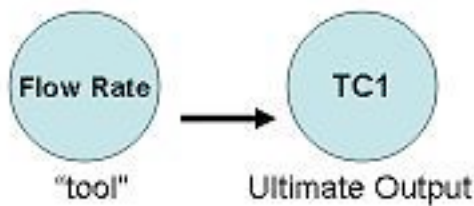
This “tool” can be any physical property of the system: temperature, pressure, surface area, flow regime, flow rate, etc. of any part of any physical component of the system. The “tool” doesn’t need to be something read by a sensor, though it can be (as it is in this example, the temperature of the heated fluid leaving the heat exchanger is read by sensor TC1).

For instance, the end goal of the process of Figure 3 is to regulate the temperature of the fluid leaving a heat exchanger. In this case, the only way to physically accomplish this is to change the flow rate of the steam through the heat exchanger (this flow rate just so happens to be read by the sensor FC1).



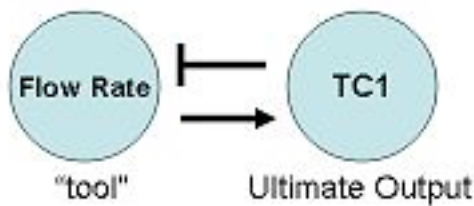
2 – Determine how the “tool” physically affects the ultimate output.

For instance, an **increased** flow rate of **steam** (read by FC1) will physically **increase** the **temperature** of the fluid leaving the heat exchanger, **TC1**.



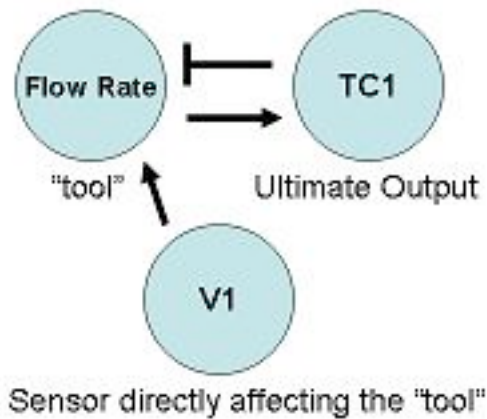
3 – Determine how the ultimate output needs to affect the “tool” to achieve the desired ultimate output change.

For instance, we presume that we would like to, in general, resist any change in TC1 (i.e. we don't want an increase in TC1 to further increase the value of TC1, that would be bad!). For this reason, we want an increase in TC1 to decrease FC1, which will then decrease TC1 (negative feedback).



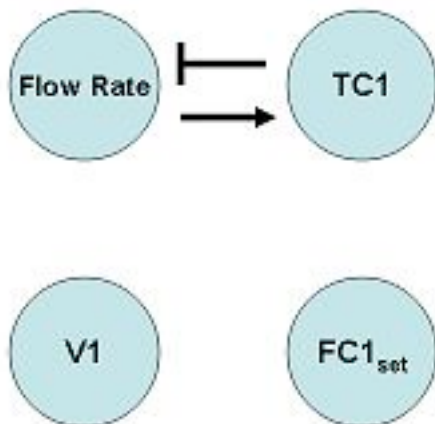
4 – Determine which valve or sensor’s output will *most* directly affect the “tool”. Also, determine how the sensor and “tool” are related.

For instance, the setting of valve V1 will most directly affect the flow rate of steam entering the heat exchanger (it is the "closest" controllable component of the process to the "tool", the steam flow rate). An increase in V1 will increase flow rate.

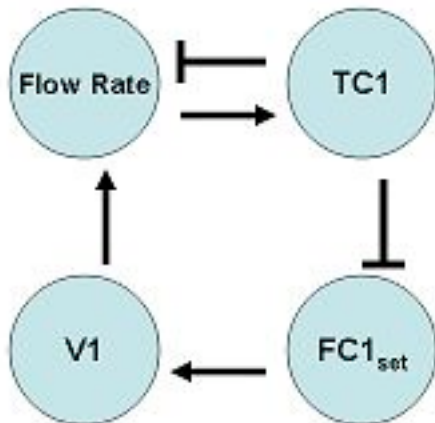


5 – **Determine all valves/sensors in between the ultimate output and valve/sensor that will directly affect the “tool”.**

For instance, between the ultimate output (TC1) and the valve (V1) that will directly affect the “tool”, there is only the FC1 sensor.



6 – **Make an incidence graph.** Make sure that you use the **set points** of the valves/sensors that directly affect the “tool”, because you cannot control what these sensors read (*you can only control their set points*). Confirm that the relationship between the “tool” and the ultimate output is consistent with the incidence graph!



7 – Use this incidence graph to **construct the algorithm**. The incidence graph is particularly helpful in determining what “sign” changes in one component should result in a the “sign” in another component. If we use incidence diagrams, and the equations for the cascade controller, we can determine a relationship between the components of the system.

For instance, if TC1 were to increase, we would want the steam flow rate to decrease, which ultimately results in a decreased temperature. An increase (a “sign” of +) in TC1 should result in a decrease in FC1_{set} (a “sign” of -). This can be seen from equation 2, where if TC1_{set} decreases, the difference between TC1_{set} and TC1 will be smaller. This causes FC1_{set} to decrease relative to its previous set point. A decrease (a “sign” of -) in FC1_{set} should result in a decrease in V1 (a “sign” of -). This is shown by equation 1, where if FC1_{set} decreases while FC1 is the same, V1 will decrease relative to its previous position. A decrease (a “sign” of -) in V1 should result in a decreased flow rate (a “sign” of -). A decrease (a “sign” of -) in steam flow rate should result in a decreased TC1 (a “sign” of -), completing the negative-feedback mechanism initially desired.

$$V_1 = V_{1,Offset} + K_{c,FC1}(FC1_{set} - FC1) + \frac{1}{\tau_{i,FC1}} \int (FC1_{set} - FC1) dt + \tau_{d,FC1} \frac{d(FC1_{set} - FC1)}{dt} \quad (1)$$

$$FC1_{set} = FC1_{Offset} + K_{c,TC1}(TC1_{set} - TC1) + \frac{1}{\tau_{i,TC1}} \int (TC1_{set} - TC1) dt + \tau_{d,TC1} \frac{d(TC1_{set} - TC1)}{dt} \quad (2)$$

3.8 Failure

A cascade system is not to be confused with a fail-safe system. The sole purpose of implementing a cascade control system is to make the system more responsive, **not** more robust.

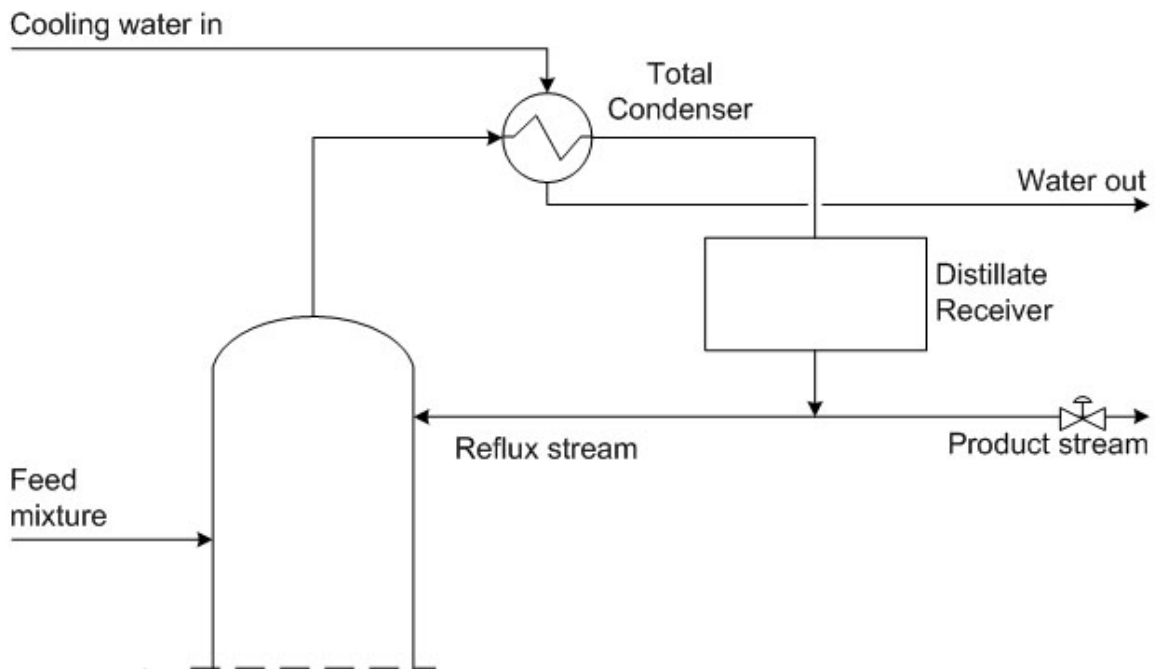
In a cascade system, if the master controller fails, the entire system will fail too. Just like for any other design, one should anticipate failure and build in redundancy. An example of redundancy could be having multiple controllers to be the master controller and then using selectors to choose which reading to use.

Alternatively, if the cascade system fails and has no built-in redundancy, there are a couple of ways to keep the cascade system running while the controller is being repaired. For example, the controller can be operated manually by an employee, or an average of previous readings can be used to temporarily send a constant signal to the system.

3.9 Worked out Example 1

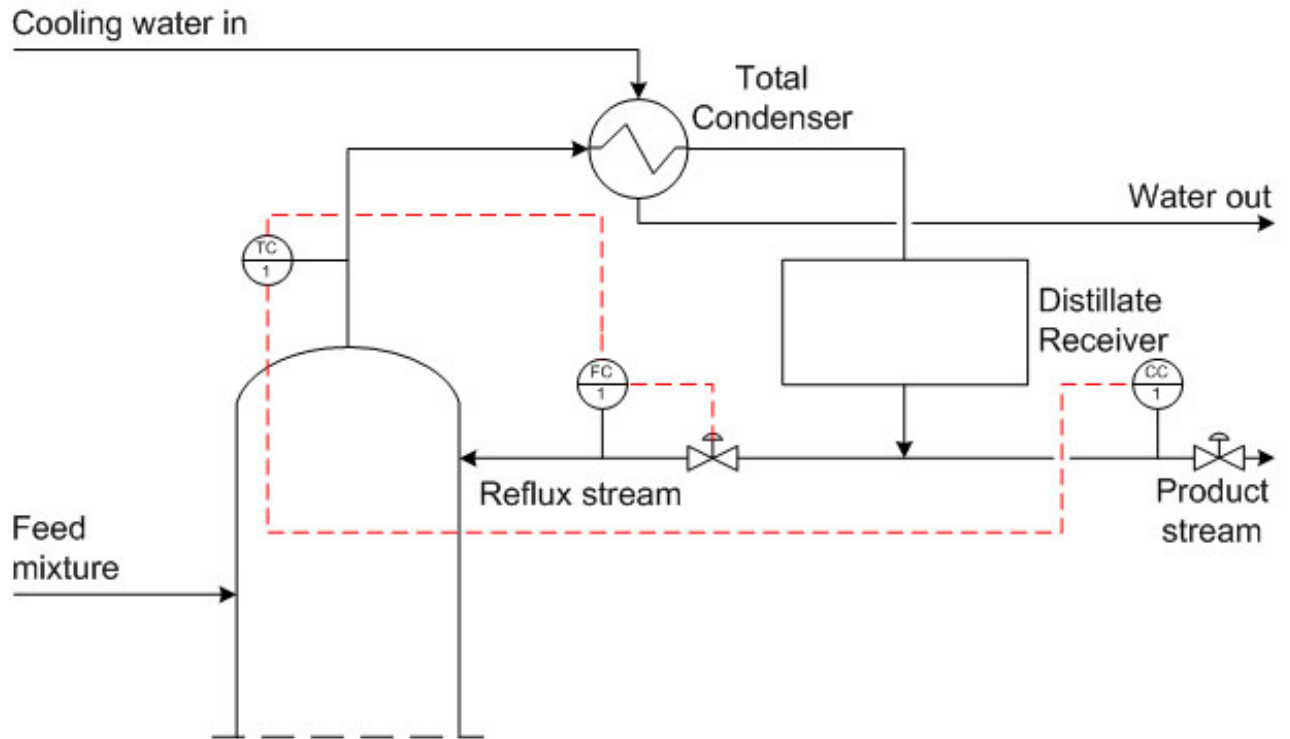
The diagram below shows the top portion of a distillation column used to separate the components of the inlet liquid mixture. Reflux is used for the column to improve the separation efficiency, as the desired product stream must have a mass fraction of component C that is greater than 0.8. At the top of the distillation column the temperature is 200°C. Components A, B, and C, which are gases at that temperature, accumulate and flow out of the top of the distillation column through the total condenser. The total condenser cools the gas stream to 150°C, causing A, B, and C to liquefy. The liquid mixture is collected in a distillate receiver. Finally, the liquid stream exits the receiver and is either collected as product or sent back to the column. A control valve is in place on the product stream to ensure that the necessary purity is attained.

On the diagram, draw the necessary controllers and valves required to implement a cascade control for the exiting stream. Also, describe the cascade control that you have implemented.



Note that this is only one possible solution to the example question. Alternatives to this solution would be to only use a composition controller with a flow controller or a temperature controller but the below solution was chosen to give an example of a multiple cascade control.

3.9.1 Solution



The system can most effectively be controlled with a cascade scheme. A composition controller can be installed to control the composition of the product stream. However, the composition controllers are typically slow to react since it takes time to analyze the samples to obtain compositions. In order to correct for the time lag of the composition controller, a temperature controller, located at the top of the distillation column, measures the temperature of the product stream giving a rough idea of the product composition. Additionally, a flow controller is needed on the reflux stream.

The input from the composition controller measures the composition of the product stream and sends a signal to the temperature controller at the top of the column. The temperature controller compares the set point to the measured temperature of the stream and outputs a signal to the flow controller on the recycle stream. The flow controller compares this set point to the measured flow rate and adjust the control valve on the recycle stream accordingly. This cascade control allows the system to react to disturbances quickly and to more effectively control the reflux process.

3.10 Worked out Example 2

You just graduated from the University of Michigan and escaped the cold winter of Ann Arbor for a sweet full-time position in Orange County. Your company manufactures a specialty drug to cure an epidemic in the penguin population in Antarctica.

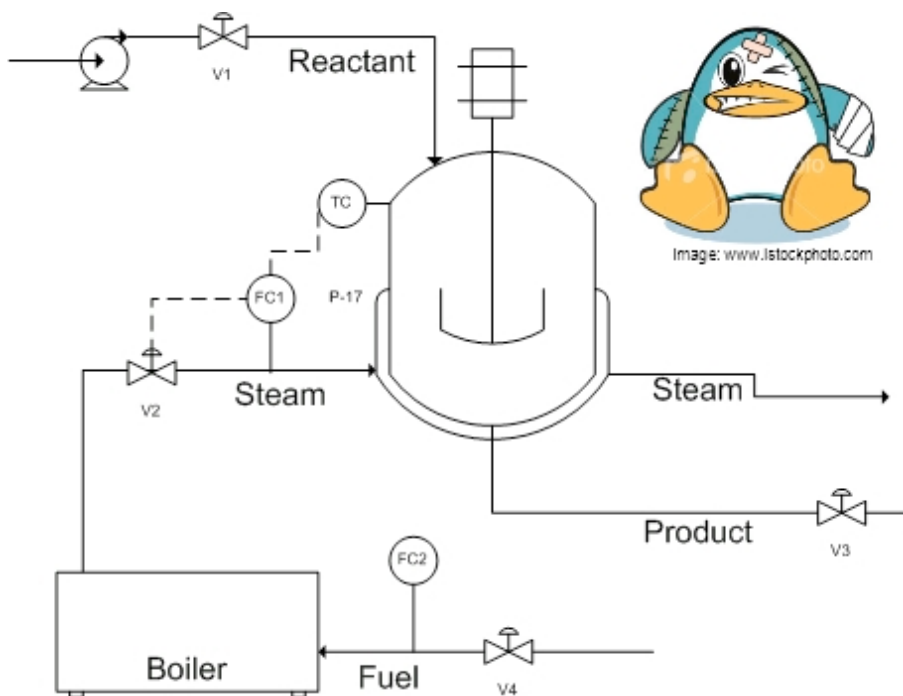
The endothermic reaction $A + B \rightarrow C$ is run in a CSTR. A and B are toxic in even dilute concentrations. Therefore, a conversion above 99.95% has to be maintained in order to ensure the safety of the process output.

Steam from a boiler is utilized to maintain the optimum reaction temperature of 100C. A PID cascade control scheme is used to maintain this temperature.

This morning, your plant manager came to you with a problem. He explained that production has been delayed because the conversion dropped below the acceptable level. He noticed that the reactor temperature was well below 100C, even though the steam valve (V2) is open completely.

As can be seen in the diagram below, a cascade control is already present in the system, but it isn't set up properly. Can you fix the problem and save the penguins?

Hint: The boiler also supplies steam to other equipment. You can increase its steam output by adding more fuel to the boiler (assume that water supply is unlimited).



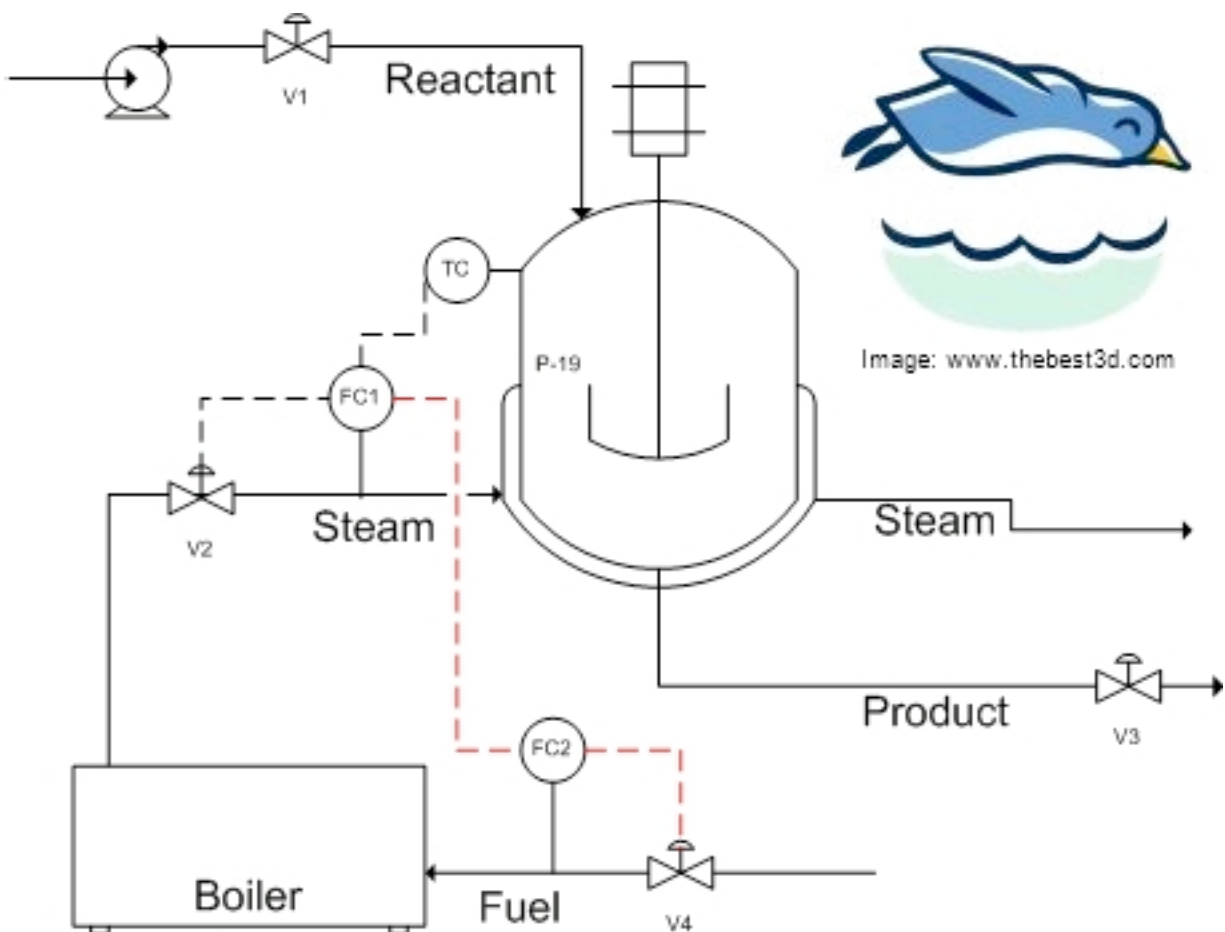
3.10.1 Solution

Before: TC is cascaded with FC1, which controls V2. (TC-->FC1-->V2) Even when V2 is open all the way, there is not enough steam to maintain the reaction at optimum temperature.

In this situation the controller surpasses the saturation limit of the actuator (V2). In other words, the controller is demanding more steam from the boiler than it can supply. A likely cause of this is a disturbance in the steam supply from the boiler because of increased steam demand from other processes. A possible solution is to increase the steam output from the boiler by adding more fuel (controlled by FC2 and V4). A side effect of this control situation would be that the I- part of a PID controller would also windup, preventing the system from responding.

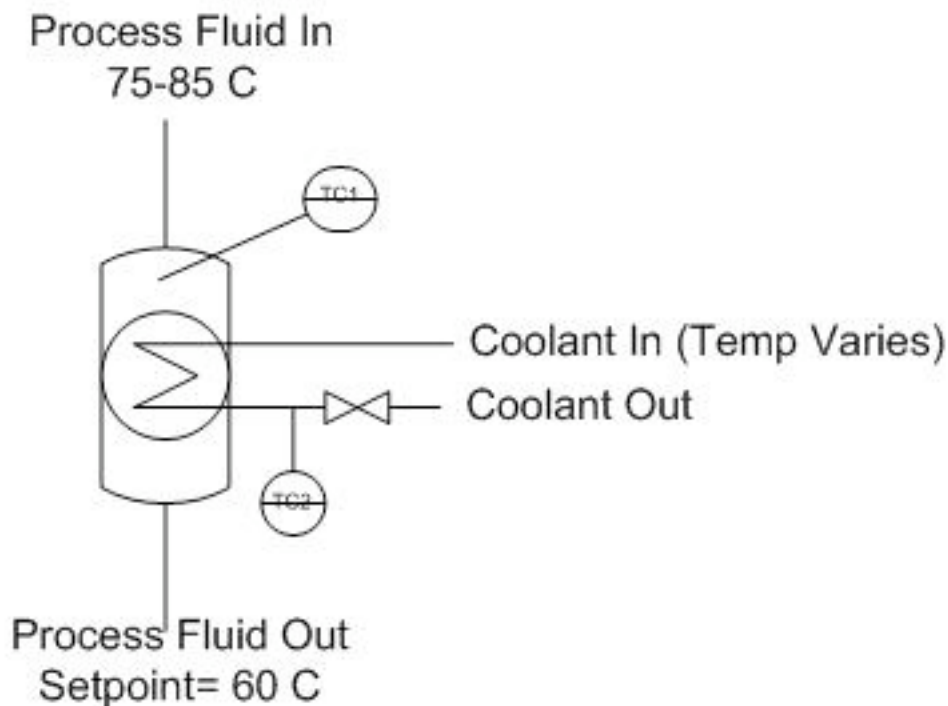
An additional control loop can be added to enable the boiler output to communicate with the fuel input. In addition to controlling V2, FC1 also controls FC2, which in turn will control V4. This additional controller is shown in the figure below.

Congratulations, you just saved the penguins!



3.11 Worked Out Example 3

You have a holding tank for a warm process fluid that is cooled by a water-filled jacket. The process stream enters at 75-85 C and should be cooled to 60 C. The temperature of the cooling water also varies, since it comes from another process, but its average temperature is about 29 C. You have thermocouples inside the holding tank and on the cooling water jacket exit stream. Unfortunately, the tank is not well mixed, so the thermocouple reading inside the tank lags behind the actual temperature of the outlet stream. When the cooling jacket is first turned on, the tank contents are initially at 70 C. Examine the dynamics of a feedback control stream versus a cascade control scheme for this system.



3.11.1 Solution

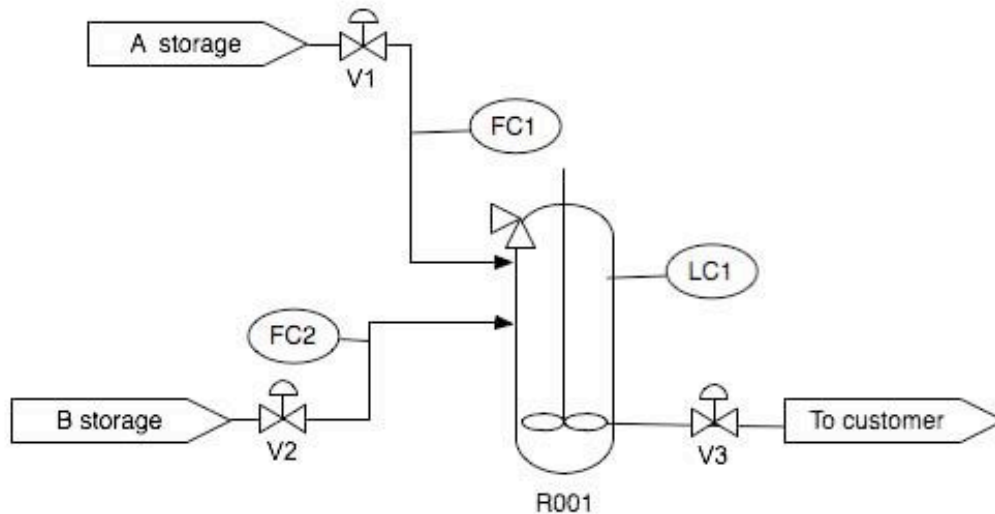
One setup for this system is given in the following Excel file: [Media:Cascade.xls](#)

Under the feedback control scheme, the flow rate of coolant is adjusted based on the temperature inside the holding tank. The system overshoots setpoints more significantly, because of the lag time before disturbances are recognized.

In cascade control, the temperature sensor in the process fluid outputs a setpoint for the jacket outlet (based on a knowledge of the process fluid setpoint and the average temperature of the cooling fluid). The signal from the temperature controller on the jacket outlet controls the flow rate of cooling fluid. Since the temperature in the cooling fluid has a shorter time lag, the process remains closer to its setpoint.

3.12 Worked Out Example 4

We have a P&ID as shown below. Write out the equations necessary to connect LC1 to FC1 to adjust v1. Which equation is the slave and which one is the master?



3.12.1 Solution

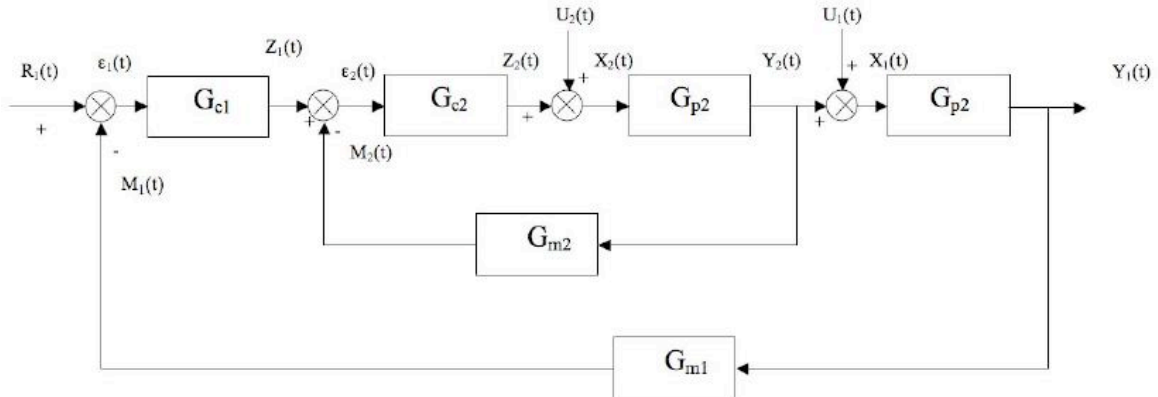
The first equation is the slave and the second equation is the master. We have to use the $FC1_{set}$ to determine what V_1 should be set as. And these are both based on the level in the tank.

$$V_1 = V_{1,offset} + K_c2(FC1_{set} - FC1) + \frac{1}{\tau_{I1}} \int (FC1_{set} - FC1) dt + \tau_{D1} \frac{d(FC1_{set} - FC1)}{dt} \quad (1)$$

$$FC1_{set} = FC1_{offset} + K_c1(LC1_{set} - LC1) + \frac{1}{\tau_{I2}} \int (LC1_{set} - LC1) dt + \tau_{D2} \frac{d(LC1_{set} - LC1)}{dt} \quad (2)$$

3.13 Worked Out Example 5

Write the general equation that describes the behavior of the cascade control system shown below. Include changes in U_1 and U_2 .



Hint: Start by writing the inner loop and outer loop equations separately.

3.13.1 Solution

For inner cycle:

$$\varepsilon_1 = Z_1 + G_{M2}Y_2$$

$$Z_2 = Z_1G_{C2} - Y_2G_{C2}G_{M2}$$

$$X_2 = U_2 + Z_2 = U_2 + Z_1G_{C2} - Y_2G_{C2}G_{M2}$$

$$Y_2 = G_{P2}X_2 = U_2G_{P2} + Z_1G_{C2}G_{P2} - Y_2G_{C2}G_{M2}G_{P2}$$

$$Y_2 = \frac{U_2G_{P2}}{1 + G_{C2}G_{M2}G_{P2}} + \frac{G_{C2}G_{P2}}{1 + G_{C2}G_{M2}G_{P2}}Z_1$$

For outer cycle:

$$Z_1 = R_1 G_{C1} - Y_1 G_{M1} G_{C1}$$

$$Y_1 = U_1 G_{P1} + Y_2 G_{P1}$$

Combining Z_1 from outer cycle with Y_2 from inner cycle:

$$Y_2 = \frac{U_2 G_{P2}}{1 + G_{C2} G_{M2} G_{P2}} + \frac{R_1 G_{C1} G_{C2} G_{P2}}{1 + G_{C2} G_{M2} G_{P2}} - \frac{Y_1 G_{C1} G_{C2} G_{M1} G_{P2}}{1 + G_{C2} G_{M2} G_{P2}}$$

Combining Y_2 above with Y_1 from outer cycle:

$$Y_1 = U_1 G_{P1} + \frac{U_2 G_{P1} G_{P2}}{1 + G_{C2} G_{M2} G_{P2}} + \frac{R_1 G_{C1} G_{C2} G_{P1} G_{P2}}{1 + G_{C2} G_{M2} G_{P2}} - Y_1 \frac{G_{C1} G_{C2} G_{M1} G_{P1} G_{P2}}{1 + G_{C2} G_{M2} G_{P2}}$$

Rearranging and solving explicitly for Y_1 :

$$Y_1 = \frac{U_1 G_{P1} + U_1 G_{C2} G_{M2} G_{P1} G_{P2} + U_2 G_{P1} G_{P2} + R_1 G_{C1} G_{C2} G_{P1} G_{P2}}{1 + G_{C2} G_{M2} G_{P2} + G_{C1} G_{C2} G_{M1} G_{P1} G_{P2}}$$

3.14 Practice Quiz

Answer the five questions below with the most appropriate solution. There is one correct answer for each question. Correct answers are awarded 4 points, whereas a loss of 2 points occurs for incorrect answers. Good luck!

1. Which of the following is never true in a process controlled by a cascade control scheme?

- a) Changes in the secondary control variable affect the primary measured variable.
- b) Disturbances in the secondary loops propagate at least four times faster than disturbances in the primary loop.
- c) One control variable is used to influence the primary and secondary measured

variables.

d) Major disturbances in the process are detected in the primary loop.

2. Which of the following is not an advantage of cascade control?

a) The system reacts to disturbances more quickly.

b) More efficient control of the primary variable.

c) It is a cheap control scheme to implement.

d) The effects of dead time and phase lag time are reduced in the system.

3. True or False: During start-up of a cascade control system, after the primary and secondary controllers are turned and placed in automatic mode, the primary controller gain should be increased to reduce system oscillations.

4. The primary loop, or outer loop, involves which of the following variables?

a) Control variable

b) Temperature variable

c) Reference variable

d) I love penguins (variable)

5. True or False: The primary loop is generally a function of the secondary loop.

3.14.1 Answers

Based on your selections, calculate your score on this quiz.

1. C- Cascade control schemes use multiple control variables for one manipulated variable.

2. C- Increased amounts of equipment and instrumentation may drive up the cost of the process.

3. False- The controller gain (K_c) should be reduced to reduce system oscillations

4. A- The best answer is (a) since the control variable may or may not be temperature. The reference variable is involved in the secondary loop. Penguins are really cute.

5. True- The output of the primary controller is the set point for the secondary controller. The output of the secondary controller adjusts the control variable.

3.14.2 Scoring

If you got...

20 points: CONGRATULATIONS! You are a cascade genius!

13-19 points: Make a list of confusing topics and bring your questions to a cascade control sage.

0-12 points: You may want to re-read this article and try again...

-10 points: Choose a new major. You may be better off in LS&A.

3.15 Sage's Corner

An example of the use of cascade control architecture and troubleshooting this control system:

<http://video.google.com/googleplayer.swf?docId=-1187011704040411738>

This is a link to the unnarrated PowerPoint slides.

[File:Cascade Control Unnarrated.ppt](#)

An example of the implementation of a cascade control system to solve a process issue.

<http://video.google.com/googleplayer.swf?docId=697386144658402357>


Unnarrated slides can be found below. [File:Cascade-](#)

[Control-1.ppt](#)

3.16 References

- Astrom, Karl J. and Haggund, Torr. "Advanced PID Control" The Instrumentation, Systems and Automation Society.
- Bequette, B. Wayne *Process Dynamics: Modeling, Analysis, and Simulation* Prentice- Hall PTR, Upper Saddle River, NJ 07458 (c) 2006.
- Mahoney, D.P., Svrcek, W.Y., and Young, B.R. (2006) *A Real-Time Approach to Process Control*, 2nd Edition. John Wiley & Sons, Ltd. [ISBN 0470025336](#)
- Industrial Controller: basic theory. Retrieved from <http://www.sapiensman.com/control/index.htm>. Last accessed on 12/12/2008

Section 4. Ratio control: What is it? When useful? When not? Common usage.

Note:  [Video lecture](#) available for this section!

Authors: Stephanie Fraley, Michael Oom, Benjamin Terrien, John Zalewski

Date Presented: October 31, 2006; Revised: November 20, 2006

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

4.1 Introduction

Ratio control architecture is used to maintain the relationship between two variables to control a third variable. Perhaps a more direct description in the context of this class is this: Ratio control architecture is used to maintain the flow rate of one (dependent *controlled feed*) stream in a process at a defined or specified proportion relative to that of another (independent *wild feed stream*) (3) in order to control the composition of a resultant mixture.

As hinted in the definition above, ratio control architectures are most commonly used to combine two feed streams to produce a mixed flow of a desired composition or physical property downstream (3). Ratio controllers can also control more than two streams. Theoretically, an infinite number of streams can be controlled by the ratio controller, as long as there is one controlled feed stream. In this way, the ratio control architecture is feedforward in nature. In this context, the ratio control architecture involves the use of an independent *wild feed stream* and a dependent stream called the *controlled feed*.

Ratio Control is the most elementary form of feed forward control. These control systems are almost exclusively applied to flow rate controls. There are many common usages of ratio controls in the context of chemical engineering. They are frequently used to control the flows on chemical reactors. In these cases, they keep the ratio of reactants entering a reaction vessel in correct proportions in order to keep the reaction conditions ideal. They are also frequently used for large scale dilutions.

4.2 Ratio Control based upon Error of a Variable Ratio

The first type of ratio control architecture uses the error of a variable ratio (R_{actual}) from a set ratio (R_{set}) to manipulate y (the *controlled stream*). R_{actual} is a ratio of the two variables *wild stream* and *controlled stream*. The controller adjusts the flow rate of stream y (*controlled stream*) in a manner appropriate for the error ($R_{actual} - R_{set}$).

The error in this system would be represented using the following equation:

$$\frac{y}{y_w} = R_{actual} \quad \text{or} \quad \frac{y_w}{y} = R_{actual}$$

$$\mathbf{Error} = R_{actual} - R_{set}$$

This error would be input to your general equation for your P, PI, or PID controller as shown below.

$$V_y = Offset + K_c(Error) + \frac{1}{\tau_I} \int (Error) dt + \tau_D \frac{d(Error)}{dt}$$

NOTE: V_y is used instead of y , because y is not directly adjustable. The only way to adjust y is to adjust the valve (V) that affects y .

4.2.1 Diagram of Ratio Dependant System

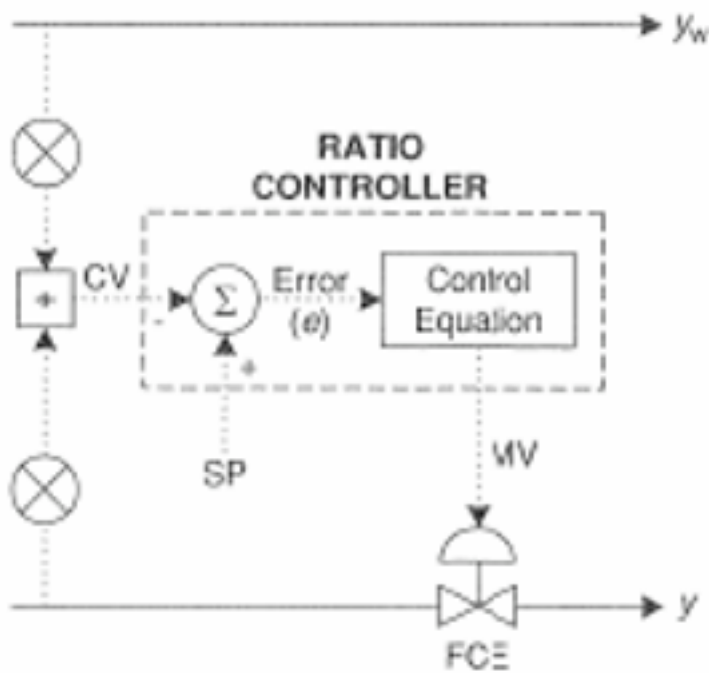


Image taken from Svreck et al.

4.3 Ratio Control based upon Error of the Controlled Stream

The second type of ratio control architecture uses the error of a setpoint (y_{set} , setpoint of the control variable) from y (controlled variable) to control, once again, y . The controller adjusts the flow rate of stream y in a manner appropriate for the error ($y - y_{set}$).

The error in this system would be represented using the following equation:

$$y_w R_{set} = y_{set} \quad \text{or} \quad \frac{y_w}{R_{set}} = y_{set}$$

$$\mathbf{Error} = y - y_{set}$$

This error would be input to your general equation for your P, PI, or PID controller as shown below.

$$V_y = \text{Offset} + K_C(\text{Error}) + \frac{1}{\tau_I} \int (\text{Error}) dt + \tau_D \frac{d(\text{Error})}{dt}$$

4.3.1 Diagram of Flowrate Dependant System

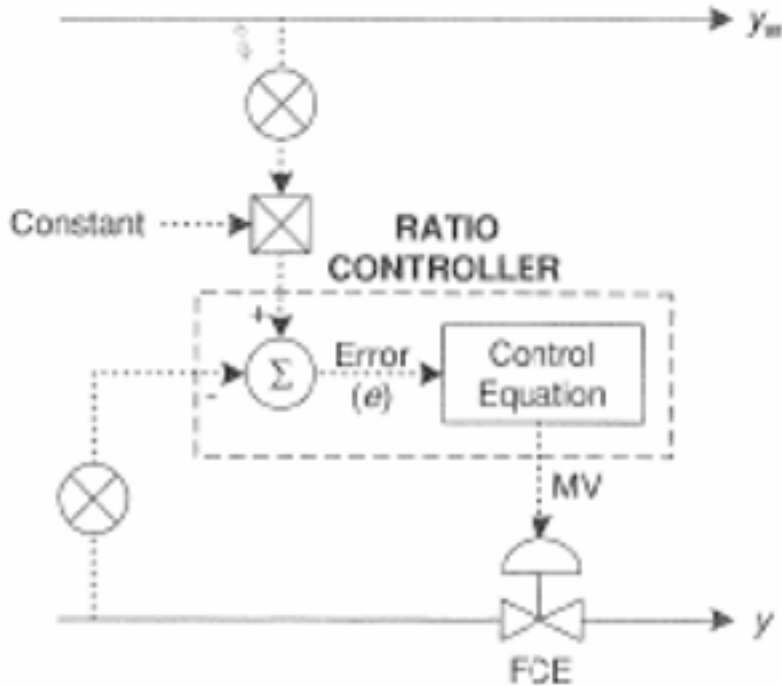


Image taken from Svreck et al.

4.4 Comparing the Two Types of Ratio Control

The main difference between the two aforementioned types of ratio control architecture is that they respond to changes in the monitored variable (R_{actual} or y - the variables through which the error is determined) differently.

The first method mentioned that defines error as $R_{actual} - R_{set}$ (monitored variable of R_{actual}) responds sluggishly when y is relatively large and too quickly when y is relatively small. This is best explained by examining the equations below.

$$R = \frac{y_w}{y} \longrightarrow \frac{\partial(R)}{\partial(y_w)} = \frac{1}{y}$$

$$R = \frac{y}{y_w} \longrightarrow \frac{\partial(R)}{\partial(y_w)} = -\frac{y}{y_w^2}$$

Unlike the first method, the second method mentioned that defines error as $y - y_{set}$ (monitored variable of y) does not respond differently depending upon the relative amounts of y (or anything else, for that matter). This is best explained by examining the equations below.

$$y = y_w R_{set} \longrightarrow \frac{\partial(y)}{\partial(y_w)} = R_{set}$$

$$y = \frac{y_w}{R_{set}} \longrightarrow \frac{\partial(y)}{\partial(y_w)} = \frac{1}{R_{set}}$$

4.5 Difficulties with Ratio Controllers

4.5.1 Steady State Issues

A common difficulty encountered with ratio controllers occurs when the system is not at steady state. Unsteady state conditions can cause a delay in the adjustment of the manipulated flow rate and thus the desired state of the system cannot be met.

Blend Stations

To overcome the difficulty with steady state, a Blend station can be used, which takes into account both the set ratio and the wild stream. As can be seen by the diagram below, the Blend station takes in the wild stream flow rate, the set ratio, and the initial set point for the wild stream (r_1) as inputs. Using a weighting factor, called gain, the Blend station determines a new set point for the manipulated stream (r_2). The relationship that determines this new set point can be seen below.

$$r_2 = \text{set ratio}[\gamma * r_1 + (1 - \gamma)y_w]$$

Where γ is the gain factor.

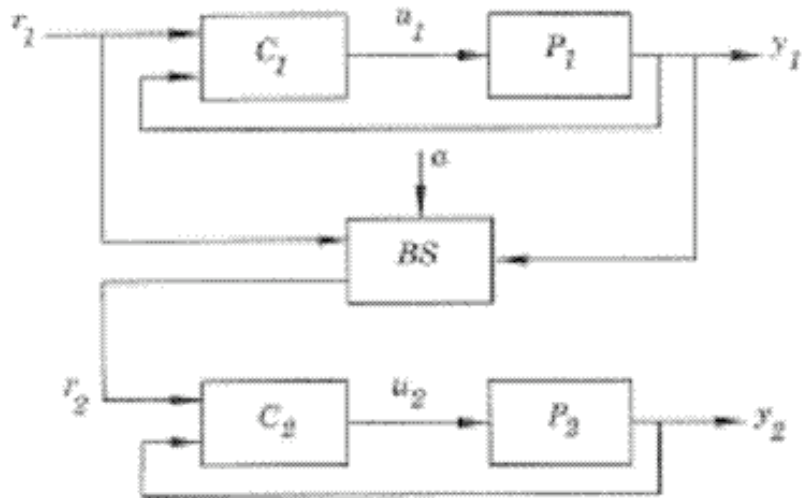


Figure 12.18 Ratio control using the Blend station (BS).

Image taken from Astrom and Hagglund article on "Advanced PID Control."

4.5.2 Accuracy Issues

Another problem (which is an issue with all "feed-forward" controllers) is that the variable under control (mix ratio) is not directly measured. This requires a highly accurate characterization of the controlled stream's valves so that the desired flow rate is actually matched.

One way to address this problem is to use two levels of PID control (Cascade Control). The first level monitors the controlled streams flow rate and adjusts it to the desired set point with a valve. The outer level of control monitors the wild stream's flow rate which adjusts the set point of the controlled stream by multiplying by the desired ratio. For example, if stream A's flow rate is measured as 7 gpm, and the desired ratio of A:B is 2, then the outer level of control will adjust B's set point to 3.5. Then the inner level of control will monitor B's flow rate until it achieves a flow rate of 3.5.

4.6 Ratio Control Schemes

The following subsections introduce three ratio controller schematics. Each schematic illustrates different ways that the controlled feed stream can be manipulated to account for the varying wild feed stream.

4.6.1 Ratio Relay Controller

The wild feed flow rate is received by the ratio relay and then multiplied by the desired mix ratio. The ratio relay outputs the calculated controlled feed flow rate which is compared to the actually flow rate of the controlled feed stream. The flow controller then adjusts the controlled feed flow rate so that it matches the set point (3).

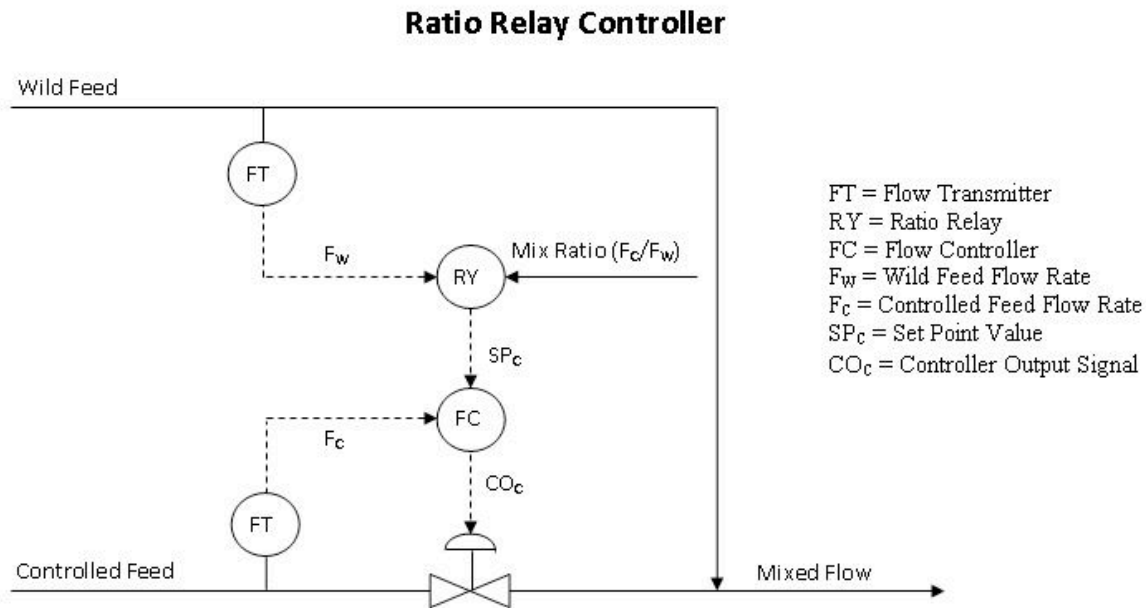


Image adapted from Houtz, Allen and Cooper, Doug "The Ratio Control Architecture"

The mix ratio (F_c/F_w) is not easy to access, so it requires a high level of authorization to change. This higher level of security may be an advantage so that only permitted people can change the mix ratio and decrease the chance that an accidental error occurs. A disadvantage is that if the mix ratio does need to be changed quickly, operation may be shut down while waiting for the appropriate person to change it.

Another disadvantage is that linear flow signals are required. The output signals from the flow transmitters, F_w and F_c , must change linearly with a change in flow rate. Turbine flow meters provide signals that change linearly with flow rates. However, some flow meters like orifice meters require additional computations to achieve a linear relationship between the flow rate and signal.

4.6.2 Flow Fraction Controller

Flow fraction and ratio relay controllers are very similar except that the flow fraction controller has the advantage of being a single-input single-output controller. A flow fraction controller receives the wild feed and controlled feed flow rates directly. The desired ratio of the controlled feed to wild feed is a preconfigured option in modern computer control systems (3).

Flow Fraction Controller

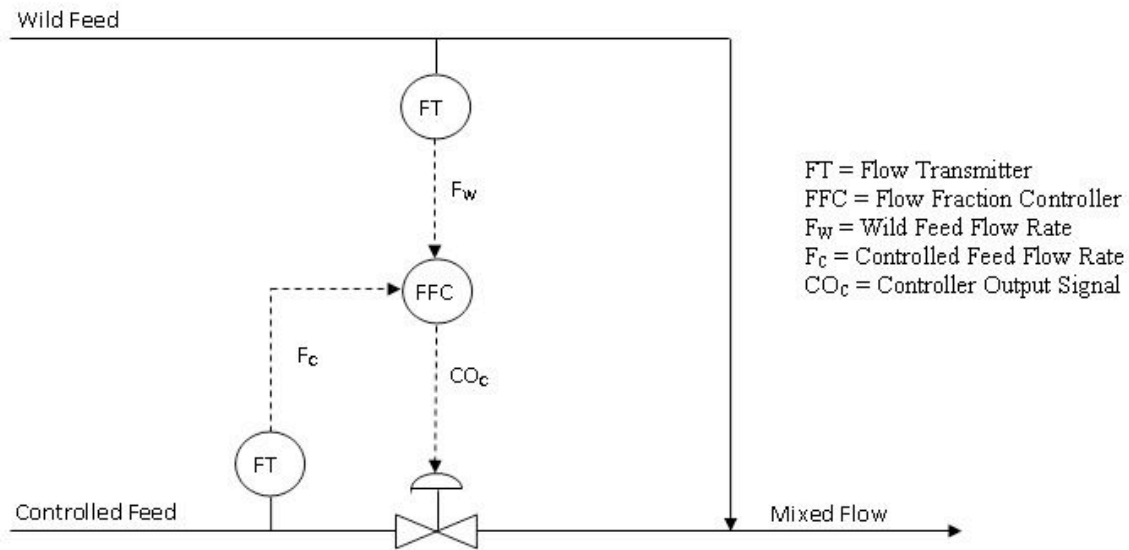


Image adapted from Houtz, Allen and Cooper, Doug "The Ratio Control Architecture"

4.6.3 Ratio Relay with Remote Input

The ratio relay with remote input model of a ratio controller is similar to the cascade control model in that it is part of a larger control strategy. The purpose of this model is to account for any unexpected or unmeasured changes that have occurred in the wild and controller feed streams. The diagram below illustrates how the composition of the mixed flow is used to change the relay ratio (3).

Ratio Relay Controller with Remote Input

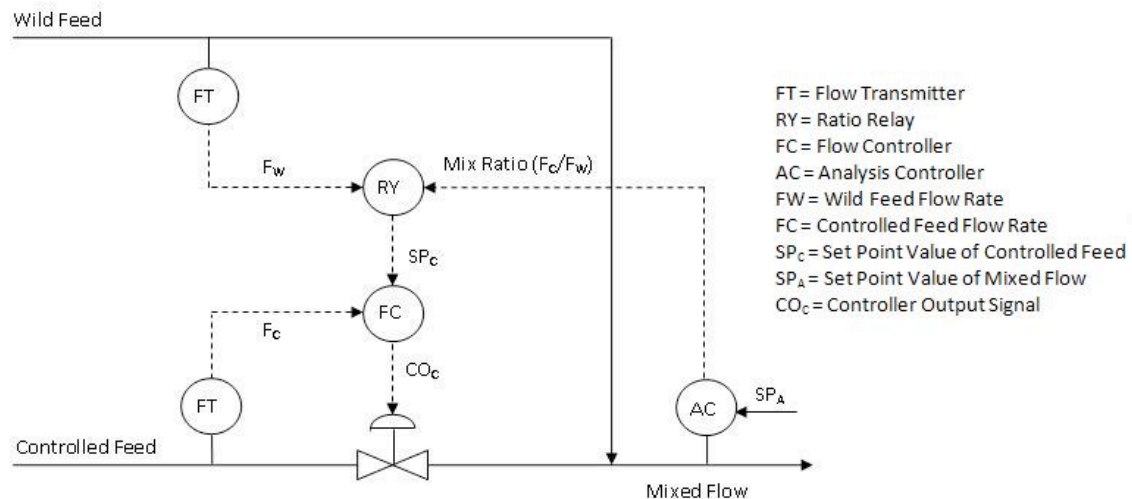


Image adapted from Houtz, Allen and Cooper, Doug "The Ratio Control Architecture"

The main advantage of having remote input is that the mix ratio is constantly being updated. A disadvantage of using an additional analyzer is that the analysis of the mixed stream may take a long time and decrease the control performance. The lag time depends on the type of sensor being used. For example, a pH sensor will most likely returned fast, reliable feedback while a spectrometer would require more time to analyze the sample.

4.7 Advantages and Disadvantages

There are some pros and cons to using ratio control where there is a ratio being maintained between two flow rates.

4.7.1 Advantages

1. Allows user to link two streams to produce and maintain a defined ratio between the streams
2. Simple to use
3. Does not require a complex model

4.7.2 Disadvantages

1. Often one of the flow rates is not measured directly and the controller assumes that the flows have the correct ratio through the control of only the measured flow rate
2. Requires a ratio relationship between variables that needs to be maintained
3. Not as useful for variables other than flow rates

4.8 Select Elements in Ratio Control

A select element enables further control sophistication by adding decision-making logic to the ratio control system. By doing so, a select variable can be controlled to a maximum or minimum constraint. The figure below depicts the basic action of both a low select and high select controller.

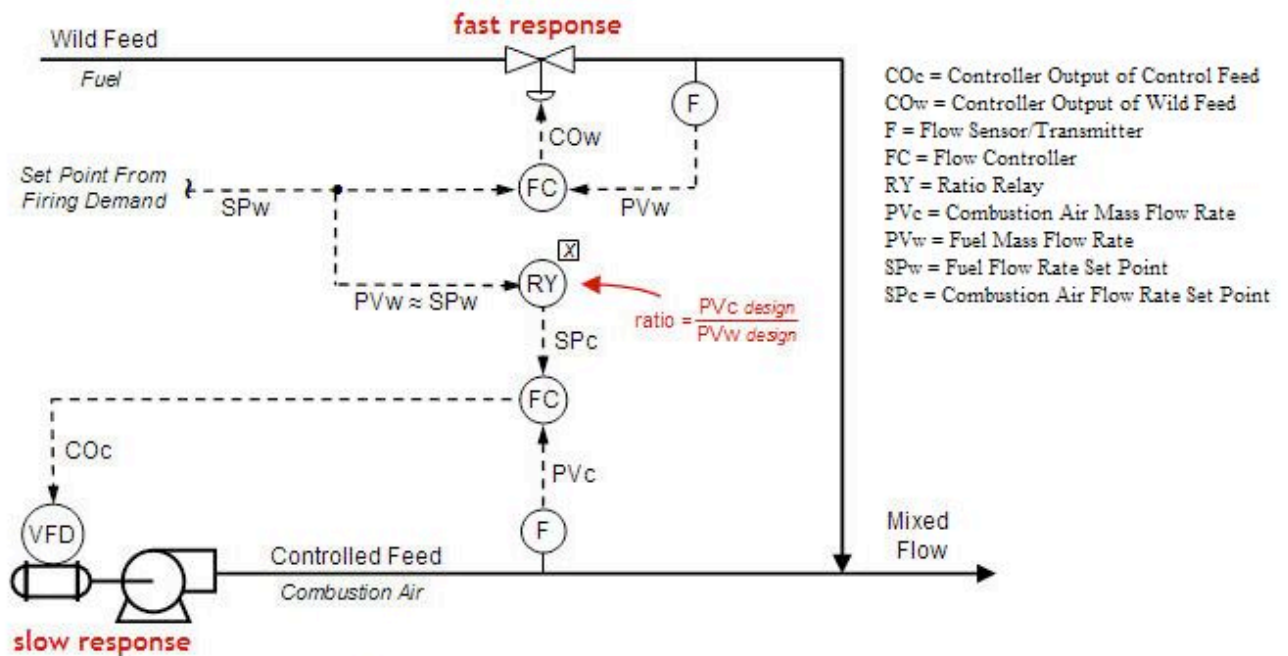


Image adapted from Houtz, Allen and Douglas Cooper

4.8.1 Single Select Override Control

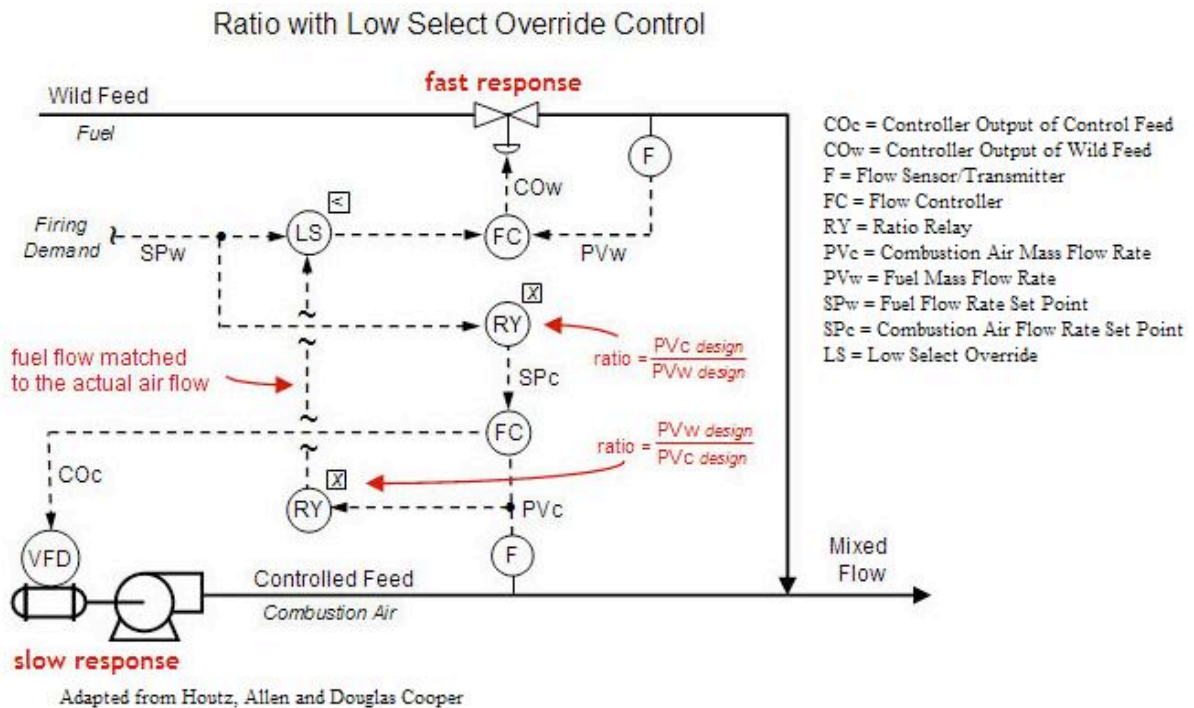
Often times, these select elements are used as an override element in ratio control. Take, for example, ratio control system (with remote input) of a metered-air combustion process in the figure below.

Ratio Control with Remote Set Point to Wild Feed Loop



Adapted from Houtz, Allen and Douglas Cooper

In this design, the fuel set point, SP_w , comes in as firing demand from a different part of the plant, so fuel flow rate cannot be adjusted freely. As the fuel set point (and therefore fuel mass flow rate, PV_w) fluctuates, a ratio relay is employed to compute the combustion air set point, SP_c . If the flow command outputs (CO_w and CO_c) are able to respond quickly, then the system architecture should maintain the desired air/fuel ratio despite the demand set point varying rapidly and often. However, sometimes the final control element (such as the valve on the fuel feed stream and blower on the combustion air feed stream in the diagram) can have a slow response time. Ideally, the flow rates would fluctuate in unison to maintain a desired ratio, but the presence of a slow final control element may not allow the feed streams to be matched at that desired ratio for a significant period of time. Valves often have quick response times, however, blowers like the one controlling the combustion air feed stream can have slow response times. A solution to this problem is to add a “low select” override to the control system, as shown in the figure below.

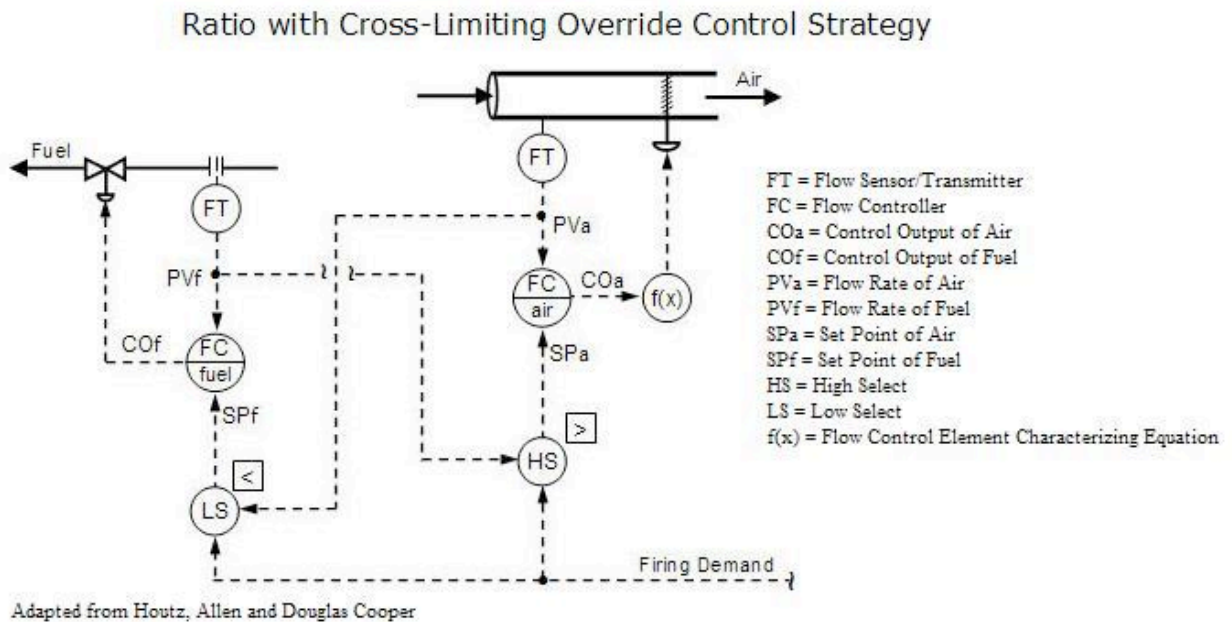


The second ratio controller will receive the actual measured combustion air mass flow rate and compute a matching fuel flow rate based on the ideal design air/fuel mixture. This value is then transmitted to the low select controller, which also receives fuel flow rate set point based from the firing demand. The low select controller then has the power to pass the lower of the two input signals forward. So, if the fuel flow rate firing demand exceeds combustion air availability required to burn the fuel, then the low select controller can override the firing demand and pass along the signal of the fuel flow rate calculated based on the actual air flow (from the second ratio relay).

This low select override strategy ensures that the proper air/fuel ratio will be maintained when the firing demand rapidly increases, but does not have an effect when the firing demand is rapidly decreasing. While the low select override can help eliminate pollution when firing demand rates increase quickly, a rapid decrease in firing demand can cause incomplete combustion (as well as increased temperature) and loss of profit.

4.8.2 Cross-Limiting Override Control

Cross-limiting override control utilizes the benefit of multiple select controls. Most commonly, a control system using the cross-limiting override strategy will implement both a high select and low select control. As a result, the system can account for quickly increasing firing demand as well as quickly decreasing firing demand. The figure below depicts a such a scenario using the inlet combustion air and fuel for a boiler as the example.

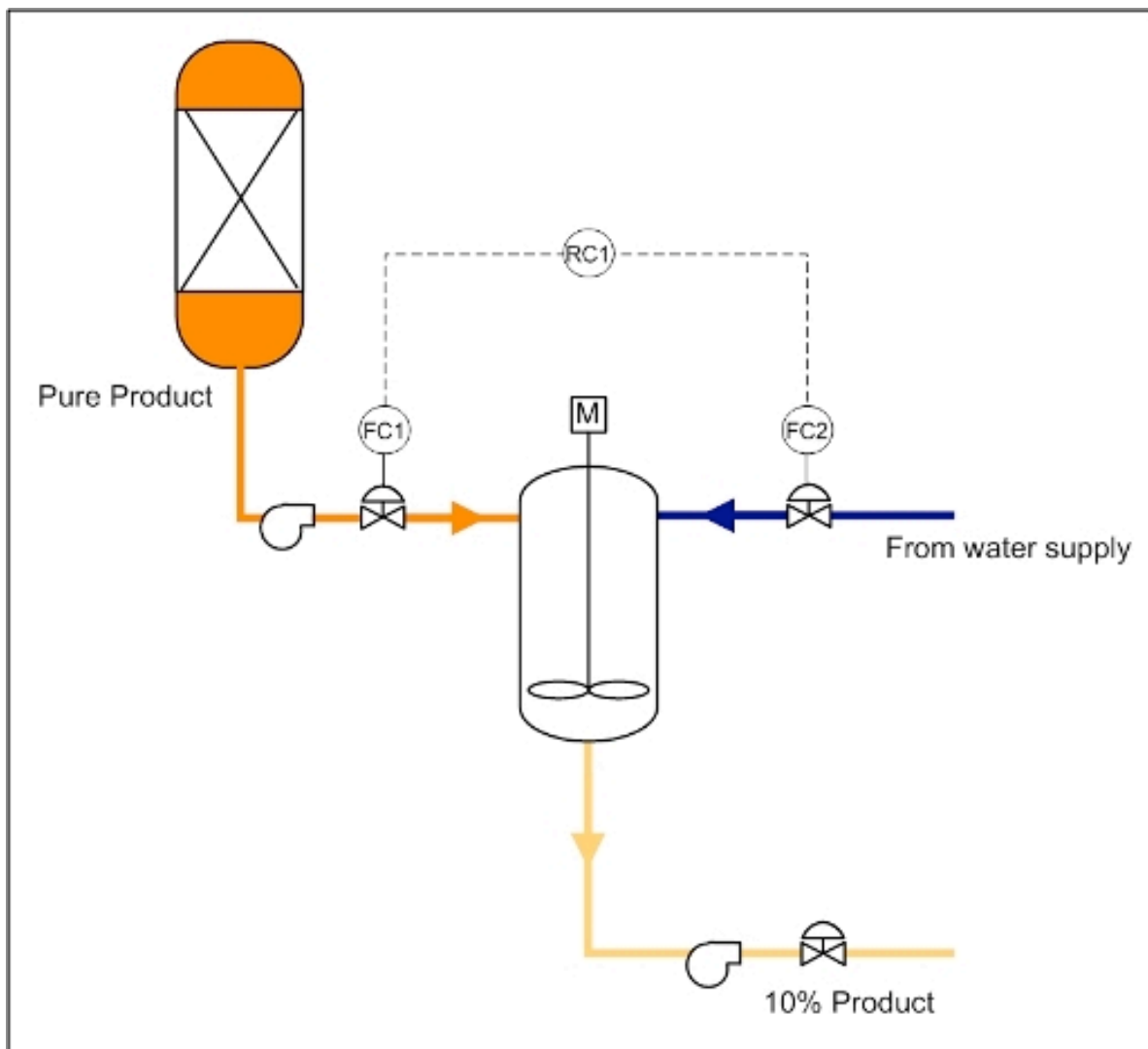


It is assumed that same firing demand enters the high select and low select control and the flow transmitters have been calibrated so that the ideal air/fuel ratio is achieved when both signals match. As a result, the set point of air will always be the greater value of the firing demand and current fuel flow signals. Likewise, the set point of fuel will always be the lower value of the firing demand and current air flow signals. So, as the firing demand increases, the set point of air will increase. At the same time, the low select will keep the set point of fuel to the signal set by the present flow or air. Therefore, the set point of fuel will not match the increasing firing demand, but will follow the increasing air flow rate as it is responding upwards. Similarly, if the firing demand decreases, the low select control will listen to the firing demand and the high select controller will not.

As a result, the firing demand will directly cause the set point of fuel to decrease while the set point of air will follow the decreasing fuel rate as it responds downwards. The cross-limiting override strategy allows for greater balance in a ratio control system.

4.9 Worked out Example 1

In the following process shown below, a concentrated solution of product is diluted continuously to be sold as a final 10% solution. Flowrates coming from the unit feeding the pure product to this mixing tank are not constant (the wild stream), and therefore a ratio controller is used to properly dilute the solution.



In this example, the ratio controller would be set to a value of $FC1/FC2 = RC1 = 9$. The ratio controller in this case would then work by the following logic:

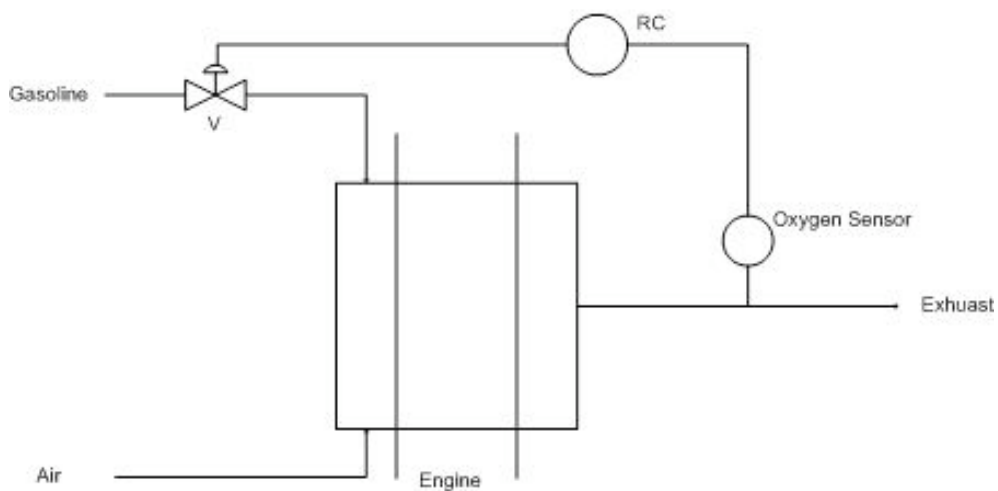
- IF $RC1 < 9$, THEN ADJUST $FC2$ DOWN
- IF $RC1 > 9$, THEN ADJUST $FC2$ UP

For an additional challenge, determine an error equation that can be related to this controller.

4.10 Worked out Example 2

One of the most common uses of a ratio controller is used for correcting the air-fuel ratio in automobiles. A specified amount of air is always taken up by the engine and the amount of fuel injected is controlled by a computer through the use of a ratio controller. The stoichiometric ratio for air to gasoline by mass is 14.7:1. There is an oxygen sensor in the exhaust manifold as well as sensors for all of the exhaust components. This sensor is connected to the valve for the fuel injection. If there is too much oxygen measured in the exhaust, then the mixture is said to be lean. Is the ratio of air to gas in the original mixture greater than or less than 14.7:1 and what should the valve controlling the fuel injection do?

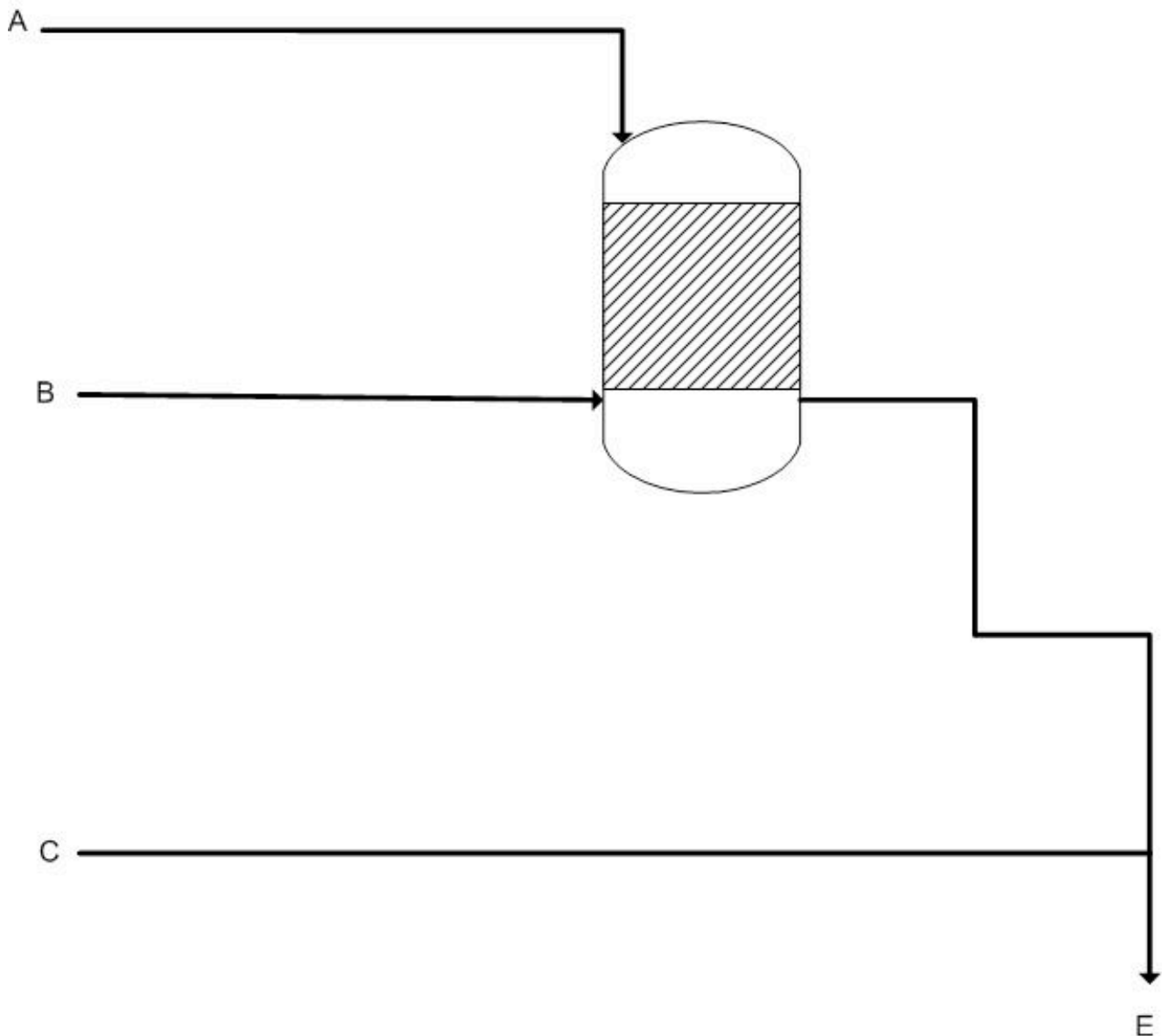
Note: This is an indirect form of a ratio controller as it is measuring a physical property of downstream in order to determine if the ratio is too high or low. Further information may be found here about [Air-fuel Ratio](#) and [Oxygen Sensors](#).



Answer: Since there is leftover oxygen in the exhaust, there must have been too much in the original mixture. The ratio of air to gas in the original mixture is greater than 14.7:1 and thus the computer should open the valve more for the fuel injection.

4.11 Worked out Example 3

Many processes in industry require multiple process streams entering at different locations in the system. A senior engineer gives you the project to design the control scheme for a new process to be implemented at the company. The process involves 2 reactions and 3 different feed streams.



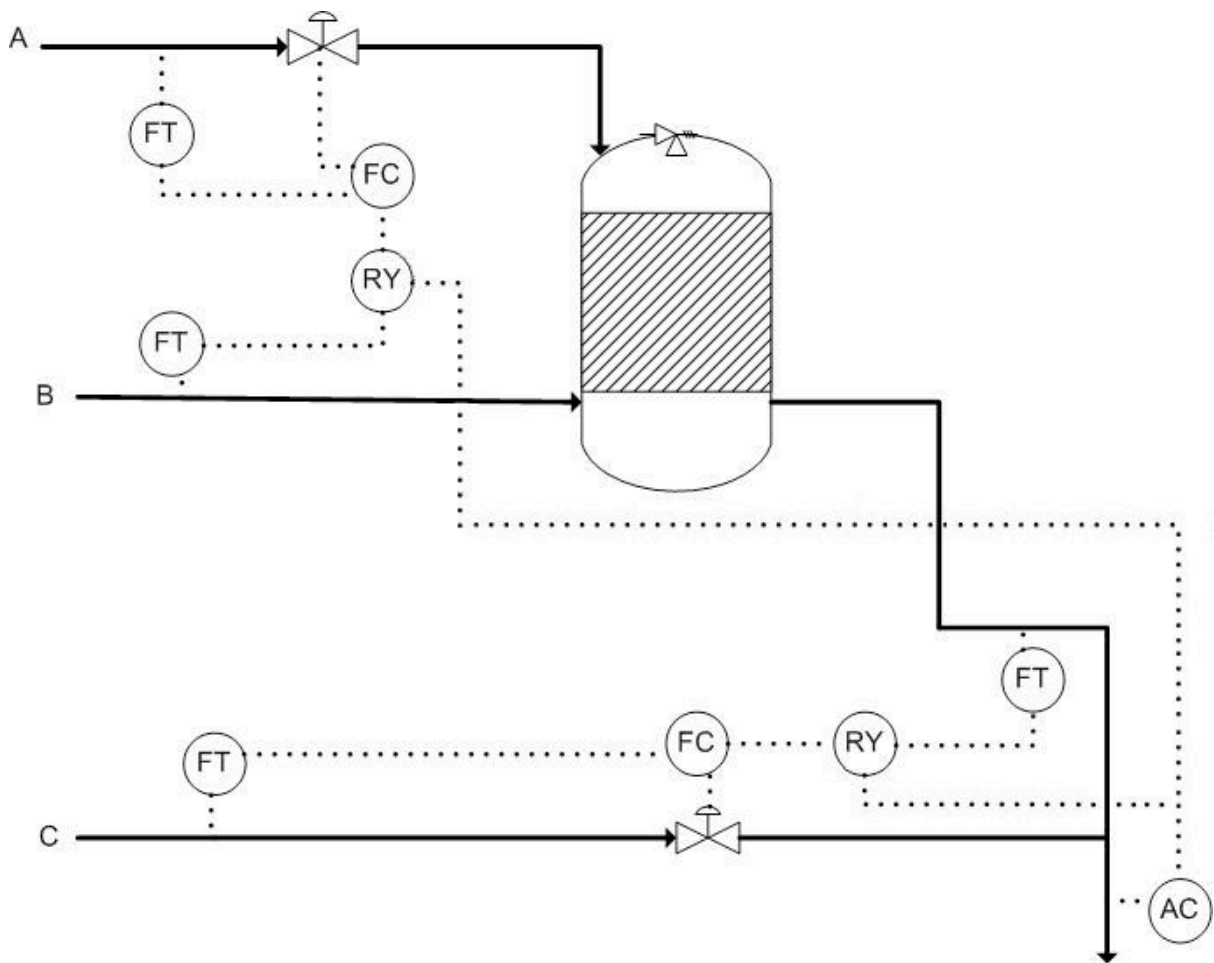
Reactions: $2A + B \rightarrow D$

$C + 3D \rightarrow E$

Assume the reactions go to 100% completion (you only need stoichiometric amounts).

Complete the P&ID with the control scheme and write the ratios (with respect to B) that the other molar flow rates will be set to. Also explain how the system will take action when it detects excess C or D in the product stream.

Solution:



A: 2 B: 1 C: 1 D: 1/3 E: 1/3

If the AC detects greater or less amounts of C expected, it will adjust the ratio setting in RY connected to C's flow controller, reducing or decreasing the ratio of C to B, respectively.

4.12 Multiple Choice Question 1

Why is a Blend Station used?

- a. to create the set point for the ratio controller
- b. to reduce lag time in adjusting flow rates
- c. to measure flow rates
- d. to multiply one flow rate by the desired ratio

4.13 Multiple Choice Question 2

How is the set ratio used in the first type of ratio controller described above?

- A. Outputs how much each stream should be flowing.
- B. It is compared against two flow rates to adjust one if needed.
- C. Tells the system to shut down.
- D. It adjusts for lag time when the system is not at steady-state.

4.14 References

- Astrom, Karl J. and Hagglund, Torr. "Advanced PID Control" The Instrumentation, Systems and Automation Society.
- Mahoney, Donald P., Svrcek, William Y. and Young, Brent R. "A Real-Time Approach to Process Control", Second Edition. John Wiley & Sons, Ltd.
- Houtz, Allen and Cooper, Doug "The Ratio Control Architecture" <http://www.controlguru.com> (<http://www.controlguru.com/2007/120207.html>)

Section 5. Summary: Summary on Control Architectures' philosophies, advantages, and disadvantages.

Summary on Control Architectures

A summary of the philosophies, advantages, and disadvantages of the different control architectures is shown below in Table 1.

Table 1. Control architectures' philosophy, advantages, and disadvantages.

	Philosophy	Advantages	Disadvantages
Feedback	Control adjusts errors as they occur	+ simple to design + no process model needed	- corrects for error after they have already occurred - usually only takes input from one sensor
Feed Forward	Control corrects errors before they occur	+ corrects possible errors before they occur + ideally can produce a perfect control where there is never any offset	- infinitely accurate models are needed - infinitely accurate measurements are needed
Ratio	Control connects two flows to maintain a constant ratio	+ generate defined ratio for given two streams + simple model	- the flow that you control is never truly measured and ratio model is assumed to be accurate - does not take into consideration of varying pressures
Cascade	Controls set points of sensors by controlling other sensors to integrate multiple information	+ responds quickly to high frequency changes + incorporate multiple sensor readings together (incidence graphs)	- can be very complex model - tuning model is difficult due to multiple set points and parameters
Mixed	Control integrating combinations of control architectures	+ pick the right combination of controls to accomplish main controlling objective + incorporate any number of sensors in a logical manner	- even more complex model than cascade alone - tuning model is even more complex than cascade alone, Zeigler-Nicholas tuning won't work by itself

Section 6. Common control loops / model for liquid pressure and liquid level

See also [ECOSSE](#)

Title: Common Control Loops / Model for liquid pressure and liquid level

Authors: Jennifersue Bowker, George Cater, Kibwe John Date Presented: 11/3/2006 Date Revised:

- [First round reviews for this page](#)

- [Rebuttal for this page](#)

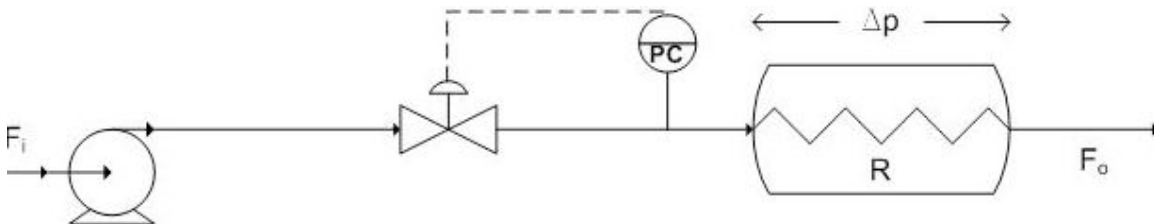
6.1 Introduction

Liquid level and liquid pressure control are fundamental aspects of many control processes because of the reliance on the stability and convenience of liquid usage. The following article will introduce the main concepts behind liquid pressure control, liquid level control, examining the loop characteristics, response, tuning and limitations. Two models are included to illustrate the application of a liquid pressure control loop and a level control loop in idealized systems.

6.2 Pressure Control Basics

Like its counterparts of temperature, level and flow, pressure is one of the most common process variables. Pressure is a key process variable as it provides a critical condition for processes such as any chemical reaction, extrusion, boiling, distillation, air conditioning and vacuuming. Poor pressure control may likely lead to problems associated with quality, safety and productivity. For example, the presence of high-pressure conditions in a sealed vessel may result in an explosion and thus it is imperative that pressure be kept under good control within its safety limits.

Liquid pressure control is one of the easier control loops in the sense that it shares many of the same characteristics of a common flow loop. The aim of the liquid pressure loop is to control the pressure at the needed set point pressure by controlling the flow with changing process needs. Because dealing with a liquid, the flow present is that of an incompressible fluid and as a result the pressure changes very quickly leading to a fast-responding process with small dead time and capacitance. This process behaves as a fixed restriction where the change in pressure is a function of the flow through the process. Illustrated below is a diagram with liquid pressure control on the pipe leading to the process.



There are a few additional considerations for the aforementioned liquid pressure loop. Firstly the controller can be proportional plus integral (PI) or integral only (I-only) if $K_c < 2$ otherwise a proportional only (P-only) controller is to be used. This controller is tuned similarly to the flow controller. Another consideration is that process gain is not constant, a square-root extractor or the highest loop gain should be used in tuning the controller. This highest loop gain is employed to prevent the process loop from ever becoming

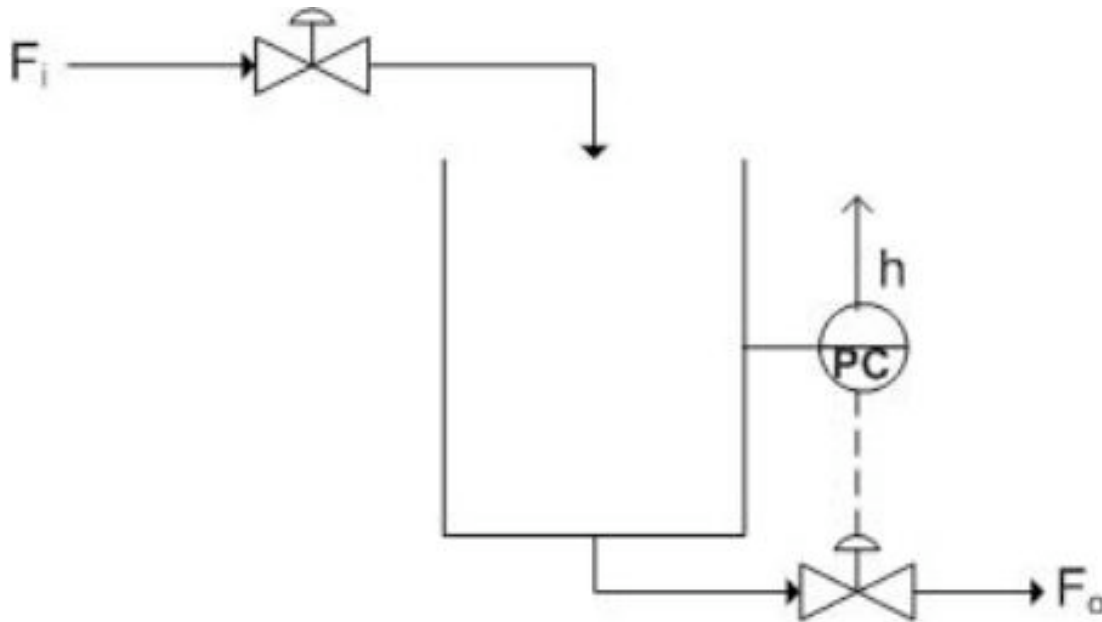
unstable. Finally, this liquid pressure loop is noisy like its flow loop counterpart and as a result it is recommended that derivative action in the controller not be used.

If you wish to see the various issues associated with pressure controllers please refer to previous wiki articles.

6.3 Level Control Basics

Controlling the level of liquid in a tank is one of the most basic requirements for a chemical process to run effectively. Most chemical engineering processes require some sort of liquid to be held for usage, and the most convenient way of ensuring the proper amount of liquid is available is through level control. A specific example of a process that requires level control is seen around the world. Water towers must have a designated amount of water within them to ensure sufficient water pressure to surrounding neighborhoods and hence liquid level control (LLC) is used.

Fortunately Liquid level control is one of the easier control loops available. The systems are fairly simple, a sensor reads the level of liquid within a tank, which then is conveyed to the controller. Subsequently, the controller changes a valve to increase or decrease the flowrate into or out of the tank, depending on the required action and controlled valve placement. Below is a figure with LLC on the pipe leaving the tank.



The ease of LLC also lies in its large capacitance and nominal dead time. Usually hold-up times vary from 5-15 minutes. Problems may arise when signal noise becomes a factor, as it usually does with level controllers. Refer to previous wiki articles to the issues associated with level controllers(), however it is important to note that a measurement of weight instead of directly measuring level can be a effective way of eliminating noise.

6.3.1 P-only Controllers

Oftentimes using a P-only controller is the best way to ensure proper level control, in most cases only a small percent error will result, and it reduces problems associated with noise. P-only controllers should only be used when gain is very small and the tank has a large capacity. This will be the basis for the rest of the wiki.

A P-only controller works off the following principle of control:

$$\text{Output} = \text{Gain} * \text{Error} + \text{Bias}$$

The output directly effects a valve to control the flowrate into or out of the tank. Refer to the previous wiki articles to learn more about P-only control.

6.3.2 Level Measurement Noise

When controlling liquid levels in drums or vessels, an important aspect to consider is that there may be noise in the level measurement due to disturbances such surface turbulence, boiling of the liquid, or agitation. Due to the existence of this noise, using a derivative action controller may not be appropriate. However, if this type of controller action is used, there are various methods that may be employed to minimize the noise.

Method 1: Use a displacer in a stilling well

Advantage: - Filters high frequency noise due to turbulence in the tank

Disadvantage: - Bobbing level due to the low-frequency movement of tank liquid into the well resulting from the formation of a U-tube between tank and well

Method 2: Use an ultrasonic level measurement with electronic filtering of the signal

Advantage: - Works well when the level response period is much lower than the noise frequency

Method 3: Use a tank weighing method

In the this method, a loading device is placed beneath the tank supports to measure the mass of the tank. Output weight values are averaged by a transmitter which are then sent to a converter which outputs the corresponding level to the controller.

Advantage: - Effectively eliminates noise in the level measurement due to turbulence

6.4 Models

The following are Excel models of Pressure and Level control in simple systems. Proportional only control is used primarily for these models. Controller noise has been eliminated for sake of simplicity.

6.4.1 Liquid Pressure Control Model

The model at hand illustrates both the feed backwards system of the liquid pressure in a pipeline of a process and its process gain relationships. This liquid pressure control loop is regulated by the position of the valve on the pipeline leading to the process. A P-only control is used here to change the valve position resulting in the need response in attaining the set point value. The following are any assumptions made and the equations used in modeling this process. An assumption is made that the process behaves like a fixed restriction such as an orifice plate whose Δp is a function of flow through the process. Another assumption that should be made is that the valve responds linearly to the flow-rate through it. In determining the process gain the following equations were used.

$$P = \Delta p + P_0$$

where P_0 is the downstream pressure at zero flow

$$\Delta p = \frac{F^2}{R^2}$$

where R is the process flow resistance

As a result we obtain:

$$P = \frac{F^2}{R^2} + P_0$$

The gain of the process is then determined by the following expression:

$$K_p = \frac{dP}{dF} = \frac{2F}{R^2}$$

A model for the feed backwards system for liquid pressure control introduced in this article is very complicated and might possibly be out of the scope of our discussion. A

possible alternative model would be very similar to the liquid level model presented below with the head in the tank determining the liquid pressure in the pipeline leaving the reactor.

The process gain model for a liquid pressure loop can be downloaded here --> [Media:Process gain model.xls](#)

6.4.2 Liquid Level Control Model

The following model represents a feed backward system of a liquid holding tank. The control loop is regulated by the exiting valve position on the pipe leaving the tank. A maximal flowrate out is assumed and the height of water in the tank does not have any effect on the flowrate out of the tank. This assumption can be made in tanks which are sufficiently wider than the pipe exiting operating with little liquid level change, as often is the case. Another assumption made is the linear response of the valve to flowrate out.

The pipe entering the tank is set by the user at a fixed flowrate. The P-only control is used to change the exiting valve position in order to cause the desired response to obtain the setpoint value. The P control follows the equation listed above and the bias is designated by the point at which the valve is open to allow a steady state to occur. Gain in Level control systems is usually low, however this can be changed by the user as well. The setpoint for the tank is determined by the user, as are the entering liquid flowrates and the maximal exiting flowrate.

The user can input a set point change in order to view the corresponding response in the controller.

Download the Level Model here --> [Media:LLCmodel.xls](#)

6.5 Worked out Examples

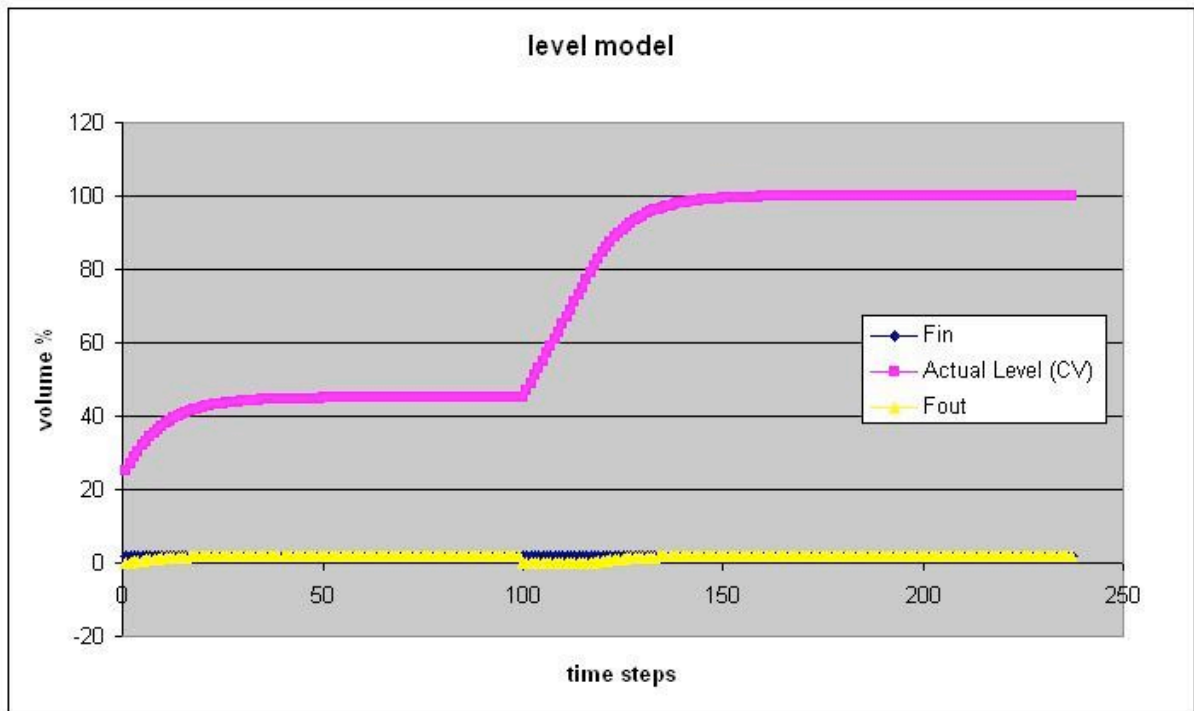
6.5.1 Question 1

Using the Liquid Level control Excel Model, what do you find when you change the level set point at a given point in time?

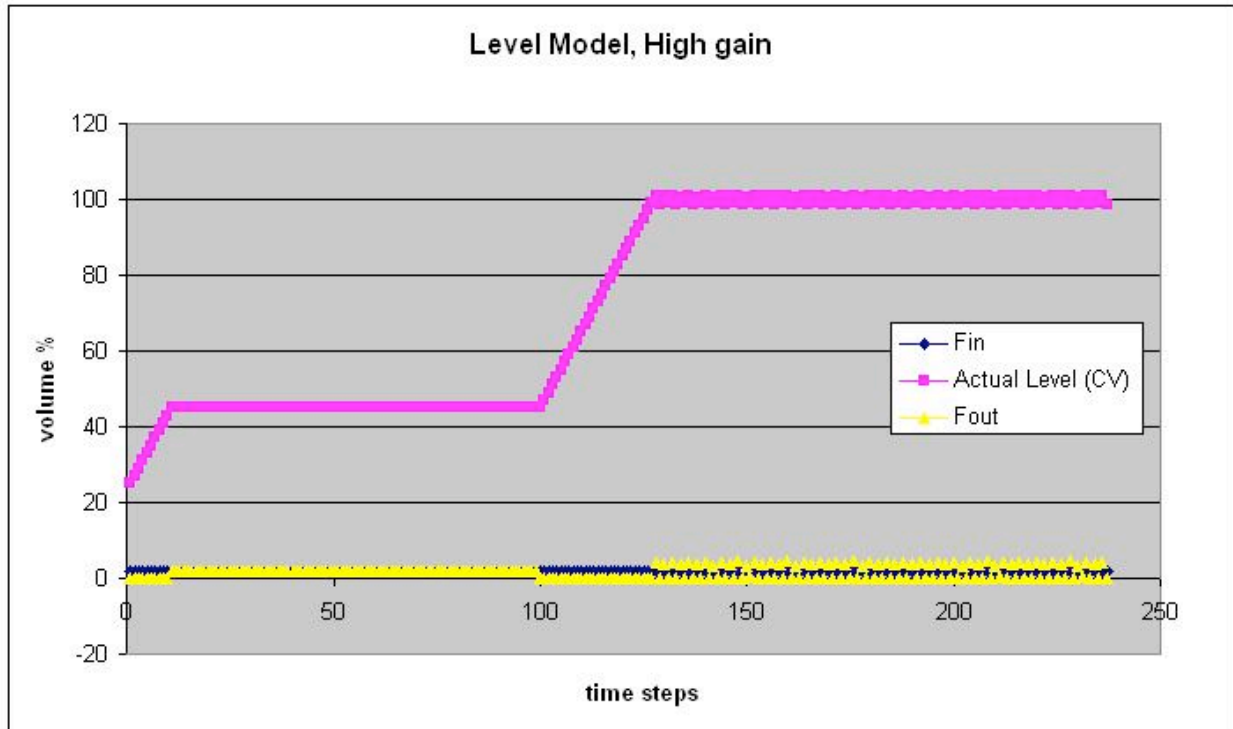
What happens if you change the gain to an large number?

6.5.2 Answer 1

When you change the level set point, you should notice a corresponding increase or decrease in the level as the P-control kicks in and beings to compensate for the error. The rate at which this set point is obtained is determined by the controller gain. At high controller gains the system responds extremely rapidly in an unreal fashion, this is why controller gain is usually small in large capacity tanks with flow control.



The above figure changes the setpoint to 100 @ t=100



The above figure uses a very high controller gain. Note the unreal response.

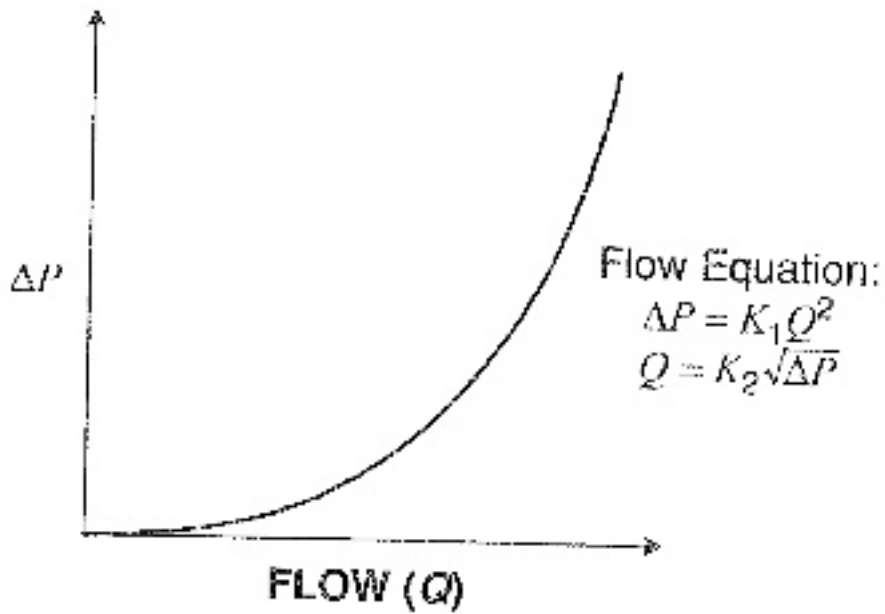
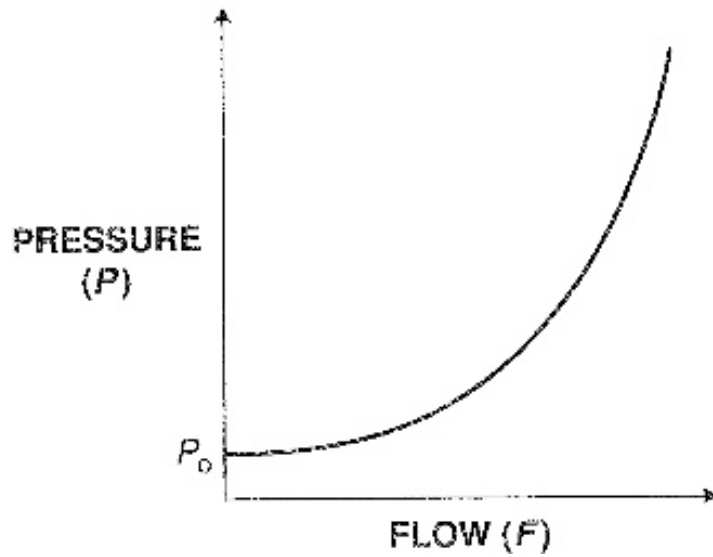
6.5.3 Question 2

What is the primary difference between the model for the process gain of the pressure flow loop introduced earlier in the article and a typical head flow response curve?

6.5.4 Answer 2

The response of pressure to flow is shaped similarly to the response of the head flow device and as a result the rules that govern the liquid pressure process gain model are in essence the same for the head flow device response. The only difference between the two response curves is that whereas the pressure varies from P_0 to 100 per cent for the process gain curve for the pressure flow loop, the pressure varies from 0 to 100 percent for the head flow device.

Below is the response for the pressure loop followed by that of head flow device.



6.6 Multiple Choice Question 1

When should P-only controllers be used in Liquid Level control?

- A) Whenever, because it's really easy.
- B) Never because it is too simple.
- C) Sometimes, when the gain is small and the tank capacity is large.
- D) None of the above

6.7 Multiple Choice Question 2

Various methods may be used to minimize the noise in a level measurement when using which type of controller action:


- A) None, you can never minimize noise in a level measurement
- B) Integral
- C) Derivative
- D) PI-control

6.8 References

- Use the [Harvard Referencing style](#) for references in the document.
- For more information on when to reference see [the following wikipedia entry](#).

Section 7. Common control loops / model for temperature control

Title: Common Control Loops: Model for Temperature Control

Note:  [Video lecture](#) available for this section!

Authors: Danesh Deonarain, Carly Ehrenberger, Georgina Mang, Teresa Misiti

Date Presented: November 2, 2006

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

7.1 Introduction

Temperature, pressure, flow, and level are the four most common process variables. Temperature is important because it provides a critical condition for processes such as combustion, chemical reactions, fermentation, drying, distillation, concentration, extrusion, crystallization, and air conditioning. Poor temperature control can cause major safety, quality, and productivity problems. Although highly desirable, it is often difficult to control the temperature because its measurement must be within a specified range of accuracy and have a specified degree of speed of response, sensitivity, and dependability. Additionally, temperature measurements must also be representative of true operating conditions in order to achieve successful automated control. The instrument selected, installation design, and location of the measuring points determine these specifications.

This article will serve as a guide to select the best location of measuring points to achieve the best automatic control. It will consider temperature control for three common process types: a CSTR, distillation column, and heat exchanger.

7.1.1 Temperature Control Loops

Before temperature control loops for specific processes are explained, we must discuss the general considerations common for all temperature control loops.

Temperature control loops can either be endothermic (requiring heat energy) or exothermic (generating heat energy). Both types are similar in that they both result in a response representing a process with a dominant capacitance plus a dead time. For both types of processes, one of the following devices is used to measure temperature:

- thermocouple
- filled thermal well system
- Resistance temperature detector (RTD)

The measurement device, or thermal well, should be selected so that it minimizes additional lag to the overall process lag. Minimizing temperature measurement lag in the temperature control loop is important in both slow and fast loops. Some general rules of thumb for reducing temperature measurement lag are:

- 1.** Use a small-diameter bulb or thermal well to minimize the thermal resistance and thermal capacity of the measuring element.
- 2.** Use a thermal well made from a material that minimizes thermal resistance and thermal capacity of the measuring element.
- 3.** Use a small pipe or orifice near the measuring device to increase velocity of the passing flow. Increasing flow will increase the rate of heat transfer between the process fluid and the measuring device.
- 4.** Place the measuring element in the liquid phase when measuring temperature in a two-phase system since thermal resistance is smaller in the liquid phase than in the vapor.
- 5.** Use a transmitter with derivative action to cancel out some of the lag in the measuring element. Compensate for this added derivative gain in the transmitter by reducing the derivative gain in the controller.

7.2 CSTR Temperature Control

7.2.1 Endothermic Reactor Temperature Control Loops

Endothermic CSTR reactors are generally easier to control than exothermic CSTR reactors because when the temperature reaches a critical minimum, the reaction does not proceed until there is adequate heat. In this sense, endothermic CSTR reactors are self-regulating. A good way to think of an endothermic CSTR's controls is that of a heat exchanger being used to heat a reaction solution. This heat exchanger's response is controlled by the dead time, so typically a PI or PID controller is used.

There are two main types of temperature control methods for endothermic CSTRs: control via steam flow rate and control via steam pressure. For the steam flow rate control case, the temperature control sends a signal to the flow control, which then controls the steam inlet valve. For the steam pressure control case, the temperature control sends a signal to the pressure control, which controls the steam inlet valve. Examples of an endothermic CSTR temperature control loop can be seen below in Figure 1 a-b.

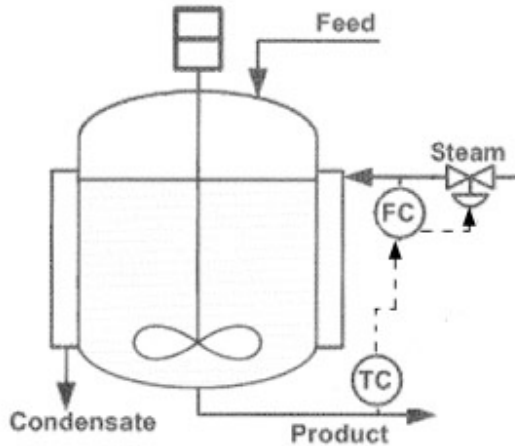


Figure 1.a. Temperature Control of an Endothermic CSTR via Steam Flow Rate

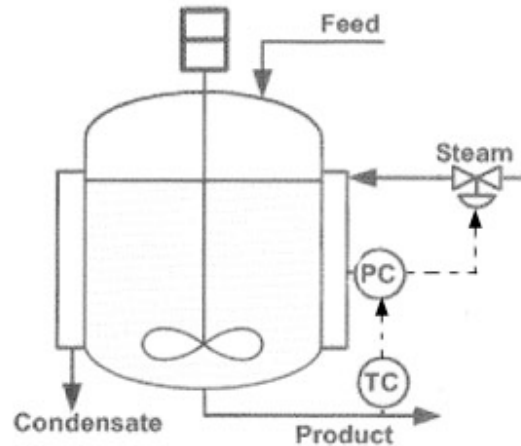


Figure 1.b. Temperature Control of an Endothermic CSTR via Steam Pressure

Image Modified From: Riggs, James B., Karim, Nazmul M.. Chemical and Bio-Process Control. Third Edition Chapter 18. Ferret Publishing.

7.2.2 Exothermic Reactor Temperature Control Loops

In an exothermic reaction, energy is released in the form of heat. In some cases, a cooling system is required to bring the temperature back to a set point and also to ensure that the temperature does not rapidly increase, or runaway. Some steps can be taken to prevent runaway temperatures, such as reducing the feed rates or concentrations of reactants. Also, the ratio of the heat transfer area to the reactor volume can be increased to help increase the controllability of the CSTR. Typically, the temperature is controlled using a PID controller, which is described in the previous section [PID Control](#).

Exothermic CSTRs are very difficult to control because they are very unstable and the temperature can easily runaway. The relationship between heat generation and temperature is non-linear, while the relationship between heat removal and temperature is linear. This relationship is illustrated in Figure 2. The stability of the temperature control loops depend on the rate at which heat can be removed from the system. For example, an exothermic CSTR that generates heat at a slow steady rate is more stable than a reactor that rapidly produces heat. In this example, the rate at which the heat can be removed from the system depends on the rate at which the temperature can be changed in the cooling jacket surrounding the CSTR.

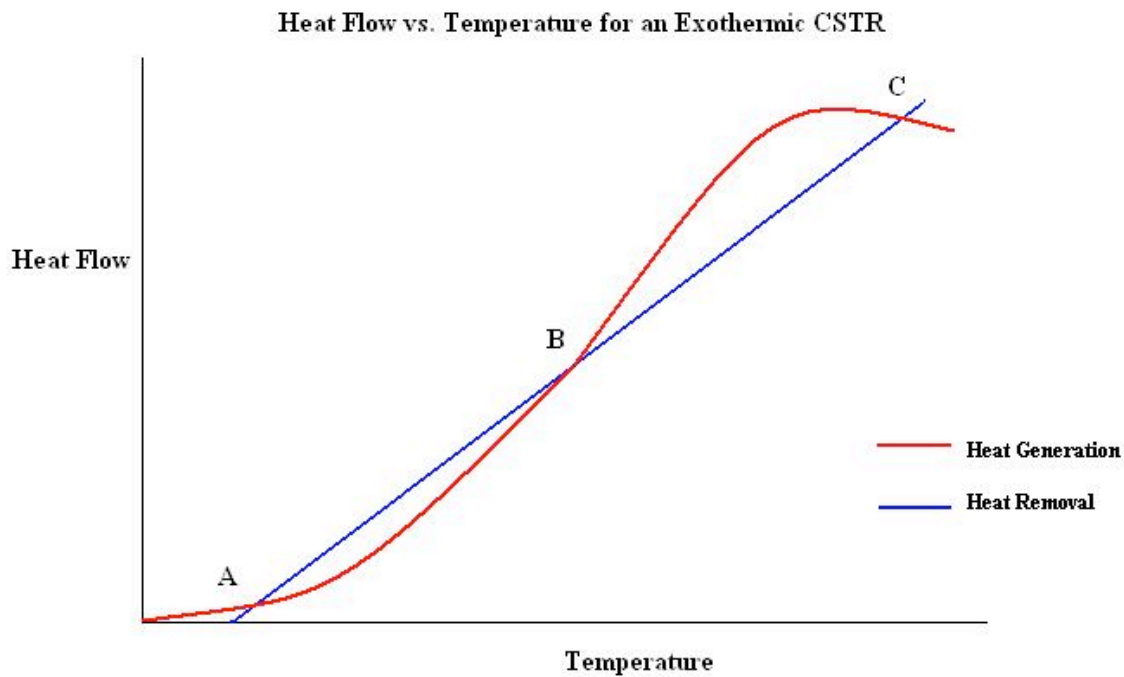


Figure 2. Heat generation or removal as a function of temperature in an exothermic CSTR

The intersections of the two curves, labeled A, B and C, represent steady state operating points. A and C are stable operation points while B is unstable. A and C are stable because as the temperature increases from this point, the rate of heat generation is less than the rate of heat removal. This means that as the temperature increases, heat is removed faster than it is generated so the temperature will be brought back down to that operating point. The same will happen if the temperature decreases from that point. As the temperature decreases, the heat generation rate is greater than the heat removal rate so the temperature will be brought back up to the operating point.

Point B is unstable because when the temperature increases from that point, the heat generation is greater than the heat removal. This means that as the temperature increases, heat is continuously added to the system and the temperature will rise until it reaches one of the stable operating points, in this case C. If the temperature decreases from point B, the heat generation rate is less than the heat removal rate so the temperature will continue to decrease until it reaches the lower, stable operating point, A.

This graph would be similar for an endothermic CSTR but there would be only one stable steady state operating point.

Very rapid exothermic reactions are the most difficult to control and they are sometimes carried out in a semi-batch reactor so the addition of reactants can be carefully controlled and runaway temperatures can be avoided.

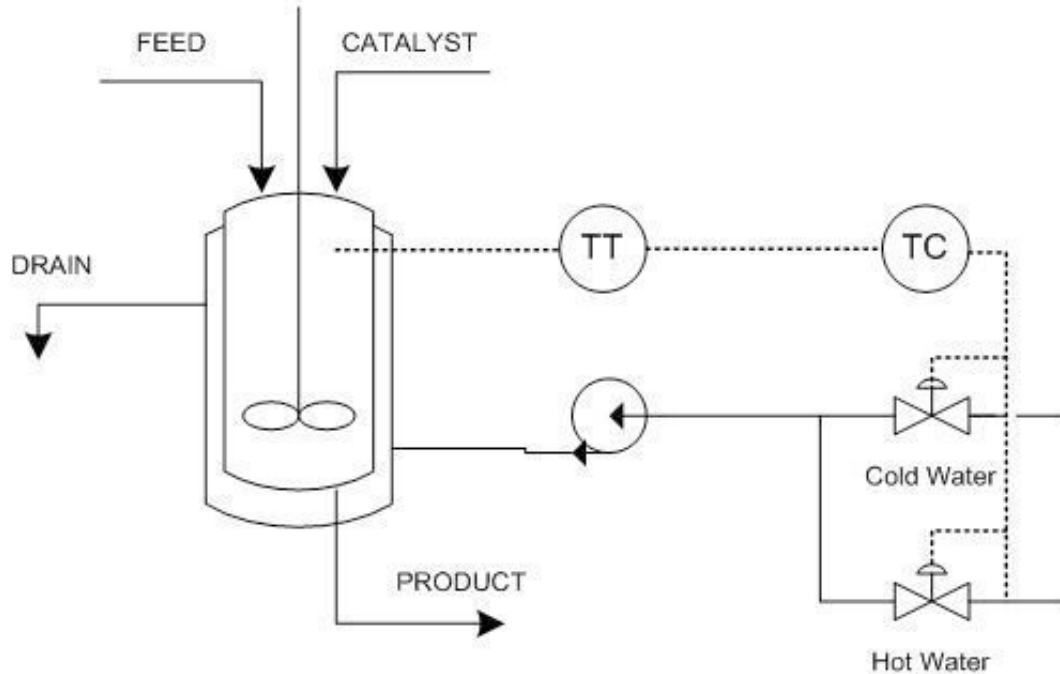


Figure 3.Temperature control loops for an exothermic CSTR

Figure 3 illustrates a common control loop for an exothermic CSTR with a cooling jacket. A temperature transmitter (TT) sends a signal to the temperature controller (TC), which controls the hot and cold water valves on the jacket. The cold and hot water are pumped into the jacket which controls the reactor at a set temperature.

7.3 Temperature Control in Distillation

In a distillation column, temperature control is used as a means to control composition because temperature sensors are cheaper, more reliable, provide continuous measurements, and respond quicker than composition analyzers. Through equilibrium relationships, temperature measurements can be used to infer composition of the product. Inferential temperature control is only effective when the relative volatility of the components is high (greater than 2.0). Temperature controllers are used as feedback composition controllers to adjust column operation to meet production requirements. They must be able to satisfy the constraints defined by production requirements at all times, even in the face of disturbances.

7.3.1 Inferential Temperature Control

To control composition via temperature, a correlation must be made between temperature in the tray and composition of the key components. Determining a correlation is challenging because the temperature-composition relationship is affected by process nonlinearity and disturbances in feed composition, flowrates, and occurrence of entrainment or fouling. For multi-component separations, temperature does not determine a unique composition, so either an online composition analyzer or periodic lab tests must be utilized to verify composition at the temperature setpoint. Additionally, the column pressure greatly affects the measurement of tray temperature. For most systems, the following linear equation can be used to correct for variations in pressure:

$$T_{pc} = T_{meas} - K_{pr}(P - P_0) \quad (\text{Eqn 1})$$

Where,

T_{pc} =corrected temperature

T_{meas} =measured tray temperature

K_{pr} =pressure correction factor

P =column pressure

P_0 =reference pressure

The pressure correction factor, K_{pr} , can be estimated using a steady-state column simulator for two different operating pressures and the equation:

$$K_{pr} = \frac{T_i(P_1) - T_i(P_2)}{P_1 - P_2} \quad (\text{Eqn 2})$$

Where,

T_i =temperature of tray i predicted by the column simulator

Successful temperature control in the column depends on the dynamic response of measuring the tray temperature with respect to the manipulated energy source used to actuate temperature. The energy source is either the reboiler or the reflux. To have tight process control means that the equivalent dead time in the loop is small compared to the shortest time constant of a disturbance with significant amplitude. According to Svreck, et al, the following observations from experimental tests are cited:

- Temperature control is made less stable by measurement lag or response times.
- The speed of response and control stability of tray temperature, when controlled by reboil heat, is the same for all tray locations.
- The speed of response and control stability of the tray temperature, when controlled by reflux, decrease in direct relation with the number of trays below the reflux tray.
- When pressure is controlled at the temperature control tray, the speed of response of the temperature control instrument can vary considerably with tray location, and is normally slower.

To achieve the best composition control, you need to determine the tray(s) whose temperature(s) show the strongest correlation with product composition. The following procedure using a steady-state column model can be used:

1. Run the column at the base conditions $(x^{BC}$ and $y^{BC})$ at steady-state and record the temperature, T_i^{BC} , of each tray.

2. Increase the impurity level in the bottoms product $(x^{BC} + \Delta x$ and $y^{BC})$, so that Δx is about 25-50% of the impurity level for the base case. Record the temperature, $T_i^{\Delta x}$, of each tray.

3. Increase the impurity level in the overhead product $(x^{BC}$ and $y^{BC} + \Delta y)$, so that Δy is about 25-50% of the impurity level for the base case. Record the temperature, $T_i^{\Delta y}$, of each tray.

4. The best tray for inferential temperature control of the stripping section will be the least sensitive to variations in the composition of the overhead product. This tray is the

one that maximizes: $\Delta T_i^{net} = (T_i^{\Delta x} - T_i^{BC}) - (T_i^{\Delta y} - T_i^{BC})$
(Eqn 3)

5. The best tray for inferential temperature control of the rectifying section will be the least sensitive to variations in the composition of the bottoms product. This tray is the one

that maximizes: $\Delta T_i^{net} = (T_i^{\Delta y} - T_i^{BC}) - (T_i^{\Delta x} - T_i^{BC})$ (Eqn 4)

6. Repeat this procedure for a range of feed compositions. Then, select the tray that maximizes the ΔT_i^{net} equations most often for the range of feed compositions.

7.3.2 Single Composition Control

Once you have determined the best tray to use for inferential temperature control, you must choose a manipulated variable (MV) that will have a significant gain on the tray temperature, and thus on the composition. Usually in distillation, the composition of only one product stream is controlled while the composition of the other product stream is allowed to drift. This is called single composition control. The chemical industry primarily uses single composition control.

When you are interested in controlling the composition of the overhead product, the reflux is used to control the purity, while the reboiler duty is held constant. The bottom composition is not directly controlled and will vary as the feed composition varies. The reflux, L , is the manipulated variable that will result in the tightest control, rather than either the distillate flowrate, D , or the reflux ratio, L/D . This is because L is the fastest-acting MV for the overhead and is the least sensitive to changes in the feed composition. This scenario is depicted below in Figure 4a.

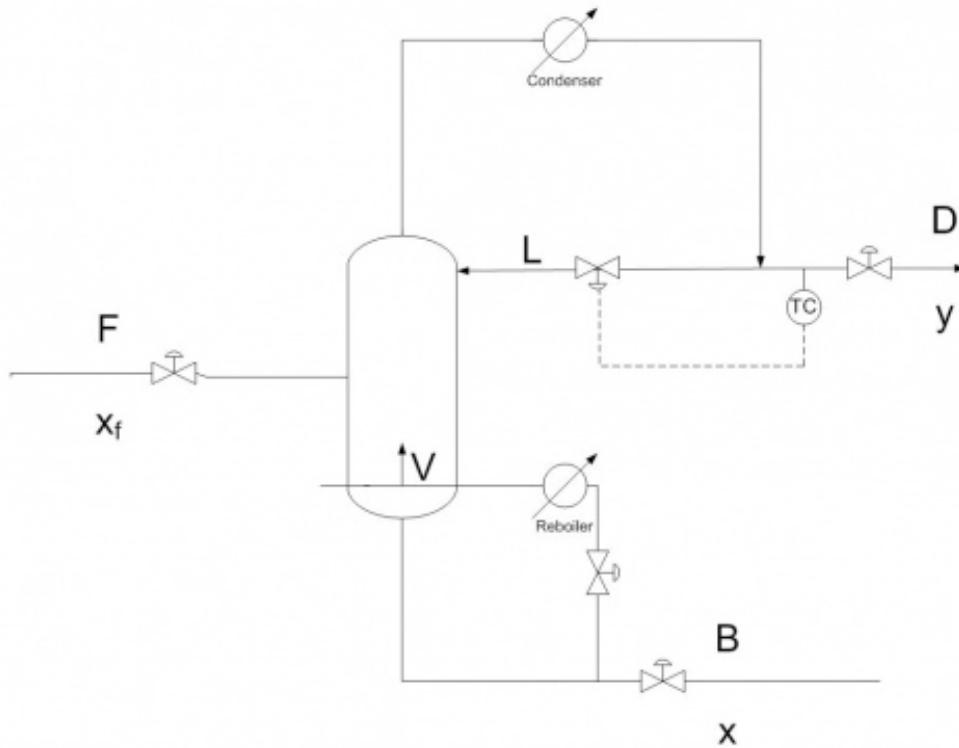


Figure 4a. Control diagram for inferential temperature-single composition control of overhead product stream by L .

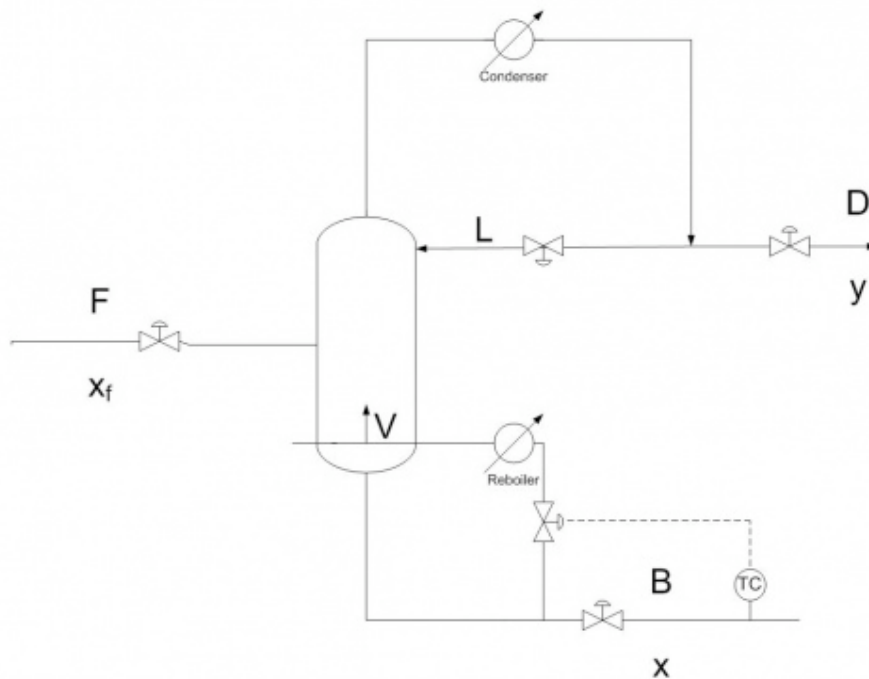


Figure 4b. Control diagram for inferential temperature-single composition control of bottom product stream by V .

When you are interested in controlling the composition of the bottom product, the boilup

rate, V , is used to control the purity, while the reflux rate is held constant. The overhead composition is not directly controlled and will vary as the feed composition varies. V is the manipulated variable that will result in the tightest control, rather than either the bottoms product flowrate, B , or the boilup ratio, V/B . This is because V is the fastest-acting MV for the bottoms and is the least sensitive to changes in the feed composition. This scenario is depicted above in 4b.

7.3.3 Dual Composition Control

Although single composition control is most commonly used, there are some industries that need to simultaneously control the composition of both the overhead and bottom product streams. This is called dual composition control and is harder to implement, tune, and maintain than single composition control. Dual composition control increases product recovery and reduces utility costs and is used for refinery columns that generally have high associated energy usage. Industries that have refineries, such as the oil industry, use dual composition control because they are interested in using both the overhead and bottom streams as product.

In dual composition control, there are many possible control configurations. The control configuration is described by the control objective and by the MV. There are four possible control objectives: bottom product x , overhead product y , reboiler level, and accumulator level. The chosen control objectives are then paired with a MV. There are a variety of choices for the MV. These include: L , D , L/D , V , B , V/B , B/L , and D/V . Therefore, in dual composition control, there are many possible configurations to consider, although most are not practical.

The most commonly used configuration for dual composition control is (L, V) which uses L to control y (overhead composition) and V to control x (bottom composition), because it provides good dynamic response, is the least sensitive to changes in feed composition, and is the easiest to implement. However, it is highly susceptible to coupling. In this configuration, depicted below, the setpoint for the reflux flow controller is set by the overhead composition controller, and the setpoint for the flow controller on the reboiler duty is set by the bottom composition controller. D is then used to control the accumulator level, and B is used to control the reboiler level.

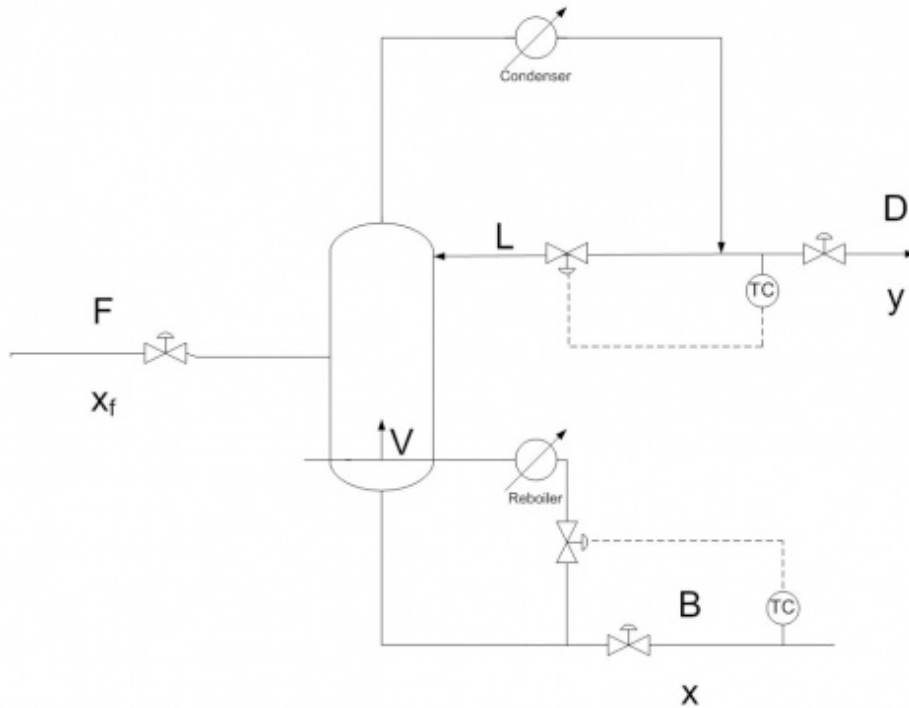


Figure 5. Control diagram for inferential temperature-dual composition configuration (L,V), the control of overhead product stream by L and bottom product stream by V.

Since there are so many possibilities for configurations, there is no clear best choice for a configuration of MVs in dual composition control in distillation columns. It is impossible to know theoretically which configuration is optimum for a particular process, but there are some rules of thumb to follow to increase the possibility of choosing a good configuration. These rules are summarized in the chart below.

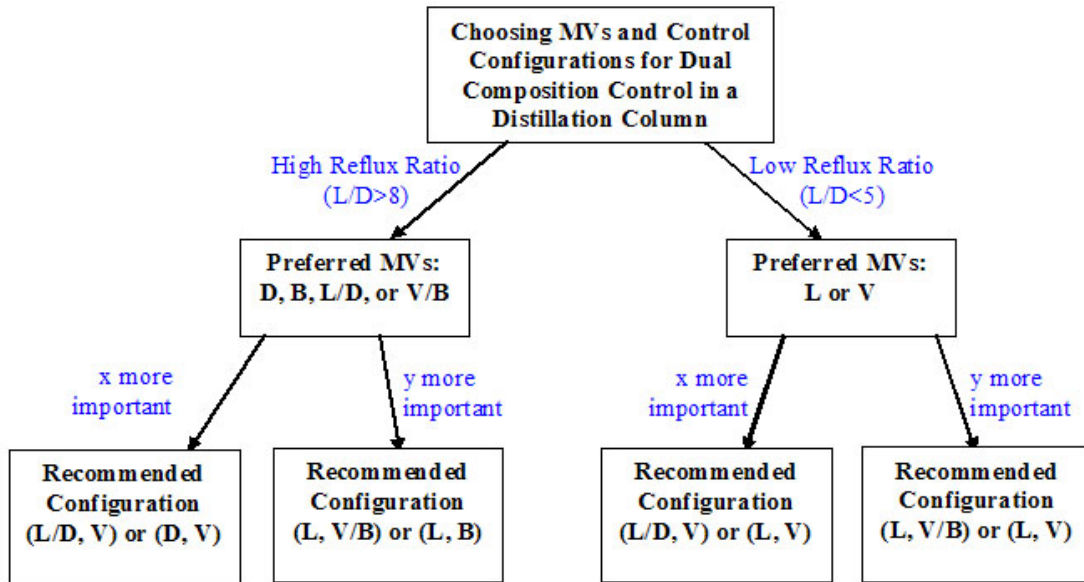


Figure 6. Chart to determine a good configuration for your process when using dual composition inferential temperature control

For the gray area where $5 < L/D < 8$, follow the rules of thumb for the closest L/D , and use experimental data to determine the best configuration for your particular process.

7.3.4 Controller Tuning and Constraints

When temperature is used for inferential composition control, a PID controller is usually used because of the significant sensor lag. Common constraints on the extent of temperature control in a distillation column include:

- Capacity of reboiler power
- Capacity of overhead condenser
- Flooding or entrainment
- Maximum (undesired) column temperature

In general, temperature control can be used to control composition in a distillation column. The temperature measuring device should be chosen to minimize the lag time. A steady-state model can be used to correct for pressure changes in the column and to determine the best tray at which to measure temperature. The choice of the MV depends on if you are operating under single or dual composition control and which product composition you want to control.

7.4 Heat Exchanger Control

In heat exchanger control, the temperature of the process exit stream is the controlled variable (CV) and can be adjusted by one of four possible manipulated variables: cool side entry stream, cool side exit stream, hot side entry stream, or hot side exit stream. The selection of where control will be implemented is a combined result of three factors:

1. Whether we want to heat or cool the process stream
2. The response time of the controller
3. The capital cost

To illustrate the selection process, first it is shown that the hot stream preferred for temperature control, then two case studies are discussed, one for heating up the process stream and the other for cooling the process stream.

7.4.1 Controlling the Cool Side Stream

It is not advisable to place temperature control on the cool side stream. This is explained below.

The particular MV in each stream is the flow rate. It is known that the temperature of the hot stream will change once the flow rate of the cool stream is adjusted.

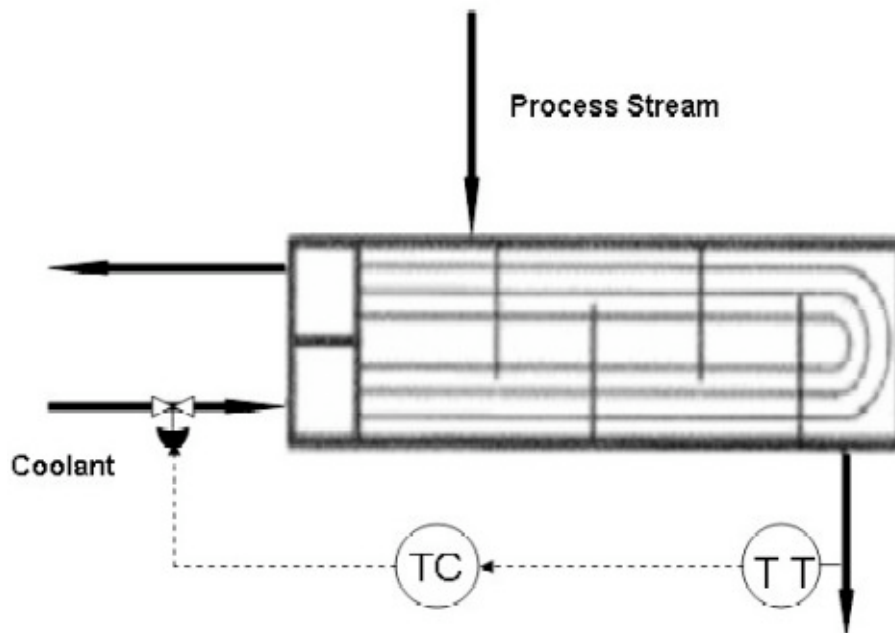


Figure 7. Image modified from Riggs & Karim, shows coolant temperature control loop for a Liquid/Liquid Heat Exchanger.

It is easier to think of the temperature change as the magnitude of the process gain (l

$T_{t+1} - T_t$ l). This just is the magnitude of the temperature change over a way the discussion can be general for both heating or cooling the process stream.

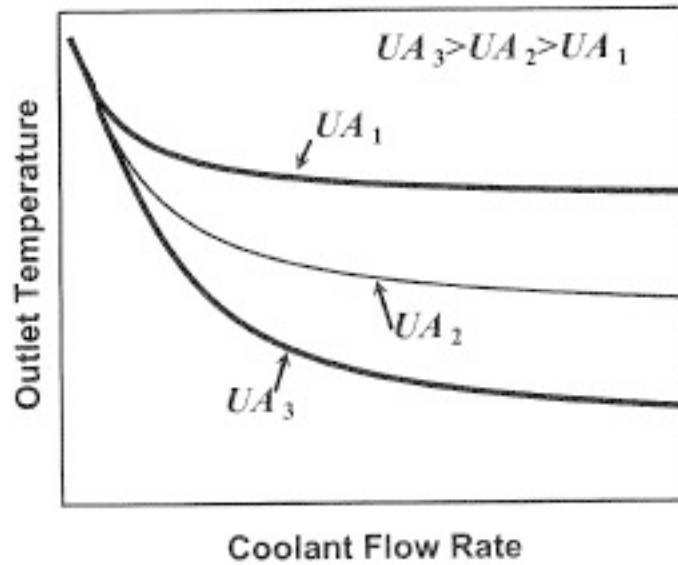


Figure 8. Taken from Riggs & Karim, demonstrates the limit that increasing the flow rate of the coolant stream has on the exit temperature of the process stream for three heat exchanger areas

As the rate of the cool stream is increased from zero, the magnitude of the process gain continuously decreases. Above a certain rate, the gain will not be a measurable change in the process stream temperature. Because of this, *making the coolant stream the MV will make the process uncontrollable at a critical point and is not a good idea.*

7.4.2 Controlling the Hot Side Stream

As indicated above it is never recommended to place the temperature control on the cool side stream. This reduces controls consideration to only the hot stream. There are two cases where the control can be on the hot stream; when heating up and when cooling down the process stream.

Heating Up The Process Stream

CASE STUDY 1: Steam-Heat Heat Exchanger

In this case the process stream is the cooler of the two entering streams, the previous section states that the MV would have to on the stream used to heat up the process stream.

The temperature control loop can either be the direct steam flow or the steam pressure. Both controls the amount of steam flowing into the heat exchanger by adjusting a valve, however, the preferred of the two is the steam pressure as the MV in the temperature control loop. This is because a change in the steam supply can quickly cause the internal pressure of the heat exchanger to change hence affecting the temperature exchange. The steam pressure control responds and corrects this faster than the steam flow control. This becomes especially useful for heavy duty requirements when the change in response to change in flow rate of the process stream. The two figures below show two preferred configurations;

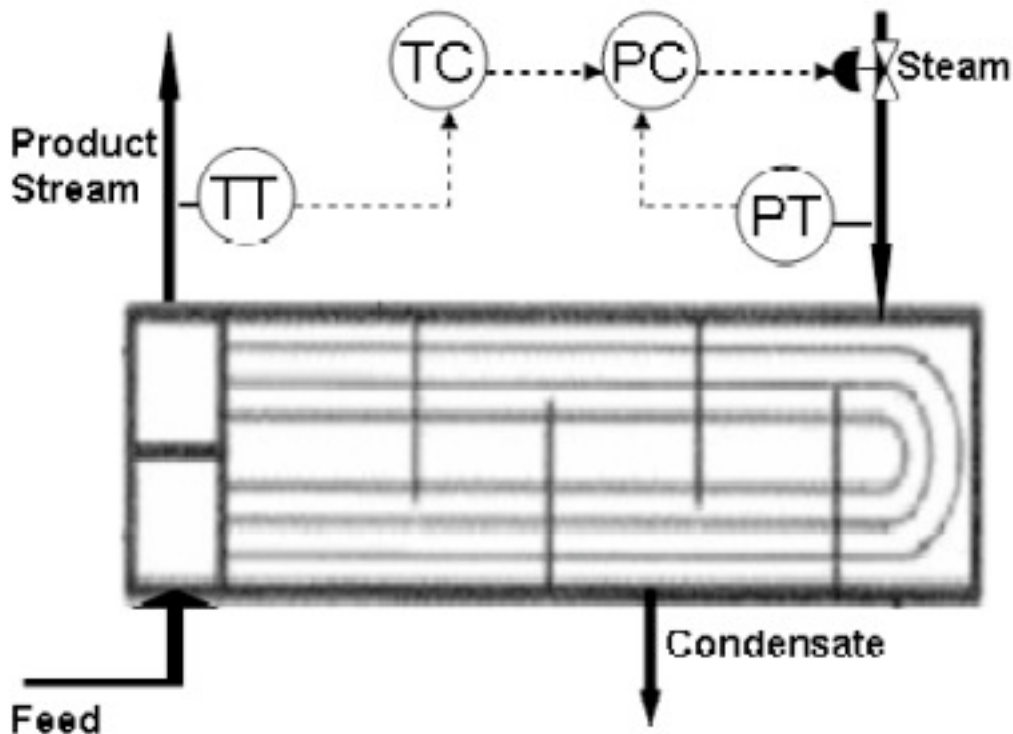


Figure 9. Image modified from Riggs & Karim, shows one arrangement for temperature control for heating up a process stream

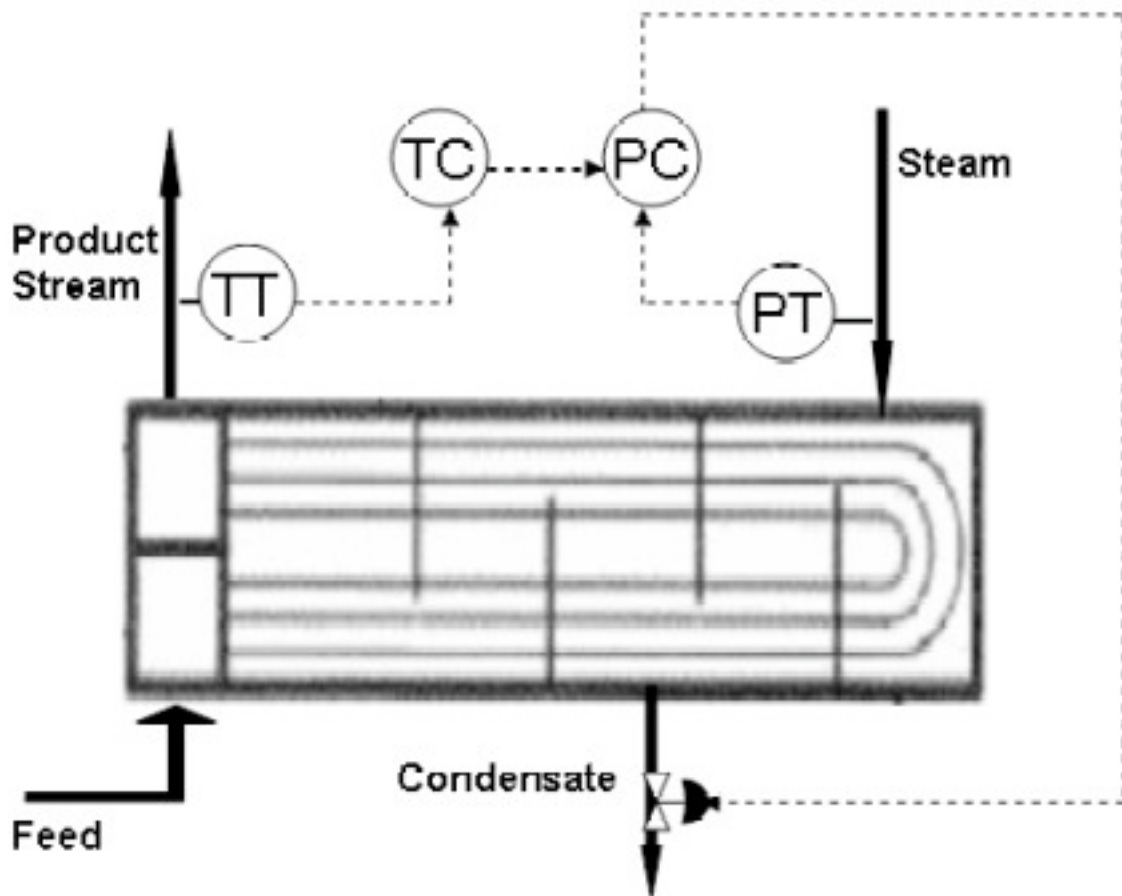


Figure 10. Image modified from Riggs & Karim, shows an alternative arrangement for temperature control for heating up a process stream

Notice that Figure 10 shows the control valve on the condensate stream. This is an acceptable control placement, however, in most practical application the first of the configurations in Figure 9 is preferred. In addition there are some ramifications to making the condensate flow the MV. The temperature loop in this case would not be as responsive as in the previous case. This is because the level responds slower than the pressure to the changes in the respective valves. The capital cost involved in placing the valve in the condensate stream is much lower that that in the steam stream because the steam stream is generally larger and requires a larger, more expensive valve. In addition a steam trap is required down stream of the condensate valve, for that configuration.

Cooling Down The Process Stream

CASE STUDY 2: Liquid/Liquid Heat Exchanger

In this case the process stream is the hotter of the two entering stream so the controls will have to be on this stream. As in case one we are setting up the temperature control loop

for varying flows in the process stream because in a plant the flow rate of this stream is dependent on a process before the heat exchanger. Hence when creating control loop for cooling down the process stream the coolant flow is kept constant (as stipulated in the section "Coolant Stream Controls") and maintain the CV at the set point. The best choice for the MV in this temperature control loop is having a feed bypass stream, as illustrated in Figure 11 below. The advantages of having this bypass stream are that the process dynamics are considerably faster with low levels of dead time and this condition is more linear, as opposed to varying the coolant flow rate. With this configuration the coolant flow rate can be maintained very high which reduced the tendency for fouling on the process fluid side of the heat-transfer surface.

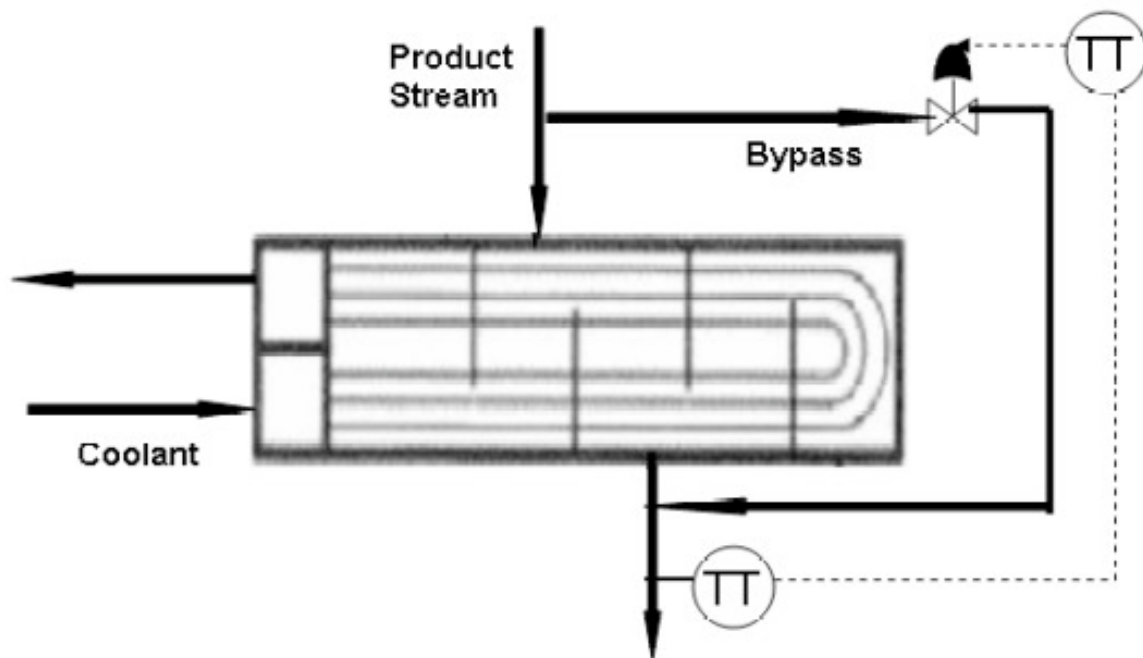


Figure 11. Image modified from Riggs & Karim, shows the common arrangement for temperature control for cooling down a process stream

7.5 Worked out Example 1

(a) Is an exothermic CSTR easier or harder to control than an endothermic CSTR? What are some reasons for this, and what are a few steps that can be taken to increase control?

(b) In Graph 1, why are points A and C stable operating points, while point B is an unstable operating point?

SOLUTION:

(a) An exothermic CSTR is harder to control. The relationship between heat generation and temperature is non-linear for an exothermic system (Graph 1). If the rate of heat generation exceeds the maximum rate of heat removal then the temperature will runaway.

An endothermic CSTR is much easier to control because these reactors are self-regulating and there is no concern for runaway temperatures.

The control of an exothermic CSTR can be increased by reducing the feed flow of the reactants, reducing the concentration of reactants and increasing the ratio of the heat transfer surface area to the reactor volume.

(b)

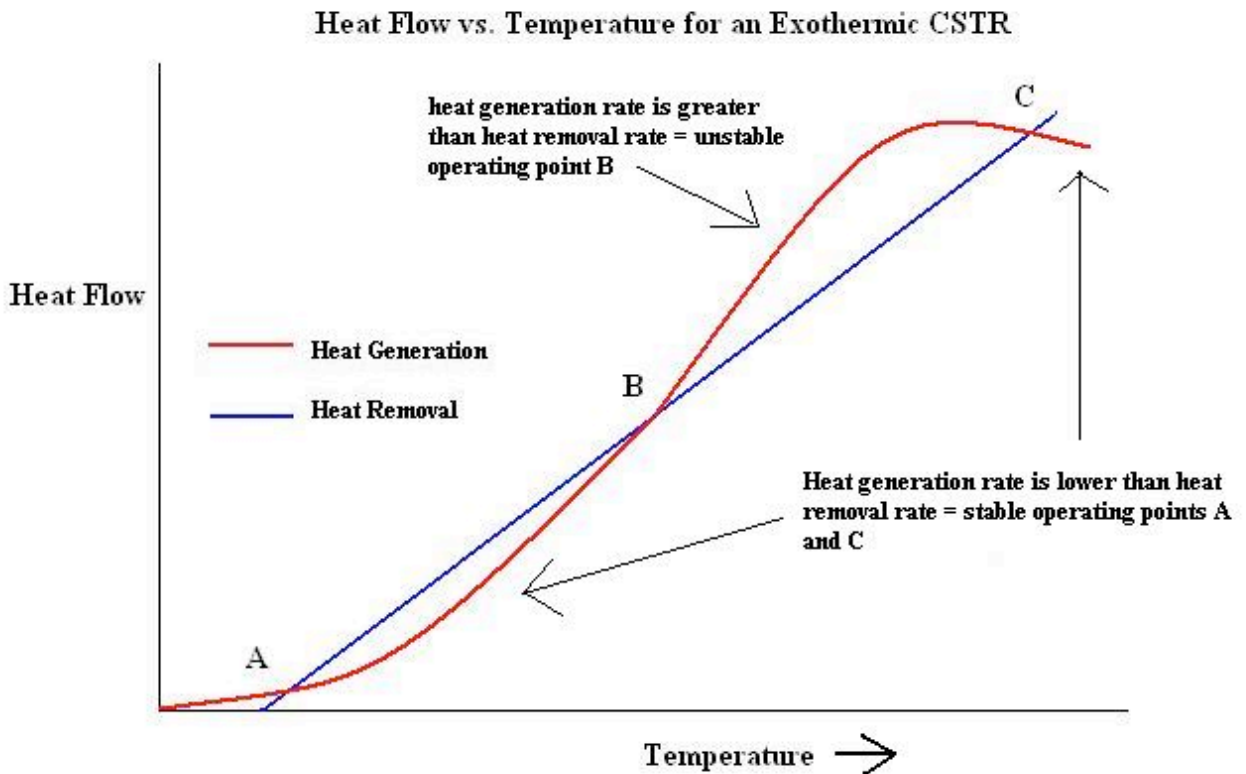


Figure E1-1. Relationship between heat generation or heat removal and temperature for an exothermic system.

Points A and C are stable because if you increase the temperature from this point, the heat generation rate is lower than the heat removal rate. If you increase the temperature from point B, the heat generation rate is higher than that heat removal rate, which is not desired. If the rate of heat generation is greater than the heat removal then the temperature is rising and could possible runaway. This is an unstable state for the reactor.

7.6 Worked out Example 2

Refer to [Heat Exchanger Modeling](#) Worked Example 1 problem statement.

After you successfully created your ODE model, you are assigned a partner who will work along with you to put temperature controls on the heat exchanger. Your partner, a new college graduate, seems to remember that in his process controls class, the best way to control a temperature loop for a heat exchanger is to make the flow rate of the coolant stream the manipulated variable. Since you are such a process guru, you know that this is not right. However, the hot shot college graduate just feels that you are over the hill and he knows his stuff.

Vary the coolant flow rate in the [Euler's Method](#) heat exchanger to demonstrate to your new partner why it is not a good idea to place the controls on the coolant side flow of a stream. Produce a process gain plot similar to that in the article to show this. Also, find the magnitude of the process gain for three different points in the plot: low, medium and high coolant flow rate, to show process gain goes to zero as the coolant flow rate increases.

SOLUTION

Note that in this case we are dealing with a liquid/liquid heat exchanger and the hot stream is the process stream. The table below summarizes the results.

Controller Flow Rate	Process Stream Exit Temperature
m ³ /s	K
0	330
0.05	288.156
0.075	279.61
0.1	274.506
0.2	266.171
0.3	263.374
0.4	262.005
0.5	261.198
0.6	260.667
0.7	260.291
0.8	260.291
0.9	259.798
1	259.626

Table E2-1. Process stream exit temperature as a function of coolant flow rate.

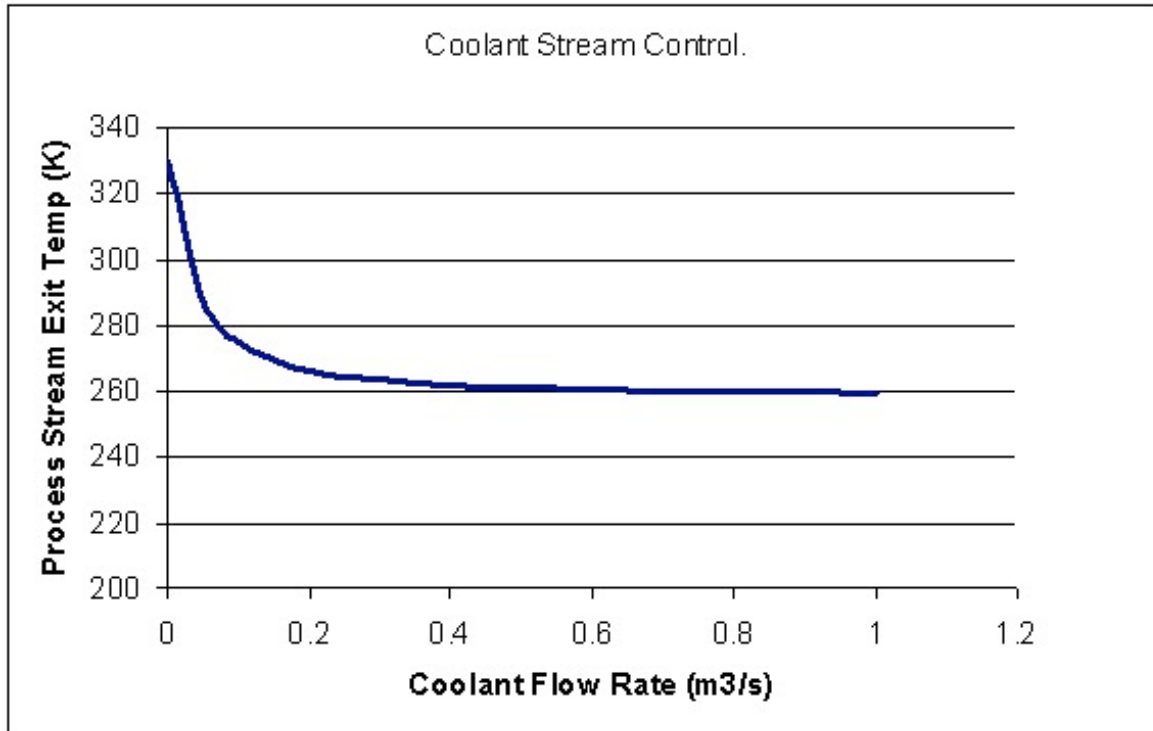


Figure E2-1. A continuous picture of how the magnitude of process gain decreases to zero as the coolant flow rate is increased.

From the graph or table above one can show that the magnitude of process gain decreases as the coolant flow rate increases. This is done as follows;

Magnitude of process gain for;

Low flow rates, choose from 0 to 0.1 m^3 / s .

$$= |330 - 274.50| = 55.5K$$

Medium flow rates, choose (same interval size) from 0.4 to 0.5 m^3 / s .

$$= |262.01 - 261.20| = 0.81K$$

High flow rates, choose (again same interval size) from 0.9 to 1 m^3 / s .

$$= |259.798 - 259.626| = 0.172 K$$

Clearly, as the flow rate increases, the magnitude of process gain decreases towards zero. This puts a limit on the amount of control of the heat exchanger if the coolant flow rate is chosen as the MV in the temperature control loop.

7.7 Multiple Choice Question 1

What two types of endothermic CSTR temperature control methods are there?

- a. steam flow rate and reactor level
- b. reactor composition and reactor level
- c. steam flow rate and steam pressure
- d. reactant flow rate and reactor level

7.8 Multiple Choice Question 2

What are temperature controllers commonly used for in distillation columns?


- a. To control composition
- b. To control reflux ratio
- c. To control pressure
- d. None of the above

7.9 References

- Svrcek, W., Mahoney, D., Young, B.. *A Real-Time Approach to Process Control*. Second Edition. John Wiley and Sons.
- Riggs, James B., Karim, Nazmul M.. *Chemical and Bio-Process Control*. Third Edition Chapter 18. Ferret Publishing.

Section 8. Common control architectures / model for reactors

Title: Common Control Architectures for Reactors

Note:  [Video lecture](#) available for this section!

Authors: Brian McQuillan, Crystal Miranda, Brandon Quigley, and John Zhang

Date Presented: Oct. 31, 2006

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

8.1 Introduction

Reactors are the central focus of many chemical plants. Many parameters must be controlled in a reactor for proper operation. Temperature is of great importance because it affects reaction rates and equilibrium relationships. A major challenge for temperature control is handling the nonlinear nature of temperature inside most reactors. Therefore, it is important to design an effective control architecture in order to ensure optimal operation of the reactor.

This article discusses the common control architectures and topologies in CSTRs. The control architectures are designed based on whether the reactor is endothermic or exothermic. The same concepts introduced in the wiki can be applied to other reactors as well. However, only CSTRs will be discussed for simplicity.

8.2 Common Topologies

Here we will introduce a few of the most common control topologies which will be examined in applications to endothermic and exothermic CSTRs below. Please refer to the specific wiki pages for each type for detail.

8.2.1 Feedback and Feed-Forward

Feedback and feed-forward refer to the direction in which the sensor information is transferred to an actuator valve. Feedback control dictates that sensor information is "fed back" to a previous part of the process. For example, the reading from a level sensor of a filling tank can be "fed back" to the valve controlling the input to the tank. Feed-forward control means the sensor information is used to control something downstream from where the reading was taken. For example, the measured flow rate of water going into an evaporator can be used to control the heating coil inside of the evaporator. For detail about these two control topologies, please see the respective pages: [Feedback Control](#) [Feed-Forward Control](#).

8.2.2 Ratio Control

Ratio Control is used when the ratio between two measured process variables has an optimal value. In the context of two input streams with optimal flow ratio going into a reactor, one stream is designated as the control stream, and one stream is designated as the wild stream. The wild stream fluctuates, and a valve on the control stream is opened or closed to maintain the ratio between the two stream flows. For detail about ratio control, see [Ratio Control](#).

8.2.3 Cascade Control

Cascade control simply means that instead of one control loop found in simple control topologies where a sensor's measurement directly controls an actuator valve, multiple loops are used so that sensors' measurements can control set points for other controllers. For example, the temperature sensor measurement of process fluid exiting a reactor can be used to modify the set point of the flow controller of steam feeding the heating jacket, which then sets the steam valve. This multiple-loop system eliminates some problems caused by variable-pressure feeds, for instance. For detail about cascade control, see [Cascade Control](#).

8.3 Disturbances to CSTRs

There are a few very common disturbances that CSTR may be subjected to. When designing a control architecture for a CSTR, you must investigate the possibility of all of these disturbances, determine the magnitude of each possible disturbance, and address how each will be handled.

- Changes in feed properties
 - flow rate
 - composition
 - temperature
- Changes in enthalpy of heat exchange medium
- Change in heat transfer properties (ex: fouling)

8.4 Disturbances to PFRs

Plug Flow Reactors (PFRs) behave differently than CSTRs and will have different properties to consider when designing a control architecture for them. The biggest difference is that the temperature, flows, and compositions will all vary along the reactor. There is danger of exceeding a design limitation in temperature or flow in certain parts of the PFR, so control of the reactor is important along its length. To design a control architecture for a PFR, the following disturbances and changes to the system must be addressed:

- Temperature control in multiple places along reactor (hot spots can easily occur in PFRs)

- Flow control in multiple places along the reactor
- Inlet/outlet pressures
- Feed property disturbances:
 - flow rate
 - composition
 - temperature
- Changes in enthalpy of heat exchange medium
- Change in heat transfer properties (ex: fouling)

8.5 Endothermic Reactors

DISCLAIMER: All reactors shown possess two controllers. We realize that in the real-world a reactor would require more than two temperature controllers but we are concerned primarily with the common placement of controllers outside of the reactor in this wiki. Thank you and continue reading.

Endothermic reactors tend to be easier to control than exothermic ones because they are much less prone to runaway. There are two commonly used methods to control an endothermic CSTR. These two methods are differentiated by the variables they manipulate. In the first method, the steam pressure in the reactor jacket is the manipulated variable, whereas in the second method, the steam flowrate is the manipulated variable. In endothermic reactors, as well as exothermic ones as we will later see, feedback is the most common type of control system used. This is done to ensure that changes are being based on what is actually happening in the reactor and not what is predicted to happen. This is important in the endothermic case to ensure that the proper amount of heat is being added to the reactor to obtain a desired conversion. Feedback is more useful for control since the amount of heat needed can change quickly based on the amount or concentration of reactants being added. Generally the temperature control of the reactor is independent of the reactant feed, so the system needs a way to adjust to changes within reactant feed, and this is accomplished by using feedback control in the streams that control the temperature (i.e. the steam feed stream).

8.5.1 Controlled by Steam Pressure

Heat duty can be more effectively removed with the use of steam pressure as the manipulated variable because changes in the heat duty of the reactor will cause an immediate change in the steam pressure. By using the steam pressure, it also linearizes the temperature control system which is not the case when the steam flowrate is the manipulated variable. Using the steam pressure as the manipulated variable does not provide a direct measurement of the heat load, the amount of heat needed by the reactor. If a direct measurement is required, a steam flow indicator can be installed which would allow for the direct measurement of the applied heat load. An added benefit, which those of you who have worked with the temperature controller in ChE 460 might have noticed, is that often times the pressure of steam being provided by the utilities plant is variable. By using the steam pressure as the manipulated variable the control system will automatically adjust to this type of disturbance from the source. If a large change in

steam pressure were to occur, the pressure controller would measure this change, and the control scheme would intake the change in steam pressure and translate this into an appropriate change in the valve setting.

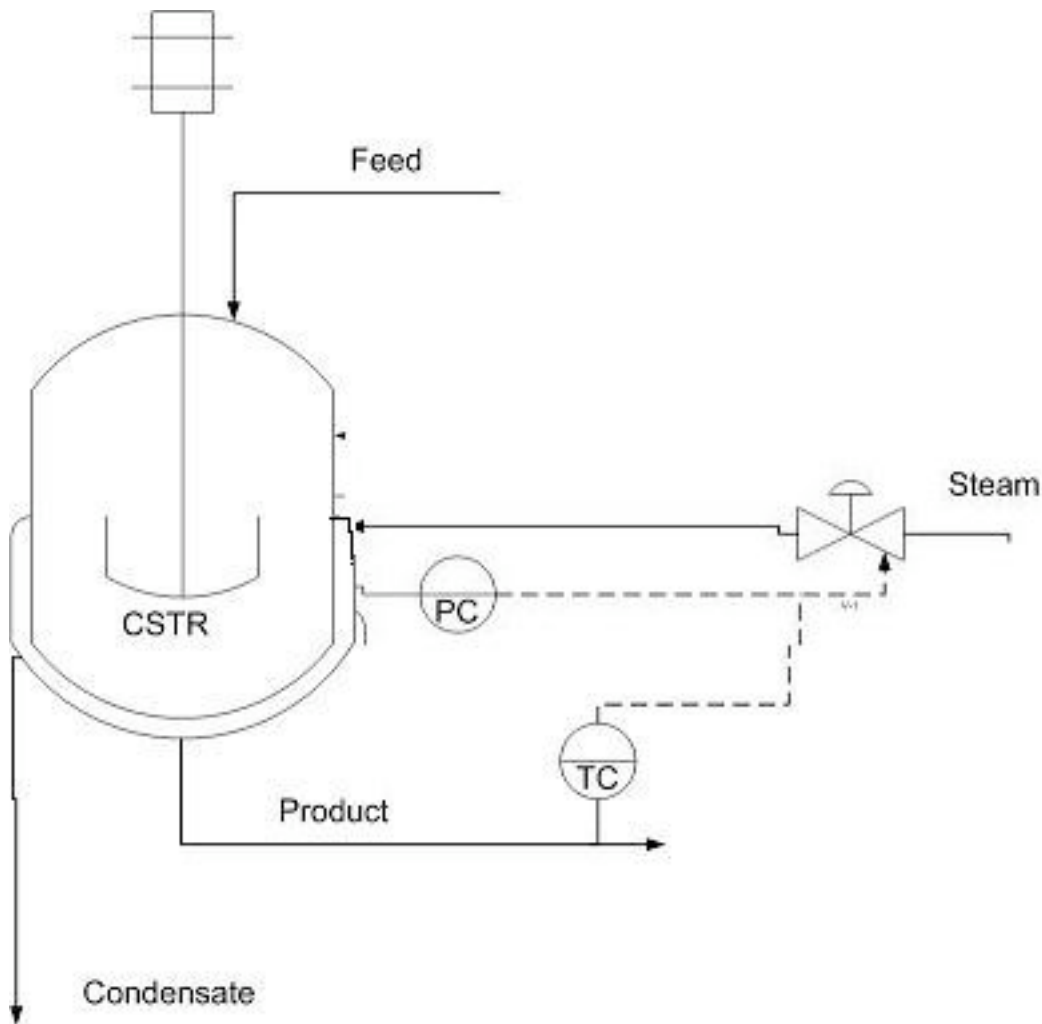


Image Modified From: Riggs, James B., Karim, Nazmul M.. Chemical and Bio-Process Control. Third Edition Chapter 18. Ferret Publishing.

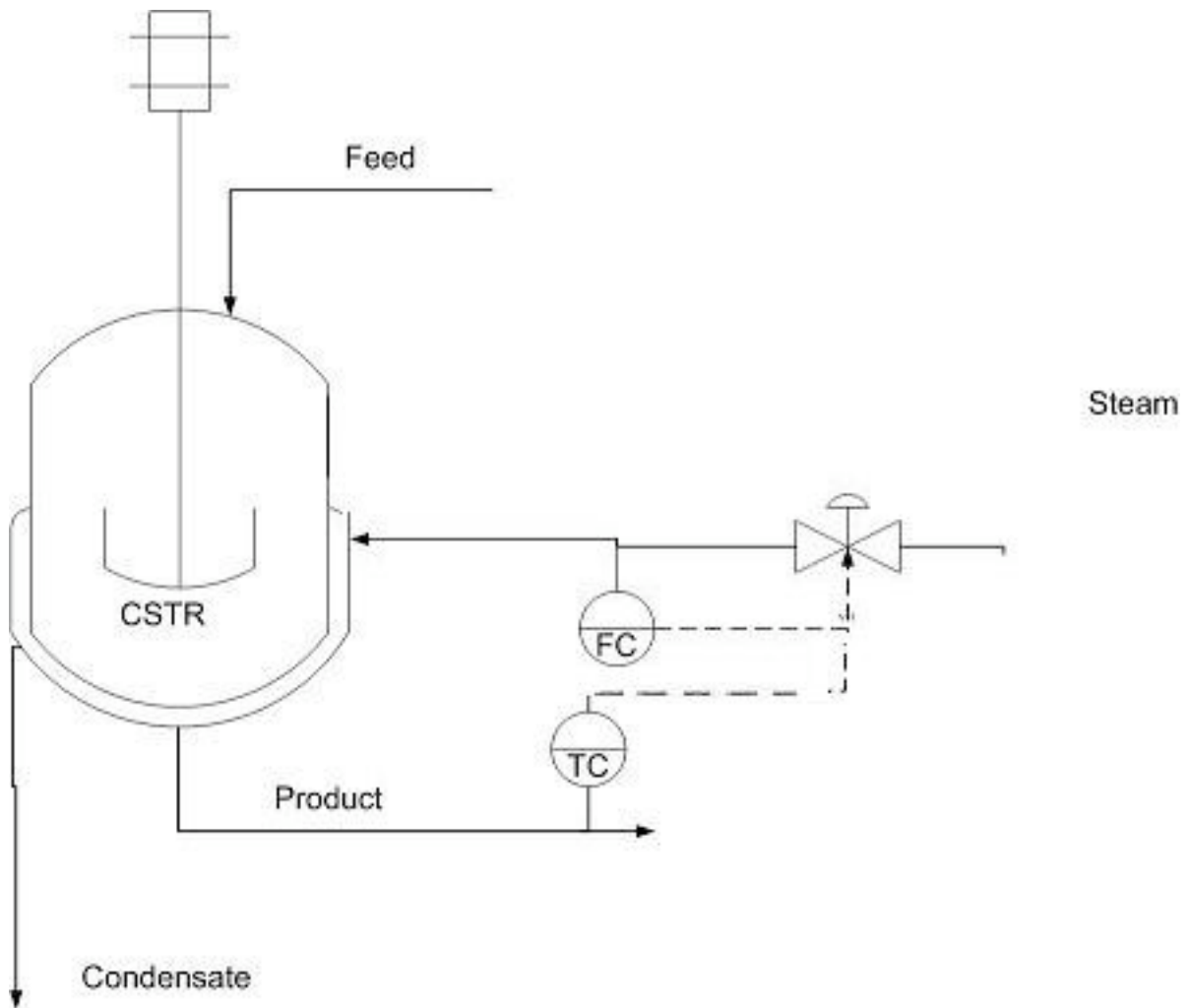
As can be seen in the figure above, when steam pressure is used as the manipulated variable the control system is run in a feedback mode. One of two things can control the amount of steam fed into the jacket. The first is the temperature of the product, and the second is the steam pressure in the jacket. As mentioned above, a change in the heat duty required by the reactor will quickly change the steam pressure which is why it is commonly used over the steam flowrate.

Notice that there are two controllers that are responsible for adjusting the steam valve. The pressure controller is sensitive to changes in the heat duty required by the reactor and

is used to adjust the steam according to the needs of the temperature controller on the product stream. This is a prime example of cascade control. The temperature of the product stream would output a setpoint to the pressure controller for the amount of steam needed to attain the desired temperature setpoint. The pressure controller would then communicate to the valve what needs to be done in order to achieve this temperature setpoint based on the steam pressure.

8.5.2 Controlled by Steam Flowrate

The second method for controlling an endothermic CSTR is by manipulating the steam flow rate. Using flow rate as the manipulated variable makes the control system prone to changes in heat load and changes in the enthalpy of supplied steam. These changes require direct action of the temperature control system. One advantage of using flowrate as the manipulated variable is that heat load is directly measured, and thus, conversion is directly measured.



As can be seen in the figure above the system works in a feedback mode when the steam flowrate is used as the manipulated variable. The temperature of the product stream is the

primary factor in adjusting the amount of steam fed into the system, and therefore this system is less responsive to changes in the amount of heat duty required for the process.

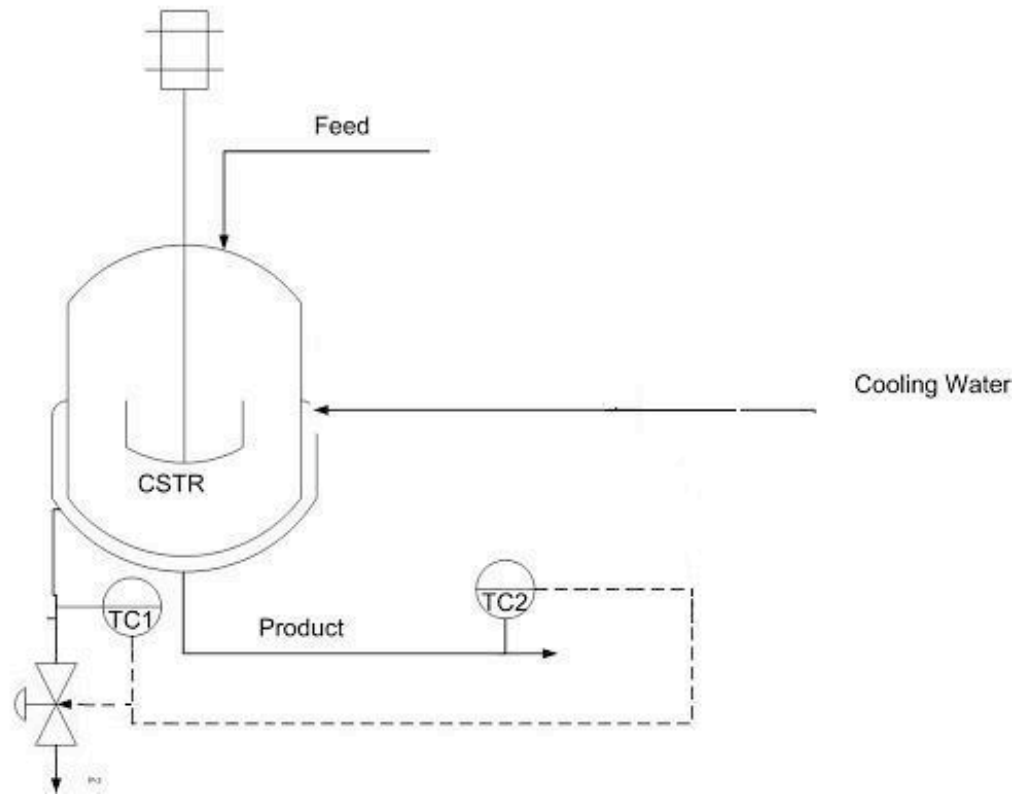
Note here that there are again two controllers used to adjust the steam valve. This setup is similar to the previous case, but now the flow controller is the "slave" controller to the temperature controller. The cascade control scheme is again at work!

Control Architecture for Endothermic Reactor		
Manipulated Variable	Advantage	Disadvantage
Steam pressure	More responsive to changes in heat duty	No direct measurement of heat load
	Linearizes temperature control system	
Steam flowrate	Heat load and conversion directly measured	Less responsive to changes in heat duty

8.6 Exothermic Reactors

Exothermic reactors are harder to control because safety is dependent on heat removal. There are two common control architectures for an exothermic CSTR based on the temperature of the coolant. The first method uses the outlet temperature of the coolant as the manipulated variable, while the second method uses the inlet temperature of the coolant. Just like the endothermic reactors, feedback control is very commonly used when controlling the temperature of exothermic reactors. The reasoning for feedback control in the exothermic case is slightly different but similar to that of endothermic reactors. In endothermic reactors we wanted to ensure that the proper amount of heat was being supplied to our reactor, and if the amount needed changed; we needed a way to adjust our temperature accordingly. In the exothermic case we need to ensure that we are removing the proper amount of heat, not only to ensure an optimal reaction temperature, but also to prevent a runaway reaction. Therefore, we need to know what is actually going on within the reactor instead of forecasting possible temperature changes within it. Cascade control is also used. In this case the temperature of the product stream outputs a setpoint to the temperature controller whether it be located on the outlet or inlet coolant feed. The "slave" controller can then adjust the valve position based on the temperature of the coolant water.

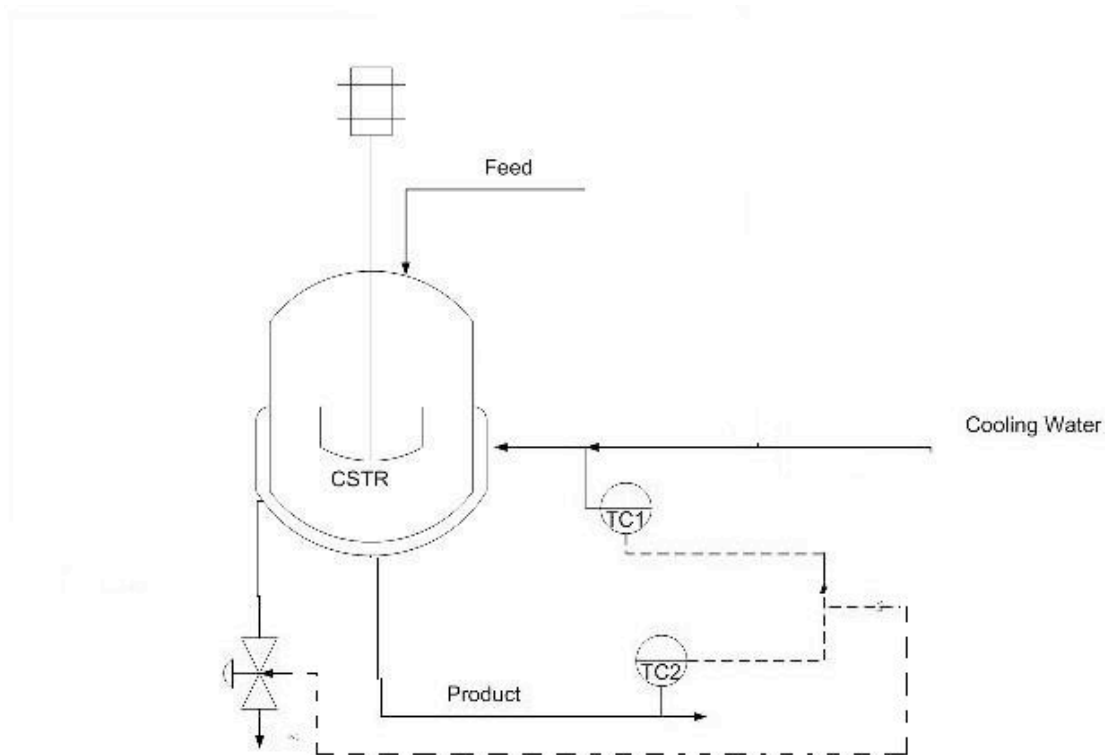
8.6.1 Controlled by Outlet Coolant Temperature



The figure above shows the control architecture for CSTR reactor temperature controlled by outlet coolant temperature in a feedback mechanism. There is a temperature control on both the product stream and outlet coolant temperature. Both of the temperature controls are used to control the valve on the inlet coolant stream. The advantage of this setup is that it responds faster to fouling on heat-transfer surfaces than the setup with the temperature controller on the inlet. This is because in order for the inlet temperature to adjust to fouling, the fouling must first affect the temperature of the product stream. Therefore the fouling has less direct effect on the controller, but in this case fouling will immediately affect the temperature of the exiting cooling water. However, this setup has the disadvantage of responding slower to changes in the inlet coolant temperature.

As can be seen in the above diagram you will notice that again cascade control is utilized in this particular system. The temperature sensor on the product stream provides information on whether the stream needs to be cooled more or less and outputs a setpoint to the temperature controller on the recycle stream. This controller can then take into account the temperature of the recycled coolant water and make an adjustment to the amount of fresh coolant water that is added to the system.

8.6.2 Controlled by Inlet Coolant Temperature



As seen in the figure above, the control configuration for CSTR reactor temperature is controlled by inlet coolant temperature in a feedforward mechanism. There are temperature controls on both the product stream and inlet coolant temperature; both of the controls are used to control the valve on the inlet coolant stream. One advantage of this setup is that it responds faster to changes in inlet coolant temperature. A disadvantage is that it responds slower to fouling on heat-transfer surfaces.

8.6.3 More on Exothermic Reactors

How do you decide which exothermic reactor control architecture to use? It depends on whether a faster response to fouling on heat-transfer surfaces or a faster response to changes in inlet coolant temperature is more important.

In addition to stabilizing the temperature within an exothermic reactor, it is often a goal to maximize production rate. This can be achieved by placing a valve on the feed stream. As the temperature control adjusts the cold water valve, the cold water valve position is then communicated to the feed valve and adjusts it.

Cascade control is again utilized. In this case the secondary or "slave" controller is located in a different location, which is the only difference between the two scenarios.

Control Architecture for Exothermic Reactor		
Manipulated Variable	Advantage	Disadvantage
Outlet coolant temperature	Faster response to fouling on heat-transfer surfaces.	Slower response to changes in inlet coolant temperature
Inlet coolant temperature	Faster response to changes in inlet coolant temperature	Slower response to fouling on heat-transfer surfaces

8.7 Worked out Example 1

As part of a community outreach program, your company is sponsoring a haunted house. The haunted house is being constructed on site in an old, dilapidated warehouse located on the plant property. You have been put in charge of designing a scene in which a witch is creating a witch's brew. It has been proposed that you use a reaction between "Witch's Brew Deluxe", a commercial compound used in the haunted house industry, dry ice, and water.

Dry Ice + "Witch's Brew Deluxe" + Water --> Bubbles + Mist

The manufacturer of "Witch's Brew Deluxe" supplies optimal conditions for real life cauldron imitation at 30°C water temperature. Temperatures in excess of this result in a surplus of cauldron bubbles and mist which impair the visual experience. Temperatures below this do not allow for large enough reaction rates and do not produce any steam or bubbles.

The reaction is highly endothermic, so a supply of steam has been diverted from the main plant to supply heat to the reactor. However, due to the great distance this steam is traveling, the supply steam pressure is highly variable. An uncovered, jacketed CSTR is available for use as a cauldron. A mixture of water and "Witch's Brew Deluxe" is constantly fed into the reactor, and solid dry ice is manually feed by the operator.

What control scheme is most suitable for temperature control and why? Specifically, what should you use as the manipulated variable?



SOLUTION

Because the steam supply pressure will vary greatly, a steam pressure control architecture is preferred. By monitoring the jacket pressure, changes in steam supply pressure will immediately be observed and corrected for.

8.8 Worked out Example 2

You have just recently taken a job offer from a haunted engineering firm run by a group of witches located in Salem, Massachusetts. As the new guy on the job they

would like your input on which variable they should treat as the manipulated variable for the reactor temperature controller. Their reactor is an exothermic CSTR. The following reaction is what takes place within this CSTR.

3 frog's legs + 2 cow hooves --> 4 moles of magic elixir

The magic elixir is generally used as a wart remover but also shows promise as an antacid.

The head witch at the plant tells you that significant fouling occurs on the heat transfer surfaces because the city only allows them access to dirty water with high mineral content because they are witches and generally considered substandard citizens. She (the head witch) also points out that they have recently developed a spell to maintain the inlet temperature and pressure of their coolant water.

Which variable should be the manipulated one and why?'

SOLUTION

The correct manipulated variable for the reactor temperature controller would be the outlet coolant temperature. This allows for a quicker response to fouled heat-transfer surfaces. Since the head witch told you that inlet temperature and pressure are constant, the configuration's weakness to changes in these two parameters can be overlooked.

8.9 Multiple Choice Question 1

Which type of REACTION is generally much easier to control?

- a) Endothermic
- b) Distillation of alcohol
- c) Cold Fusion
- d) Exothermic

8.10 Multiple Choice Question 2

By using the _____ as the manipulated variable, it linearizes the temperature control system which is not the case when the steam flowrate is the manipulated variable.

- a) feed flow rate

- b)** steam pressure
- c)** product composition
- d)** rate of mixing


8.11 *References*

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Chapter 12. MIMO Control

Section 1. Determining if a system can be decoupled

Title: Determining if a System can be Decoupled

Note:  [Video lecture](#) available for this section!

Authors: Wen Chung Lim, James Bennett, Jamila Grant, Ajay Bhasin
Date Presented: 11/07/06

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

1.1 Introduction

A system of inputs and outputs can be described as one of four types: SISO (single input, single output), SIMO (single input, multiple output), MISO (multiple input, single output), or MIMO (multiple input, multiple output).

Multiple input, multiple output (MIMO) systems describe processes with more than one input and more than one output which require multiple control loops. Examples of MIMO systems include heat exchangers, chemical reactors, and distillation columns. These systems can be complicated through loop interactions that result in variables with unexpected effects. Decoupling the variables of that system will improve the control of that process.

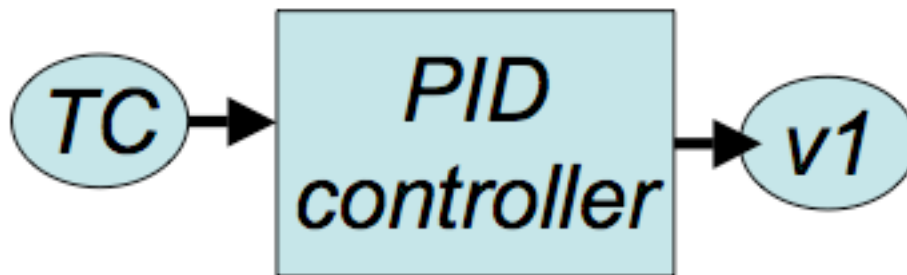
An example of a MIMO system is a jacketed CSTR in which the formation of the product is dependent upon the reactor temperature and feed flow rate. The process is controlled by two loops, a composition control loop and a temperature control loop. Changes to the feed rate are used to control the product composition and changes to the reactor temperature are made by increasing or decreasing the temperature of the jacket. However, changes made to the feed would change the reaction mass, and hence the temperature, and changes made to temperature would change the reaction rate, and hence influence the composition. This is an example of loop interactions. Loop interactions need to be avoided because changes in one loop might cause destabilizing changes in another loop. To avoid loop interactions, MIMO systems can be decoupled into separate loops known as single input, single output (SISO) systems. Decoupling may be done using several different techniques, including restructuring the pairing of variables, minimizing interactions by detuning conflicting control loops, opening loops and putting them in manual control, and using linear combinations of manipulated and/or controlled variables. If the system can't be decoupled, then other methods such as [neural networks](#) or [model predictive control](#) should be used to characterize the system.

There are two ways to see if a system can be decoupled. One way is with mathematical models and the other way is a more intuitive educated guessing method. Mathematical

methods for simplifying MIMO control schemes include the [relative gain array \(RGA\)](#) method, the Niederlinski index (NI) and singular value decomposition (SVD). This article will discuss the determination of whether a MIMO control scheme can be decoupled to SISO using the SVD method. It will also discuss a more intuitive way of decoupling a system using a variation of the RGA method.

1.1.1 Definitions of Input and Output System Types

1. SISO- *Single Input, Single Output*



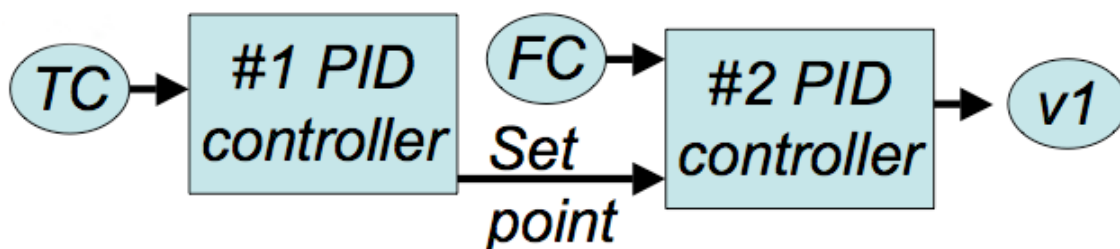
These systems use data/input from one sensor to control one output. These are the simplest to design since they correspond one sensor to one actuator. For example, temperature (TC) is used to control the valve state of v1 through a PID controller.

2. SIMO- *Single Input, Multiple Output*



These systems use data/input from one sensor to control multiple outputs. For example, temperature (TC) is used to control the valve state of v1 and v2 through PID controllers.

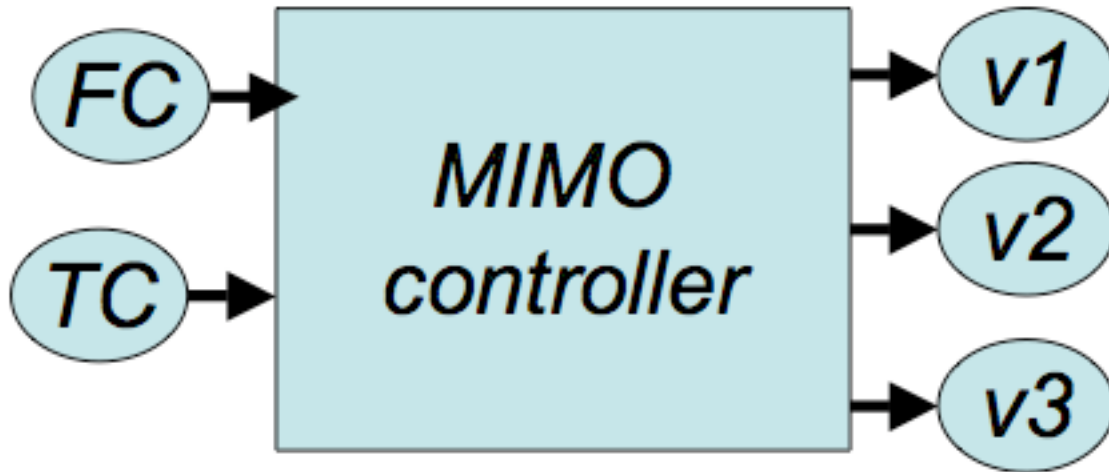
3. MISO- *Multiple Input, Single Output*



These systems use data/input from multiple sensors to control one output. For example, a cascade controller can be considered MISO. Temperature (TC) is used in a PID controller

(#1) to determine a flow rate set point i.e. FCset. With the FCset and FC controller, they are used to control the valve state of v1 through a PID controller (#2).

4. MIMO- *Multiple Input, Multiple Output*



These systems use data/input from multiple sensors to control multiple outputs. These are usually the hardest to design since multiple sensor data is integrated to coordinate multiple actuators. For example, flow rate (FC) and temperature (TC) are used to control multiple valves (v1, v2, and v3). Often, MIMO systems are not PID controllers but rather designed for a specific situation.

1.2 Singular Value Decomposition

Singular value decomposition is a useful mathematical way to determine if a system will be prone to interactions due to sensitivity problems that result from small errors in process gains. It is a matrix technique that determines if a system is able to be decoupled.

1.2.1 Two input two output system

The SVD method starts with the steady state gain matrix, which is obtained from the relative gain array (RGA) method for a given 2 input-2 output control loop system:

$$[G] = \begin{bmatrix} g_{1,1} & g_{1,2} \\ g_{2,1} & g_{2,2} \end{bmatrix},$$

Using [G], we obtain the eigenvalues for the system. This can be done through two methods; either the eigenvalues can be obtained through numerical software as described in the [Eigenvalues and Eigenvectors](#) section or the eigenvalues can be calculated by hand. The hand calculations are shown here. [G] gives the following values for the system, which have been derived from theoretical work and are used to find the eigenvalues:

$$b = g_{11}^2 + g_{12}^2 \text{-----(1)}$$

$$c = g_{11}g_{21} + g_{12}g_{22} \text{-----(2)}$$

$$d = g_{21}^2 + g_{22}^2 \text{-----(3)}$$

b, c, and d are parameters created for this method that do not have a direct physical meaning. Using the formulas below with the values of b, c, and d gives the eigenvalues for the system:

$$\lambda_1 = s_1^2 = \frac{b + d + \sqrt{(b - d)^2 + 4c^2}}{2} \text{-----(4)}$$

$$\lambda_2 = s_2^2 = \frac{bd - c^2}{s_1^2} \text{-----(5)}$$

s_1 and s_2 are the positive square roots of the respective eigenvalues. The condition number CN is defined as the ratio of the larger of the two values to the smaller value:

$$CN = \frac{s_1}{s_2} \text{ if } s_1 \geq s_2, \text{ or } CN = \frac{s_2}{s_1} \text{ if } s_2 \geq s_1$$

The greater the CN value, the harder it is for the system in question to be decoupled. As a rule of thumb, a system with a CN number of more than 50 is impossible to decouple. Such a system has manipulated variables which all have significant and similar relative impact on the controlled variables they affect and hence the control equations for the system cannot be restructured to obtain a simpler control system. In the worst case scenario for a two input two output system, using the exact same control variable twice would give a CN number of infinity, because both control variables would have the same effect on the controlled variables. An ideal system would have a CN number of one, where each control variable controls a single distinct output variable.

1.2.2 MIMO systems with two or more inputs and outputs

To use this method, it is necessary to know how to create a transpose matrix. A transpose matrix is created by writing the columns of the original matrix as the rows of the transpose matrix. Mathematically, the transpose matrix is denoted by $[A]^T$, where $[A]$ is

$$\begin{bmatrix} i & j \\ k & l \end{bmatrix}^T = \begin{bmatrix} i & k \\ j & l \end{bmatrix}$$

the original matrix. An example is shown here:

To use singular value decomposition on systems with two or more inputs and outputs, the $m \times m$ steady state gain matrix $[G]$ of the form

$$[G] = \begin{bmatrix} g_{1,1} & g_{1,2} & \cdots & g_{1,m} \\ g_{2,1} & g_{2,2} & \cdots & g_{2,m} \\ \vdots & & & \\ g_{n,1} & g_{n,2} & \cdots & g_{n,m} \end{bmatrix}$$

is broken down into the form:

$$G = U\Sigma V^T$$

Where:

* U is an $m \times m$ matrix, the column vectors of which are the unit eigenvectors of the $m \times m$ matrix GG^T , G^T being the transpose matrix of G .

* V is an $m \times m$ matrix, the column vectors of which are the unit eigenvectors of the $m \times m$ matrix G^TG .

* Σ is an $m \times m$ diagonal matrix containing singular values, where the values are arranged in descending order from the top left most corner to the bottom right corner.

$$\Sigma = \begin{bmatrix} s_1 & 0 \\ 0 & s_2 \end{bmatrix} \text{ for a 2 input 2 output system if } s_1 \geq s_2, \text{ or}$$

$$\Sigma = \begin{bmatrix} s_2 & 0 \\ 0 & s_1 \end{bmatrix} \text{ for a 2 input 2 output system if } s_2 \geq s_1.$$

The CN number can then be determined by the ratio of the largest value in Σ to the smallest value. Notice in the previous two input two output example, there was no need to calculate the eigenvalue matrix Σ for a two by two matrix, since the eigenvalues can be calculated directly with the parameters b, c , and d .

For more information on how to derive the three matrices U, Σ and V by hand, refer to the [Eigenvalues and Eigenvectors](#) section.

Mathematica can also be used to find U, Σ and V for a given $m \times m$ Matrix G . This is accomplished by typing in the command

Map[MatrixForm, {u, w, v} = SingularValueDecomposition[G]],

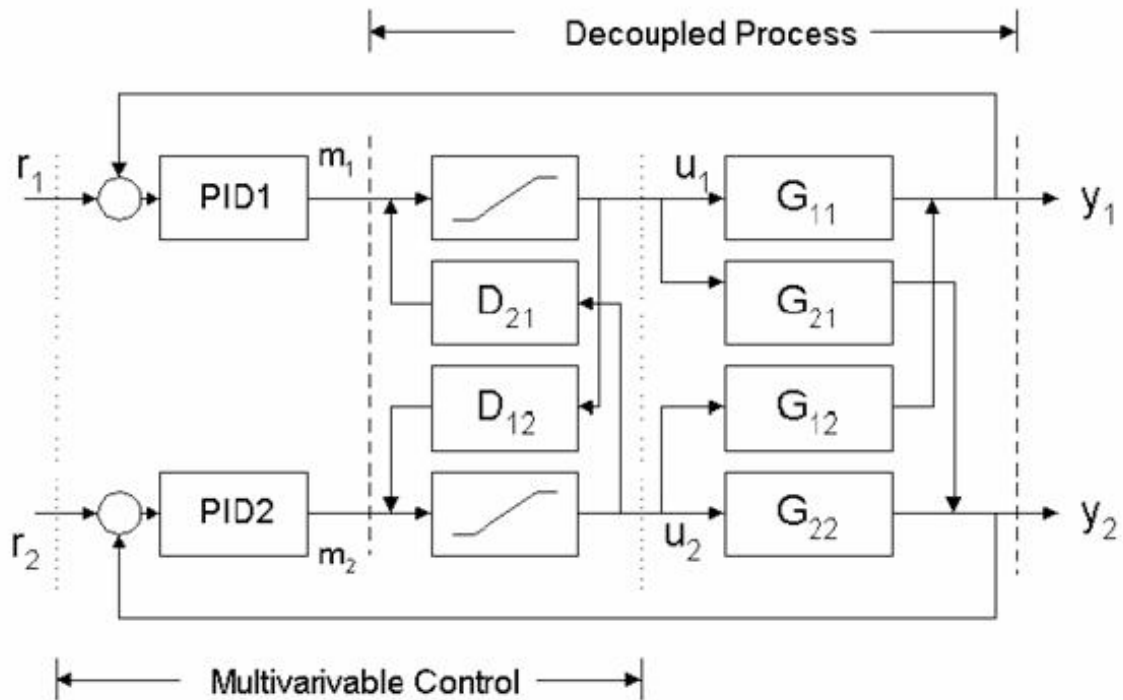
giving U, Σ and V in that order.

1.2.3 Intuitive decoupling using the RGA

With this technique, the first step is to construct the RGA by placing all of the controllers in manual, changing the value of the output manually, and then recording the final value of the controller after making the change. This will give the gain matrix, which is then multiplied by its inverse to give the relative gain matrix. The goal here is to pair measurements and control valves so that the relative gain elements are close to 1, and all other combinations are close to zero. A value between 0 and 1 tells that the net effect of the other loops on this pairing is to change the measurement signal in the same direction as the control valve signal (cooperation). A value greater than one means that the measurement signal will go in the opposite direction of the control valve signal (conflict). Finally a relative gain element less than zero means that the net effect is conflict, but here the gain will change sign, not the measurement signal. Therefore, if a loop is stable when the other loops are in manual, it will probably not be stable when the other loops are in automatic, and vice versa. To intuitively decouple this system then would require a guess and check of different pairings, with the goal being to get the pairings to a relative gain element close to one. If this is not possible and no pairings give a value close to one, then the system will need to be decoupled using decoupling control.

1.2.4 Decoupling a system using decoupling control

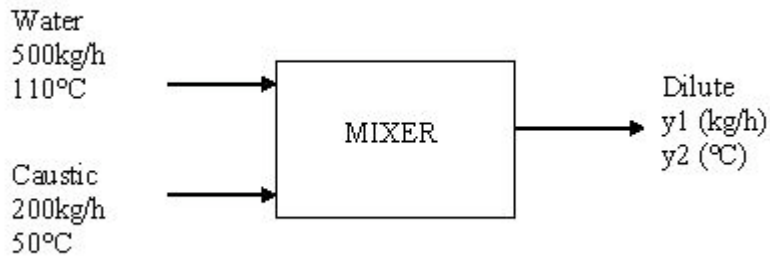
The goal of decoupling control is to eliminate complicated loop interactions so that a change in one process variable will not cause corresponding changes in other process variables. To do this a non-interacting or decoupling control scheme is used. In this scheme, a compensation network called a decoupler is used right before the process. This decoupler is the inverse of the gain array and allows for all measurements to be passed through it in order to give full decoupling of all of the loops. This is shown pictorially below.



For a simple jacketed reactor example, if changing the flow rate of reactant to obtain a desired composition also increases the reactor temperature by five degrees, the decoupler would decrease the temperature of the jacket to decrease the temperature inside the reactor by five degrees, offsetting the original change. This jacket temperature decrease also changes the composition inside the reactor, so a properly designed controller accounts for both effects in the control scheme to obtain the desired composition without changing the reactor temperature.

1.3 Worked out Example 1

Hot water at 110°C is pumped into a mixer at 500 kg/h. The water is used to dilute a concentrated caustic substance at 50°C flowing in at 200 kg/h. Below is a diagram of the process. Check, by the singular value decomposition method, to see if decoupling of the system is feasible. Assume that the heat capacities of both streams are the same with no heat of mixing.



Solution :

From the question you know:

$$T_1 = 383.15 \text{ K}$$

$$T_2 = 323.15 \text{ K}$$

$$m_1 = 500 \text{ kg/h}$$

$$m_2 = 200 \text{ kg/h}$$

$$y_1 = \text{outgoing mass flow rate (kg/h)}$$

$$y_2 = \text{temperature of outflowing stream (K)}$$

From mass balances you know:

$$y_1 = (m_1 + m_2)$$

$$y_2 = \frac{T_1 m_1 + T_2 m_2}{y_1}$$

So:

$$y_1 = 700 \text{ kg/h}$$

$$y_2 = 366.01 \text{ K}$$

The steady state gain matrix (G) needs to be calculated as explained in the [RGA method](#):

$$G = \begin{bmatrix} g_{1,1} & g_{1,2} \\ g_{2,1} & g_{2,2} \end{bmatrix}$$

$$g_{1,1} = \left. \frac{\partial y_1}{\partial m_1} \right|_{m_2=\text{constant}} = \frac{\partial}{\partial m_1}(m_1 + m_2) = 1$$

$$g_{2,1} = \left. \frac{\partial y_2}{\partial m_1} \right|_{m_2=\text{constant}} = \frac{\partial}{\partial m_1} \left(\frac{T_1 m_1 + T_2 m_2}{m_1 + m_2} \right) = \left[\frac{(T_1 - T_2)m_2}{(m_1 + m_2)^2} \right]$$

$$g_{1,2} = \left. \frac{\partial y_1}{\partial m_2} \right|_{m_1=\text{constant}} = \frac{\partial}{\partial m_2}(m_1 + m_2) = 1$$

$$g_{2,2} = \left. \frac{\partial y_2}{\partial m_2} \right|_{m_1=\text{constant}} = \left[\frac{(T_2 - T_1)m_1}{(m_1 + m_2)^2} \right]$$

By plugging in all known values, the steady state gain matrix becomes:

$$G = \begin{bmatrix} 1 & 1 \\ 0.0245 & -0.0612 \end{bmatrix}$$

From here you can solve for the values b, c, d λ_1 , λ_2 , s_1 and s_2 by using the equations (1) through (5) in the wiki:

$$b = g_{11}^2 + g_{12}^2 = 1^2 + 1^2 = 2$$

$$c = g_{11}g_{21} + g_{12}g_{22} = (1)(.0245) + (1)(- .0612) = -0.0367$$

$$d = g_{21}^2 + g_{22}^2 = .0245^2 + - .0612^2 = 0.004346$$

$$\lambda_1 = \frac{b + d + \sqrt{(b - d)^2 + 4c^2}}{2} = \frac{2 + .004346 + \sqrt{(2 - .004346)^2 + 4(-.0367)^2}}{2} = 2$$

$$\lambda_2 = \frac{bd - c^2}{\lambda_1} = \frac{(2)(.004346) - (-.0367)^2}{2^2} = 0.003673$$

$$s_1 = \sqrt{\lambda_1} = \sqrt{2} = 1.414$$

$$s_2 = \sqrt{\lambda_2} = \sqrt{.003673} = 0.0606$$

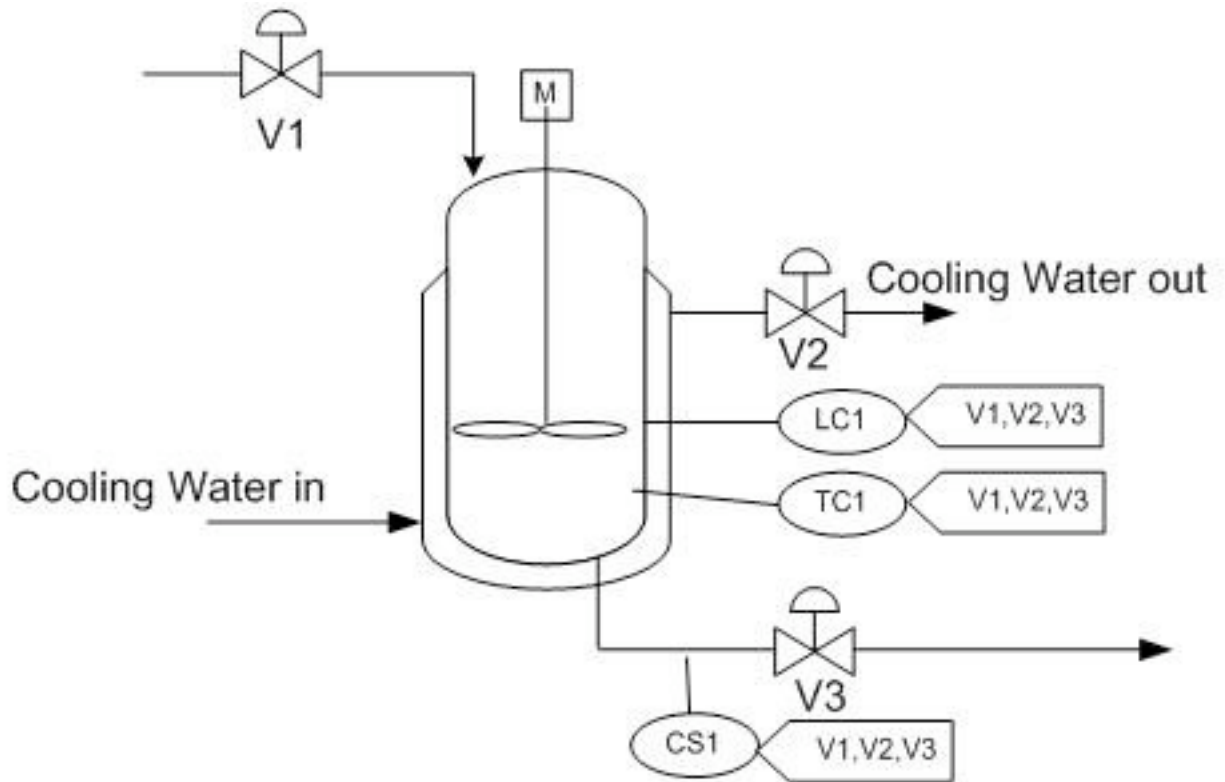
$$\Sigma = \begin{bmatrix} 1.414 & 0 \\ 0 & 0.0606 \end{bmatrix}$$

$$CN = \frac{s_1}{s_2} = 23.33$$

CN is less than 50, therefore decoupling for this system is feasible.

1.4 Worked out Example 2

A jacketed reactor with a single feed stream (Stream 1) is monitored by 3 proportional (P) controllers as indicated in the figure.



These controllers all act as inputs to each of 3 valves according to the relationships:

$$V_1 = \frac{1}{3}C_1 + \frac{7}{15}C_2 + \frac{1}{5}C_3$$

$$V_2 = \frac{4}{15}C_1 + \frac{4}{15}C_2 + \frac{1}{3}C_3$$

$$V_3 = \frac{1}{5}C_1 + \frac{4}{15}C_2 + \frac{1}{3}C_3$$

Where:

$C_1 = K_{c1}e_1(t) + b_1$, C_1 is the output from the level controller

$C_2 = K_{c2}e_2(t) + b_2$, C_2 is the output from the temperature controller

$C_3 = K_{c3}e_3(t) + b_3$, C_3 is the output from the composition sensor

Is it feasible to decouple this system?

Solution :

The gain array is calculated according to the [RGA method](#) and is:

$$G = \begin{bmatrix} 1/3 & 7/15 & 1/5 \\ 4/15 & 4/15 & 1/3 \\ 1/5 & 4/15 & 1/3 \end{bmatrix}$$

Input the following commands in *Mathematica* for SVD analysis:

```
G = {{1/3, 7/15, 1/5}, {4/15, 4/15, 1/3}, {1/5, 4/15, 1/3}}
G = G*1.0 Map[MatrixForm,
{u,w,v}=SingularValueDecomposition[G]]
```

The output of the SVD decomposition is the following:

$$U = \begin{bmatrix} -0.657043 & -0.75205 & 0.052116 \\ -0.552104 & 0.432979 & -0.712538 \\ -0.513299 & 0.496941 & 0.699696 \end{bmatrix},$$
$$\Sigma = \begin{bmatrix} 0.897525 & 0 & 0 \\ 0 & 0.193259 & 0 \\ 0 & 0 & 0.0392887 \end{bmatrix},$$
$$V = \begin{bmatrix} -0.522439 & -0.18542 & -0.832273 \\ -0.658174 & -0.532849 & 0.531864 \\ -0.542094 & 0.825646 & 0.156343 \end{bmatrix}$$

The condition number is calculated from the highest and lowest values of the Σ matrix:

$$CN = \frac{0.897525}{0.0392887} = 22.844$$

$CN < 50$, therefore the system may be decoupled.

As a more complicated problem, consider how this problem would change if the controllers used a cascade control style. For a P controller, the output may be similar to:

$$C_2 = K_{c2}e_2(t) + b_2 = K_{c2} * (LC_{actual} - f(C_1)) + b$$

What if we used a PID controller instead?

1.5 Multiple Choice Question 1

The CN, or condition number

- Is the ratio of the smaller number (s_2) to the larger number (s_1)
- Determines the feasibility of decoupling a system.
- Is the unit eigenvectors of the $m \times m$ matrix $G^T G$
- Is always less than 50.

Answer : b

1.6 Multiple Choice Question 2

For MIMO systems

- Control loops are isolated
- Each controlled variable is only manipulated by one variable
- Decoupling the system makes it more complicated
- Manipulated variables may affect several controlled variables

Answer : d

1.7 Sage's Corner

<http://www.youtube.com/v/j-heeeVmEAM>
[Unnarated Powerpoint Presentation](#)


1.8 References

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Section 2. MIMO control using RGA

See also [ECOSSE](#)

Note:  [Video lecture](#) available for this section!

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Date Presented: 7 November 2006; Revised: 1 November 2007

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

2.1 Introduction

Single variable **I**ntput or Single variable **O**utput (SISO) control schemes are just one type of control scheme that engineers in industry use to control their process. They may also use MIMO, which is a **M**ulti-**I**ntput-**M**ulti-**O**utput control scheme. In MIMO, one or more manipulated variables can affect the interactions of controlled variables in a specific loop or all other control loops. A MIMO control scheme is important in systems that have multiple dependencies and multiple interactions between different variables- for example, in a distillation column, where a manipulated variable such as the reflux ratio could directly or indirectly affect the feed flow rate, the product composition, and the reboiler energy. Thus, understanding the dependence of different manipulated and controlled variables in a MIMO control scheme could be extremely helpful in designing and implementing a control scheme for a process.

One method for designing and analyzing a MIMO control scheme for a process in steady state is with a **R**elative **G**ain **A**rray (RGA). RGA is useful for MIMO systems that can be decoupled (see the article about [determining if a system can be decoupled](#)). For systems that cannot be decoupled, [model predictive control](#) or [neural networks](#) are better choices of analysis tool than RGA. A good MIMO control scheme for a system that can be decoupled is one that can control a process variable without greatly affecting the other process variables. It must also be stable with respect to dynamic situations, load changes, and random disturbances. The RGA provides a quantitative approach to the analysis of the interactions between the controls and the output, and thus provides a method of pairing manipulated and controlled variables to generate a control scheme.

2.2 What is RGA?

Relative Gain Array is an analytical tool used to determine the optimal input-output variable pairings for a multi-input-multi-output (MIMO) system. In other words, the RGA is a normalized form of the gain matrix that describes the impact of each control variable on the output, relative to each control variable's impact on other variables. The process interaction of open-loop and closed-loop control systems are measured for all possible input-output variable pairings. A ratio of this open-loop 'gain' to this closed-loop 'gain' is determined and the results are displayed in a matrix.

$$RGA = \Lambda = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \cdots & \lambda_{1n} \\ \lambda_{21} & \lambda_{22} & \cdots & \lambda_{2n} \\ \vdots & & & \\ \lambda_{n1} & \lambda_{n2} & \cdots & \lambda_{nn} \end{bmatrix}$$

The array will be a matrix with one column for each input variable and one row for each output variable in the MIMO system. This format allows a process engineer to easily compare the relative gains associated with each input-output variable pair, and ultimately to match the input and output variables that have the biggest effect on each other while also minimizing undesired side effects.

2.2.1 Understanding the Results of the RGA

- The closer the values in the RGA are to 1 the more decoupled the system is
 - The maximum value in each row of the RGA determines which variables should be coupled or linked
 - Also each row and each column should sum to 1
-
- Example

The table below includes the RGA results. The values highlighted in red are the maximum values in the row. These values indicated that the valve for that row should be used to control the variable that is listed in the corresponding column.

RGA

P	T	F	Ca	Cb	Valves
0.903911	0.015328	0.021940	0.015397	0.043423	V1
0.084549	0.228626	-0.0313343	0.230685	0.487474	V2
0.001492	0.139518	-0.002314	0.763468	0.097835	V3
-0.027496	0.584721	0.029974	-0.025906	0.438707	V4
0.037542	0.031807	0.981733	0.016356	-0.067439	V5

V1->P
V2->Cb
V3->Ca
V4->T
V5->F

2.3 Calculating RGA

There are two main ways to calculate RGA:

- (1) Experimentally determine the effect of input variables on the output variables, then compile the results into an RGA matrix.
- (2) Use a steady-state gain matrix to calculate the RGA matrix.

Method (1) should be used when it is possible to carry out the experiments as detailed in the **Calculating RGA with Experiments** section. This method will generally yield the most accurate RGA matrix of the system because it is based on actual data taken from the operating control system. If performing these extensive experiments is not possible, method (2) can be used. If a process model is available, method (2) can be used with no experimental data. If there is no process model available, some experimental data must be taken (though less extensively than in method (1)) and used in conjunction with method (2).

2.3.1 Method 1: Calculating RGA with Experiments

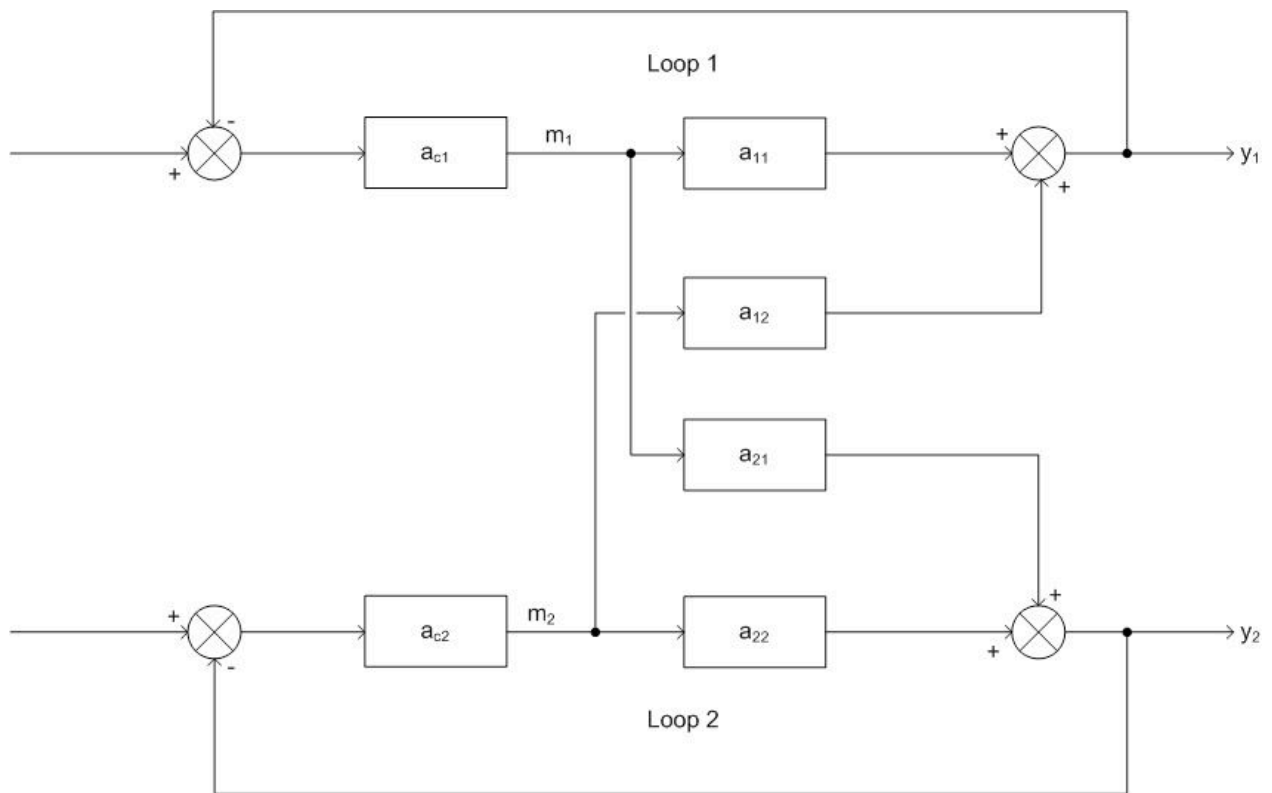
This method of calculating the RGA can be used when it is possible to run experiments on each of the input-output pairings. Below is a step-by-step explanation of how to experimentally compile the RGA for a simple MIMO system.

The simplest MIMO system is one that has two inputs and two outputs. Remember that by definition, a change in one of the inputs in a MIMO system will change *both* of the outputs. This system can be expressed mathematically as written below.

$$y_1 = a_{11}m_1 + a_{12}m_2$$

$$y_2 = a_{21}m_1 + a_{22}m_2$$

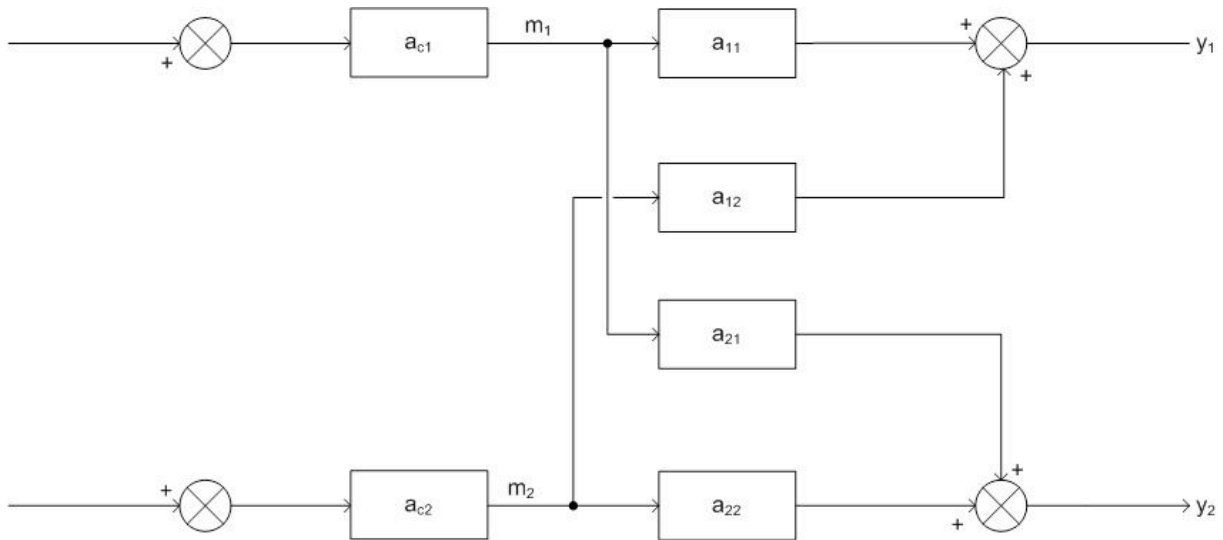
Where y_i is the output for loop i , the m variables are the inputs for each loop, and the a variables are the transfer functions. It also helps to see this system as a control diagram, as shown here.



Clearly, both y_1 and y_2 are affected by both inputs (m_1 and m_2). Because of this, there are two choices for control. y_1 could be controlled by m_1 , or y_1 could be controlled by m_2 . y_2 would then be controlled by the input that is not controlling y_1 . For a MIMO system with n input variables, there are $n!$ possible control configurations. The question is: Which configuration will give you the best control? The answer can be determined by finding the relative gain array (RGA). There are a few ways to determine the RGA, one of which is by doing two experiments, repeated for every possible configuration. The RGA can be assembled from the data collected. These experiments are explained below using the above drawing and the configuration where m_1 controls y_1 .

Experiment 1

For the first experiment, the objective is to observe the effect of m_1 on y_1 . To do this, *all* of the loops must be open. In other words, the feedback loop is removed and the system is run manually with no control. This configuration is shown below.



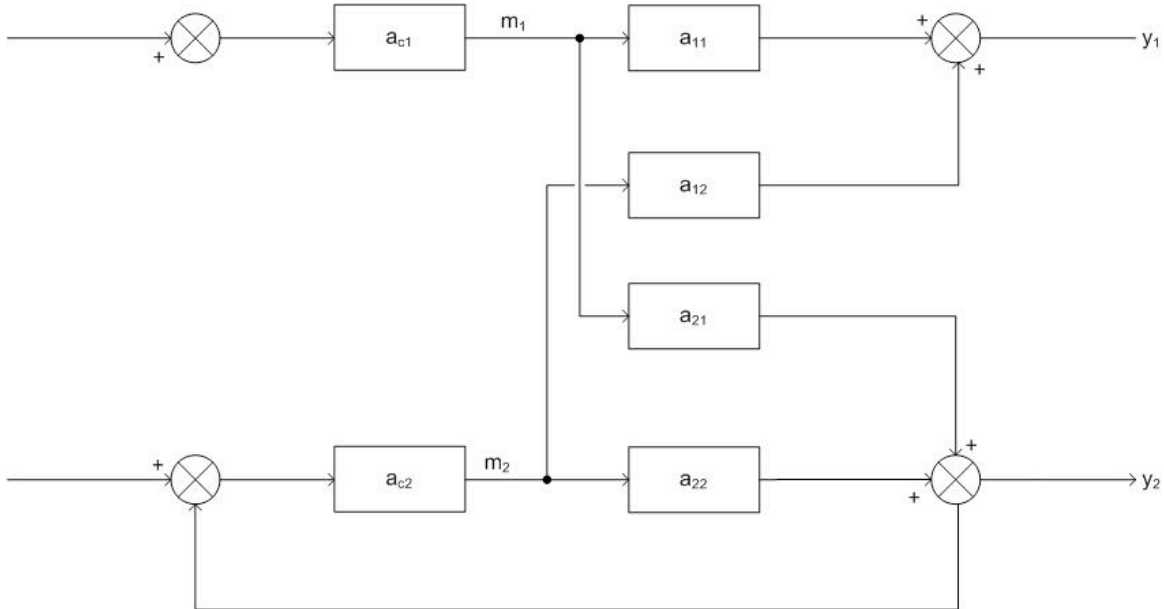
Now, since the system is under manual control, it is possible to introduce a step change Δm_1 while keeping m_2 constant. Because m_2 is held constant, the change in y_1 , Δy_1 , can be attributed entirely to m_1 . Although a change in m_1 will also affect y_2 , it is the relationship between m_1 and y_1 that must be observed at this point. Then, the gain of y_1 with respect to m_1 with all loops open is defined as g_{11} . The calculation of g_{11} is shown below.

$$g_{11} = \frac{\Delta y_1(\text{all} - \text{loops} - \text{open})}{\Delta m_1(\text{all} - \text{loops} - \text{open})}$$

The final objective of experiment one is obtaining the value g_{ij} where the controlled variable i is controlled by manipulated variable j .

Experiment 2

The goal of experiment two is to determine the effect of m_2 on y_1 . To do this, loop 1 must remain open, but all other loops remain closed. This configuration is shown below.



Now, the *same* step change that was introduced to m_1 in experiment one must be introduced again. The difference is, now loop 2 is in *perfect control* which means that when m_1 changes, it affects y_2 , so the control loop on loop two will adjust m_2 in order to compensate and keep y_2 constant. When m_2 changes it, in turn, affects y_1 . It is this change that is being observed. The amount y_1 changes is Δy_1 and the amount m_1 was stepped up is Δm_1 . Now:

$$g_{11}^* = \frac{\Delta y_1(\text{only} - \text{loop} - \text{one} - \text{open})}{\Delta m_1(\text{only} - \text{loop} - \text{one} - \text{open})}$$

The objective of experiment two is to obtain this value of g_{ij}^* where controlled variable i is being controlled by manipulated j .

Compiling the Array

Once the experiments are run for every possible configuration, the results can be used to compile the relative gain array (RGA). To do this, we first have to find the *relative gain*.

The relative gain is the ratio of g_{ij} to g_{ij}^* and is represented by λ_{ij} .

$$\lambda_{ij} = \frac{g_{ij}}{g_{ij}^*} = \frac{\left(\frac{\delta y_i}{\delta m_j}\right)_{all-loops-open}}{\left(\frac{\delta y_i}{\delta m_j}\right)_{only-loop-i-open}}$$

The value for λ must be computed for every possible combination of i and j . After every value is found, the RGA matrix can be formed:

$$RGA = \Lambda = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \cdots & \lambda_{1n} \\ \lambda_{21} & \lambda_{22} & \cdots & \lambda_{2n} \\ \vdots & & & \\ \lambda_{n1} & \lambda_{n2} & \cdots & \lambda_{nn} \end{bmatrix}$$

2.3.2 Method 2: Calculating RGA with Steady-State Gain Matrix

Sometimes it is not convenient or possible to perform the experiments described above on every control pairing possibility in the system. If that is the case, a *steady-state gain matrix* can be used to determine the RGA. If a process model is available, the steady-state gain matrix can be calculated from the model equations. If a process model is not available, the steady-state gain matrix can be calculated from experimental data (fewer experiments are required than when the RGA is calculated directly from experimental data as above). Once the steady-state gain matrix is calculated, it can be used to compute the RGA. Beware that a RGA has to have the same number of controlled variables and manipulated variables (same number of inputs and outputs) to be in an $m \times m$ matrix form.

Process Model Available

If a process model is available, the steady-state gain matrix relates the manipulated variables to the controlled variables according to the following equation:

$$\mathbf{y} = \mathbf{Gm}$$

where \mathbf{y} is a vector of the controlled variables:

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

\mathbf{m} is a vector of the manipulated variables:

$$\mathbf{m} = \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_n \end{bmatrix}$$

and G is the steady-state gain matrix:

$$G = \begin{bmatrix} g_{11} & g_{12} & \cdots & g_{1n} \\ g_{21} & g_{22} & \cdots & g_{2n} \\ \vdots & & & \\ g_{n1} & g_{n2} & \cdots & g_{nn} \end{bmatrix}$$

The values of g_{ij} are calculated by taking partial derivatives of the equations governing the controlled variables. Specifically:

$$g_{ij} = \frac{\partial y_i}{\partial m_j}$$

During differentiation, hold constant all manipulated variables other than m_j . To fill in matrix G with numerical values, simply substitute the appropriate steady state values for the process into the expressions derived from differentiation.

Now that the steady-state gain matrix has been found, the RGA can be calculated with just a little bit more math. However, now that you have the steady state gain matrix, this might be a good time to determine if your system can even be decoupled! See the article on [singular value decomposition](#) for methods to check this. Assuming SVD gives a

condition number of less than about 50, we can proceed to calculation of the RGA. First, define a matrix R to be the transpose of the inverse of matrix G :

$$R = (G^{-1})^T$$

The calculation of the **inverse** of a matrix is quite complicated for anything larger than a 2x2 matrix. Fortunately Mathematica will do this with the following command for a square matrix M :

Inverse[M]

The **transpose** of a matrix is when the rows become columns and the columns become rows. For a square matrix, this just means reflecting across the diagonal running from the top left to the bottom right corner of the matrix. The **transpose** can be found in Mathematica with the following command:

Transpose[M]

The RGA can now be obtained one element at a time according to this equation:

$$\lambda_{ij} = g_{ij}r_{ij}$$

Note that this is not your usual matrix multiplication! Here you multiply corresponding elements of the G and R matrices to get the corresponding element of the RGA. This is the type of multiplication Mathematica does with the standard multiplication operator.

See Example 1 below for a worked-out RGA calculation using this approach.

Process Model Not Available

In case there is no process model available and it is not feasible to determine the RGA by carrying out both experiments necessary for full experimental determination, it still may be possible to develop a steady-state gain matrix experimentally which can then be used to derive the RGA. In this case, just carry out experiment 1 as described above to determine the elements of the steady-state gain matrix:

$$g_{ij} = \frac{\Delta y_i}{\Delta m_j} \text{ with all loops open}$$

Each element of the steady-state gain matrix can be determined this way, and then the RGA can be calculated from the steady-state gain matrix as shown in the previous section.

2.4 Interpreting the RGA

There are some important properties and guidelines in understanding and analyzing the RGA, and what the different values of the RGA mean:

1) **All elements of the RGA across any row, or down any column will sum up to one:**

$$\sum_{i=1}^n \lambda_{ij} = \sum_{j=1}^n \lambda_{ij} = 1$$

This makes calculating the RGA easier because:

- in 2X2 case, only 1 element must be calculated to determine all elements
- in 3X3 case, only 4 elements must be calculated to determine all elements

and so on.

2) The λ_{ij} calculated from steady-state matrix is dimensionless and unaffected by scaling.

3) Each of the rows in the RGA represent one of the outputs. Each of the columns represent a manipulated variable.

- **If $\lambda_{ij} = 0$:** The manipulated variable (m_j) will have no effect on the output or the controlled variable (y_i).
- **If $\lambda_{ij} = 1$:** The manipulated variable m_j affects the output y_i without any interaction from the other control loops in the system. From the definition of λ_{ij} , this implies that the gain loop with all loops open is equal to the gain loop with all other loops closed, ie: $g_{11} = g^*_{11}$.
- **If $\lambda_{ij} < 0$:** The system will be unstable whenever m_j is paired with y_i , and the opposite response in the actual system may occur if other loops are opened in the system.
- **If $0 < \lambda_{ij} < 1$:** This implies that other control loops (m_j - y_i) are interacting with the manipulated and controlled variable control loop.

Three different relationships based on $\lambda=0.5$ imply different interpretations of pairing and the RGA:

- **If $\lambda_{ij} = 0.5$:** The control pairing effect is equal to the retaliatory effect of other loops.

- **If $\lambda_{ij} < 0.5$:** The other control loops are influencing the control pair, and the influence from the other control loops are greater than the influence from the control pair.
- **If $\lambda_{ij} > 0.5$:** This means that the control pair has a greater influence on the system than the other control loops.
- **If $\lambda_{ij} > 1$:** The open-loop gain of the control pair is greater than the gain with all other loops closed, ie: $g_{11} > g_{11}^*$. The positive value of RGA indicates that the control pair is dominant in the system, but the other loops are still affecting the control pair in the opposite direction. The higher the value of λ_{ij} , the more correctional effects the other control loops have on the pair.

λ_{ij}	Possible Pairing
$\lambda_{ij} = 0$	Avoid pairing m_j with y_i
$\lambda_{ij} = 1$	Pair m_j with y_i
$\lambda_{ij} < 0$	Avoid pairing m_j with y_i
$\lambda_{ij} = \text{or} < 0.5$	Avoid pairing m_j with y_i
$\lambda_{ij} > 1$	Pair m_j with y_i

2.5 NI Analysis with RGA

NI, the Niederlinski Index, is a calculation used to analyze the stability of the control loop pairings using the result of the RGA, evaluated at Steady State:

$$NI = \frac{|G|}{\prod_{i=1}^n g_{ii}}$$

A negative NI value indicates instability in the control loop. For a 2×2 matrix, a positive NI value indicates stability in the pairings, but this is not necessarily true for larger matrices! For matrices larger than 2×2 , a conclusion can only be drawn from a negative NI, which indicates instability. NI should not be used for systems that have time delays (dead time), as the NI stability predictions assume immediate feedback to the controller. However, the index can be adapted for systems with dead time, although that application is beyond the scope of this article.

Here's an example NI calculation: given the steady state gain matrix

$$G = \begin{bmatrix} -0.002 & 0.001 \\ 0.002 & 0.003 \end{bmatrix}$$

the NI can be calculated from the following expression:

$$NI = \frac{(-0.002 \times 0.003) - (0.001 \times 0.002)}{-0.002 \times 0.003} = 1.333$$

Since this is a 2 × 2 matrix, the positive value of the NI indicates stability in the control loop pairings.

2.6 Optimizing a MIMO Control Scheme: Pairing Rules

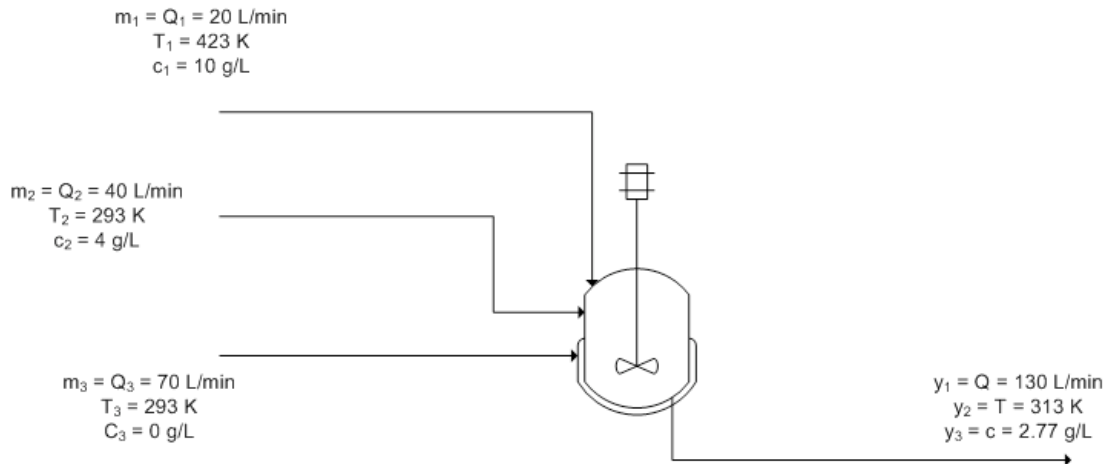
The goal of the RGA and NI analysis is to quantitatively determine the optimal variable pairing for a given process. Some basic rules to remember when attempting to obtain an optimal pairing of control loops in a system are:

- **Rule 1:** The **positive** RGA elements that are closest to 1.0 should have the corresponding manipulated and controlled variables paired. When the CN number is large, implying a less decoupled system, one should look for the max RGA elements.
- **Rule 2:** If the NI value is negative, the loop pairing for that control system configuration is unacceptable.

2.7 Worked Out Example 1

A blending unit is used to dilute and cool down the product stream of a reactor. Three streams are combined in the mixer: the hot, concentrated stream from the reactor, a room temperature stream containing none of the product A, and a second room temperature stream containing some A produced elsewhere in the process. It is desired to control the flow rate, temperature, and concentration of A in the product stream by manipulating the flow rates of the three input streams. A schematic of the process follows, filled in with the steady state values of flow rate, temperature, and concentration. The manipulated

variables are indicated with the letter m and the controlled variables are indicated with the letter y :



The equations used to model the system are:

$$y_1 = m_1 + m_2 + m_3$$

$$y_2 = \frac{T_1 m_1 + T_2 m_2 + T_3 m_3}{y_1} = \frac{T_1 m_1 + T_2 m_2 + T_3 m_3}{m_1 + m_2 + m_3}$$

$$y_3 = \frac{c_1 m_1 + c_2 m_2 + c_3 m_3}{y_1} = \frac{c_1 m_1 + c_2 m_2 + c_3 m_3}{m_1 + m_2 + m_3}$$

Calculate the RGA using the steady-state gain matrix method and use it to determine the best control scheme for the system.

2.7.1 Solution

First you must take the partial derivatives of the control variable equations in order to determine the elements of the steady-state gain matrix:

$$g_{11} = \frac{\partial y_1}{\partial m_1} = 1$$

$$g_{21} = \frac{\partial y_2}{\partial m_1} = \frac{(T_1 - T_2) m_2 + (T_1 - T_3) m_3}{(m_1 + m_2 + m_3)^2}$$

$$g_{31} = \frac{\partial y_3}{\partial m_1} = \frac{(c_1 - c_2) m_2 + (c_1 - c_3) m_3}{(m_1 + m_2 + m_3)^2}$$

$$g_{12} = \frac{\partial y_1}{\partial m_2} = 1$$

$$g_{22} = \frac{\partial y_2}{\partial m_2} = \frac{(T_2 - T_1) m_1 + (T_2 - T_3) m_3}{(m_1 + m_2 + m_3)^2}$$

$$g_{32} = \frac{\partial y_3}{\partial m_2} = \frac{(c_2 - c_1) m_1 + (c_2 - c_3) m_3}{(m_1 + m_2 + m_3)^2}$$

$$g_{13} = \frac{\partial y_1}{\partial m_3} = 1$$

$$g_{23} = \frac{\partial y_2}{\partial m_3} = \frac{(T_3 - T_1) m_1 + (T_3 - T_2) m_2}{(m_1 + m_2 + m_3)^2}$$

$$g_{33} = \frac{\partial y_3}{\partial m_3} = \frac{(c_3 - c_1) m_1 + (c_3 - c_2) m_2}{(m_1 + m_2 + m_3)^2}$$

Now you can substitute in the given steady state values of the variables to find the numerical values of g_{ij} , obtaining:

$$g_{11} = 1$$

$$g_{21} = \frac{11}{13}$$

$$g_{31} = \frac{47}{845}$$

$$g_{12} = 1$$

$$g_{22} = -\frac{2}{13}$$

$$g_{32} = \frac{8}{845}$$

$$g_{13} = 1$$

$$g_{23} = -\frac{2}{13}$$

$$g_{33} = -\frac{18}{845}$$

In matrix form:

$$G = \begin{bmatrix} 1 & 1 & 1 \\ \frac{11}{13} & -\frac{2}{13} & -\frac{2}{13} \\ \frac{47}{845} & \frac{8}{845} & -\frac{18}{845} \end{bmatrix}$$

Now calculate matrix R :

$$R = (G^{-1})^T = \begin{bmatrix} \frac{2}{13} & \frac{4}{13} & \frac{7}{13} \\ 1 & -\frac{5}{2} & \frac{3}{2} \\ 0 & \frac{65}{2} & -\frac{65}{2} \end{bmatrix}$$

You can now calculate the RGA by multiplying matrices G and R piecewise, according to the formula:

$$\lambda_{ij} = g_{ij}r_{ij}$$

So the RGA is:

$$\text{RGA} = \begin{bmatrix} \frac{2}{13} & \frac{4}{13} & \frac{7}{13} \\ \frac{11}{13} & \frac{5}{13} & -\frac{3}{13} \\ 0 & \frac{4}{13} & \frac{9}{13} \end{bmatrix}$$

Note that all rows and columns sum to 1, as they should.

Now it's time to determine the optimal control scheme for the system. The closer an element in the matrix is to 1, the better the pairing is between the manipulated and controlled variables represented by that element. With this in mind, we can immediately see that m_1 , the flow rate of stream 1, should be used to control y_2 , the temperature of the

output stream, because the value of λ_{21} is the closest to 1 in the matrix ($\frac{11}{13}$). Next in line is λ_{33} , with a value of $\frac{9}{13}$. This indicates that m_3 , the flow rate of stream 3, should control y_3 , the concentration of A in the product stream. So far so good, but what should control y_1 , the flow rate of the product stream? The best option would be m_3 , but this is already controlling the concentration of A in the product, so the next best option is m_2 , the flow rate of stream 2. This is not optimal because the relative gain is less than 0.5, but it is the best option available given the constraints of the system.

2.8 Worked Out Example 2

In a distillation column, reflux rate (R) and steam rate (S) are used to control the compositions in the distillate (x_D) and the bottom product (x_B). The control loops are opened in order to conduct experiment one as described above, and the following set of data is collected:

Trial	R (kg/min)	S (kg/min)	x_D	x_B
1	75	20	0.96	0.05
2	85	20	0.94	0.06
3	95	20	0.92	0.08

4	85	15	0.95	0.06
5	85	25	0.97	0.03

Calculate the RGA for this system, and determine which is the best pairing between the manipulated (R and S) and controlled variables (x_D and x_B).

2.8.1 Solution

From the experiment data, it is observed that the reflux rates (R) are constant for trials 2, 4 and 5, while the steam rates (S) are constant for trials 1, 2 and 3.

First, calculate the steady-state gain matrix for this system:

$$g_{11} = \frac{\Delta x_D}{\Delta R} \text{ with S constant} = \frac{0.96 - 0.94}{75 - 85} = -0.002$$

$$g_{12} = \frac{\Delta x_B}{\Delta R} \text{ with S constant} = \frac{0.05 - 0.06}{75 - 85} = 0.001$$

$$g_{21} = \frac{\Delta x_D}{\Delta S} \text{ with R constant} = \frac{0.95 - 0.97}{15 - 25} = 0.002$$

$$g_{22} = \frac{\Delta x_B}{\Delta S} \text{ with R constant} = \frac{0.06 - 0.03}{15 - 25} = 0.003$$

Organize the gain value into the matrix form and compute R:

$$G = \begin{bmatrix} -0.002 & 0.001 \\ 0.002 & 0.003 \end{bmatrix}$$

$$R = (G^{-1})^T = \begin{bmatrix} -375 & 250 \\ 125 & 250 \end{bmatrix}$$

Multiply each value in the R matrix by its corresponding gain value to obtain λ_{ij} :

$$\lambda_{11} = g_{11}R_{11}$$

λ_{ij} is then organized into the RGA matrix form:

$$RGA = \begin{bmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{3}{4} \end{bmatrix}$$

The RGA matrix indicates that the composition of the distillate (x_D) would be best controlled by the reflux flow (R); while x_B would be best controlled by the steam rate (S) from the reboiler.

2.9 Worked Out Example 3: Using Mathematica

An example problem based from Fall 2008 second exam:

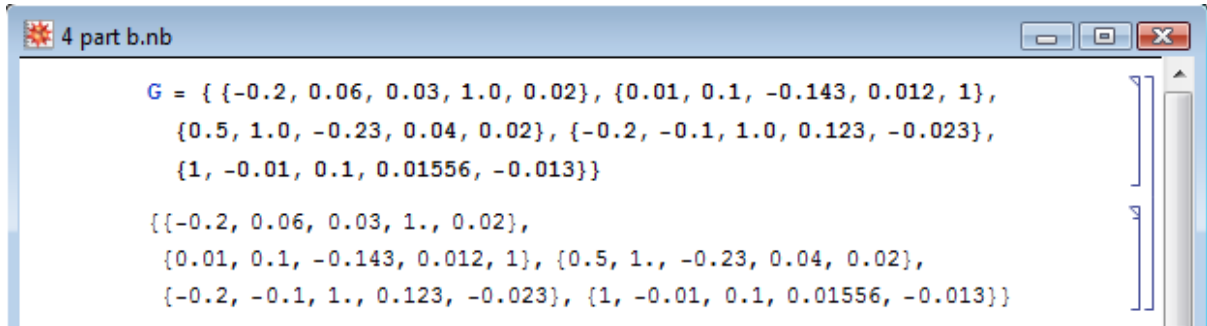
"Imagine that you are developing a control scheme for a new low temperature reactor system. The physics governing the system is complicated, so you decide to start out with an experiment on the system to see if you can develop a simple set of SISO controllers. To evaluate this possibility, you begin with your five valves at their steady state operating conditions ($v_1=0.5$, $v_2=0.55$, $v_3=0.5$, $v_4=0.6$, $v_5=0.4$) and measure the five key variables of this process T_1 , T_2 , T_3 , P_1 and P_2 . Next you slightly adjust each valve to see the steady state effects on each output variable"

As an approximation, you fit this model to the following system:

$$\begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ P_1 \\ P_2 \end{bmatrix} = \begin{bmatrix} -0.2 & 0.06 & 0.03 & 1.0 & 0.02 \\ 0.01 & 0.1 & -0.143 & 0.012 & 1.0 \\ 0.5 & 1.0 & -0.23 & 0.04 & 0.02 \\ -0.2 & -0.1 & 1.0 & 0.123 & -0.023 \\ 1.0 & -0.01 & 0.1 & 0.01556 & -0.013 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \\ V_5 \end{bmatrix}$$

"Perform an RGA analysis to find the best pairing between valves (v_1 , v_2 , v_3 , v_4 , and v_5) and outputs (T_1 , T_2 , T_3 , P_1 , and P_2)."

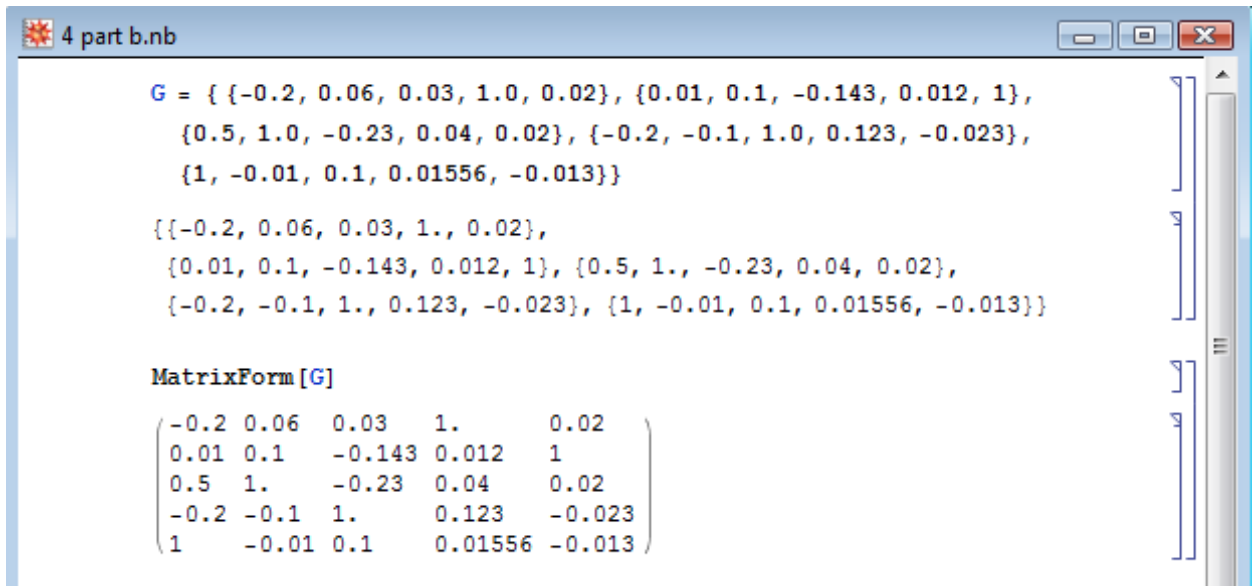
In Mathematica, you can input the matrix of coefficients by the following:



```
G = { {-0.2, 0.06, 0.03, 1.0, 0.02}, {0.01, 0.1, -0.143, 0.012, 1},  
      {0.5, 1.0, -0.23, 0.04, 0.02}, {-0.2, -0.1, 1.0, 0.123, -0.023},  
      {1, -0.01, 0.1, 0.01556, -0.013}}  
  
{{-0.2, 0.06, 0.03, 1., 0.02},  
 {0.01, 0.1, -0.143, 0.012, 1}, {0.5, 1., -0.23, 0.04, 0.02},  
 {-0.2, -0.1, 1., 0.123, -0.023}, {1, -0.01, 0.1, 0.01556, -0.013}}
```

Note: I assign the matrix of coefficients to the variable, G.

It can be viewed in a matrix form in Mathematica by using function, "MatrixForm[]":



```
G = { {-0.2, 0.06, 0.03, 1.0, 0.02}, {0.01, 0.1, -0.143, 0.012, 1},  
      {0.5, 1.0, -0.23, 0.04, 0.02}, {-0.2, -0.1, 1.0, 0.123, -0.023},  
      {1, -0.01, 0.1, 0.01556, -0.013}}  
  
{{-0.2, 0.06, 0.03, 1., 0.02},  
 {0.01, 0.1, -0.143, 0.012, 1}, {0.5, 1., -0.23, 0.04, 0.02},  
 {-0.2, -0.1, 1., 0.123, -0.023}, {1, -0.01, 0.1, 0.01556, -0.013}}
```

MatrixForm[G]

$$\begin{pmatrix} -0.2 & 0.06 & 0.03 & 1. & 0.02 \\ 0.01 & 0.1 & -0.143 & 0.012 & 1 \\ 0.5 & 1. & -0.23 & 0.04 & 0.02 \\ -0.2 & -0.1 & 1. & 0.123 & -0.023 \\ 1 & -0.01 & 0.1 & 0.01556 & -0.013 \end{pmatrix}$$

With the gain matrix, G, you can use the a singular value decomposition (SVD) of the gain matrix to determine how linearly dependent the model is. The linearity is based on the condition number (CN). Mathematica has a built-in function to do singular value decomposition. The following shows how to do singular value decomposition for this example.

```

4 part b.nb *

G = { {-0.2, 0.06, 0.03, 1.0, 0.02}, {0.01, 0.1, -0.143, 0.012, 1},
      {0.5, 1.0, -0.23, 0.04, 0.02}, {-0.2, -0.1, 1.0, 0.123, -0.023},
      {1, -0.01, 0.1, 0.01556, -0.013}}

Out[1]= {{-0.2, 0.06, 0.03, 1., 0.02},
         {0.01, 0.1, -0.143, 0.012, 1}, {0.5, 1., -0.23, 0.04, 0.02},
         {-0.2, -0.1, 1., 0.123, -0.023}, {1, -0.01, 0.1, 0.01556, -0.013}}

In[2]:= MatrixForm[G]
Out[2]/MatrixForm=

$$\begin{pmatrix} -0.2 & 0.06 & 0.03 & 1. & 0.02 \\ 0.01 & 0.1 & -0.143 & 0.012 & 1 \\ 0.5 & 1. & -0.23 & 0.04 & 0.02 \\ -0.2 & -0.1 & 1. & 0.123 & -0.023 \\ 1 & -0.01 & 0.1 & 0.01556 & -0.013 \end{pmatrix}$$


In[3]:= N[Map[MatrixForm, {u, w, v} = SingularValueDecomposition[G]]]
Out[3]= {

$$\begin{pmatrix} 0.189269 & -0.625065 & 0.637289 & 0.219648 & -0.345091 \\ -0.202216 & -0.64526 & -0.364987 & -0.639526 & -0.0232304 \\ -0.70659 & -0.12418 & 0.361949 & 0.120974 & 0.58281 \\ 0.47824 & 0.153605 & 0.453547 & -0.581447 & 0.45156 \\ -0.441931 & 0.392324 & 0.352045 & -0.435941 & -0.580343 \end{pmatrix},$$


$$\begin{pmatrix} 1.39007 & 0. & 0. & 0. & 0. \\ 0. & 1.07001 & 0. & 0. & 0. \\ 0. & 0. & 1.02718 & 0. & 0. \\ 0. & 0. & 0. & 0.903883 & 0. \\ 0. & 0. & 0. & 0. & 0.712281 \end{pmatrix},$$


$$\begin{pmatrix} -0.669571 & 0.390719 & 0.302968 & -0.3424 & -0.435873 \\ -0.545916 & -0.229431 & 0.306482 & 0.146816 & 0.730651 \\ 0.454048 & 0.275622 & 0.464197 & -0.613823 & 0.354422 \\ 0.15145 & -0.572684 & 0.689899 & 0.153241 & -0.38685 \\ -0.156695 & -0.625113 & -0.350484 & -0.67893 & -0.0299283 \end{pmatrix}$$


```

The Mathematica syntax is : `N[Map[MatrixForm, {u, w, v} = SingularValueDecomposition[G]]]`. The "SingularValueDecomposition[]" pops out three arrays assigned to variable *u*, *w*, and *v* . The "Map[MatrixForm, ...]" portion pops out the three arrays into a matrix view and "N[.]" portion forces numerical values in the matrices.

To the condition number(CN), you divide the biggest value by the smallest value in matrix, *w*. The general rule thumb is that if the condition number(CN) is greater than 50, then the system/model is too difficult to decouple.

```

4 part b.nb *

G = { {-0.2, 0.06, 0.03, 1.0, 0.02}, {0.01, 0.1, -0.143, 0.012, 1},
      {0.5, 1.0, -0.23, 0.04, 0.02}, {-0.2, -0.1, 1.0, 0.123, -0.023},
      {1, -0.01, 0.1, 0.01556, -0.013}}

Out[1]= {{-0.2, 0.06, 0.03, 1., 0.02},
         {0.01, 0.1, -0.143, 0.012, 1}, {0.5, 1., -0.23, 0.04, 0.02},
         {-0.2, -0.1, 1., 0.123, -0.023}, {1, -0.01, 0.1, 0.01556, -0.013}}

In[2]:= MatrixForm[G]

Out[2]/MatrixForm=

$$\begin{pmatrix} -0.2 & 0.06 & 0.03 & 1. & 0.02 \\ 0.01 & 0.1 & -0.143 & 0.012 & 1 \\ 0.5 & 1. & -0.23 & 0.04 & 0.02 \\ -0.2 & -0.1 & 1. & 0.123 & -0.023 \\ 1 & -0.01 & 0.1 & 0.01556 & -0.013 \end{pmatrix}$$


In[3]:= N[Map[MatrixForm, {u, w, v} = SingularValueDecomposition[G]]]

Out[3]= {

$$\begin{pmatrix} 0.189269 & -0.625065 & 0.637289 & 0.219648 & -0.345091 \\ -0.202216 & -0.64526 & -0.364987 & -0.639526 & -0.0232304 \\ -0.70659 & -0.12418 & 0.361949 & 0.120974 & 0.58281 \\ 0.47824 & 0.153605 & 0.453547 & -0.581447 & 0.45156 \\ -0.441931 & 0.392324 & 0.352045 & -0.435941 & -0.580343 \end{pmatrix},$$


$$\begin{pmatrix} 1.39007 & 0. & 0. & 0. & 0. \\ 0. & 1.07001 & 0. & 0. & 0. \\ 0. & 0. & 1.02718 & 0. & 0. \\ 0. & 0. & 0. & 0.903883 & 0. \\ 0. & 0. & 0. & 0. & 0.712281 \end{pmatrix},$$


$$\begin{pmatrix} -0.669571 & 0.390719 & 0.302968 & -0.3424 & -0.435873 \\ -0.545916 & -0.229431 & 0.306482 & 0.146816 & 0.730651 \\ 0.454048 & 0.275622 & 0.464197 & -0.613823 & 0.354422 \\ 0.15145 & -0.572684 & 0.689899 & 0.153241 & -0.38685 \\ -0.156695 & -0.625113 & -0.350484 & -0.67893 & -0.0299283 \end{pmatrix}$$

}

MatrixForm[w]


$$\begin{pmatrix} 1.39007 & 0. & 0. & 0. & 0. \\ 0. & 1.07001 & 0. & 0. & 0. \\ 0. & 0. & 1.02718 & 0. & 0. \\ 0. & 0. & 0. & 0.903883 & 0. \\ 0. & 0. & 0. & 0. & 0.712281 \end{pmatrix}$$


1.3900681280600775` / 0.7122813169144732`

1.95157

```

This illustrates that this system can be decoupled because the CN number is below 50. To determine the best pairing, RGA analysis is used in which it is a normalized form of the gain matrix, "G" that determines the impact of each control variable on its respective output e.g. how much impact does v1 have on T1, etc. The Mathematica syntax is $N[G*\text{Transpose}[\text{Inverse}[G]]]$. The RGA normalization is essential since at times, not in this case however, the values of the gain matrix may represent that a valve has great

influence on multiple variables (ie. a column may contain the highest value from multiple rows). In order to distinguish unique separations between these influences, the RGA is used to normalize the gain matrix as seen below. This allows us to determine the different magnitudes of influence the valve has on an output in order to find the predominant effect on an output. The RGA illustrates these marginal differences in impact by the valves on the variable outputs, and lets us make the best possible pairings.

```

RGA = N[G*Transpose[Inverse[G]]]

{{0.000694796, -0.00410818, -0.00396187, 1.00786, -0.00048195},
 {0.000106057, -0.00188374, -0.00365155, -0.00021153, 1.00564}, {-0.000353147, 1.02961, -0.0249849, -0.00253774, -0.00173317},
 {0.0193131, -0.0283335, 1.02029, -0.00852503, -0.00274541}, {0.980239, 0.00471643, 0.0123075, 0.00341709, -0.000680243}}

MatrixForm[RGA]

```

$$\begin{pmatrix}
 0.000694796 & -0.00410818 & -0.00396187 & 1.00786 & -0.00048195 \\
 0.000106057 & -0.00188374 & -0.00365155 & -0.00021153 & 1.00564 \\
 -0.000353147 & 1.02961 & -0.0249849 & -0.00253774 & -0.00173317 \\
 0.0193131 & -0.0283335 & 1.02029 & -0.00852503 & -0.00274541 \\
 0.980239 & 0.00471643 & 0.0123075 & 0.00341709 & -0.000680243
 \end{pmatrix}$$

The best pairing is discovered by taking the maximum value of RGA Matrix for each row.

$$\text{RGA} = \begin{bmatrix}
 0.000694 & -0.00411 & -0.00396 & \mathbf{1.0079} & -0.000482 \\
 0.000106 & -0.00188 & -0.00365 & -0.000212 & \mathbf{1.00564} \\
 -0.000353 & \mathbf{1.0296} & -0.0249 & -0.00254 & -0.00173 \\
 0.0193 & -0.0283 & \mathbf{1.0202} & -0.00853 & -0.00275 \\
 \mathbf{0.9802} & 0.00471 & 0.0123 & 0.00342 & -0.000680
 \end{bmatrix} \begin{bmatrix} V1 \\ V2 \\ V3 \\ V4 \\ V5 \end{bmatrix}$$

The bold values correspond to the valve that is the best pairing for the individual output. By looking at the bold values, V1->P2 V2->T3, V3-> P1, V4-> T1, V5-> T2.

2.10 Test Yourself!

Multiple Choice Question 1

For a MIMO control system containing 4 different manipulated and 4 different controlled variables, how many control configurations are possible for the system?

- a. 24
- b. 4
- c. 64
- d. 256

Multiple Choice Question 2

In a case of a 2x2 matrix system, if one RGA element in first row calculated to be $\frac{3}{4}$. According to the RGA properties, what is the other element in that same row?

- a. $\frac{3}{4}$
- b. $\frac{1}{4}$
- c. $\frac{2}{4}$
- d. Cannot be determined with given information.

Multiple Choice Question 3

RGA is useful for process engineers because it allows us to determine:

- a. Which matrix size to use.
- b. What eigenvalues and eigenvectors are paired.
- c. What input and output pairs to use.
- d. When feed forward control is preferred over feedback control.

2.11 Test Yourself! Answers

Multiple Choice Question 1

Answer: *a*

Explanation: Mathematically, for an $n \times n$ manipulated by controlled variable system, the number of control configurations possible will be $n!$ or n factorial. For a 4x4 variable system, $4 \times 3 \times 2 \times 1 = 24$. Physically, the number of control configurations translates to the number of possible input-output pairings.

Multiple Choice Question 2

Answer: *b*

Explanation: As explained above, all elements of the RGA across any row, or down any column should sum up to unity (one). For a 2x2 matrix, if one element in a row is $\frac{3}{4}$, the other element must be $1 - \frac{3}{4} = \frac{1}{4}$

Multiple Choice Question 3

Answer: *c*

Explanation: Using RGA, a process engineer will assess the relative gain of pairing each input with each output to minimize undesired interactions and maximize desired interactions between controlled and manipulated variables in a system. See "Interpreting the RGA" section if you are confused on how this analysis is achieved.

2.12 Sage's Corner

MIMO Control using RGA Presentation #1 #2
<http://www.youtube.com/v/cRUCIPIoPeo> <http://www.youtube.com/v/W9bOs2un-uM>

[Interpreting RGA matrices powerpoint](#)

[Slides without narration](#)


[PDF of slides](#)

2.13 References

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- Romagnoli, Jose A., Palazoglu, Ahmet. *Introduction to Process Control*, Taylor and Francis Group.
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- Edinburgh University, [Exercise: Relative Gain Arrays](#), 2006
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Section 3. MIMO using model predictive control

Title: Model Predictive Control

Note:  [Video lecture](#) available for this section!

Authors: Bradley Anderson, Aaron Bennick, Michael Saliccioli

Stewards: Sarah Hebert, Valerie Lee, Matthew Morabito, Jamie Polan

Date Presented: 11/7/06; Revised: 10/30/07

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

3.1 Introduction

This article will describe how to control a system with multiple inputs and outputs using model predictive control (MPC). MPC is a linear algebra method for predicting the result of a sequence of control variable manipulations. Once the results of specific manipulations are predicted, the controller can then proceed with the sequence that produces the desired result. One can compare this controller method to "look ahead" in chess or other board games. In look ahead, you foresee what an action might yield some time in the future using specific knowledge of the process (or game in the case of chess), and are thereby able to optimize your actions to select for the best long term outcome. MPC methods can prevent an occurrence with conventional PID controllers in which actions taken achieve short term goals, but end up very costly in the end. This phenomenon can be described as "winning the battle but losing the war."

The open ended nature of MPC allows the process control engineer use MPC to control any system for which models can be generated.

3.2 Model Predictive Control

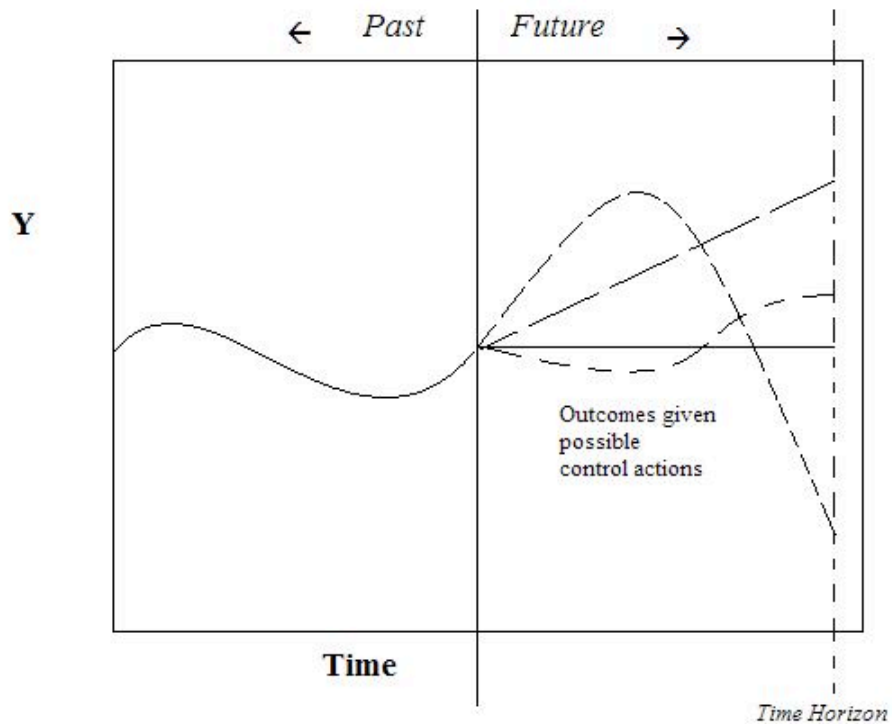
MPC is a widely used means to deal with large multivariable constrained control issues in industry. The main aim of MPC is to minimize a performance criterion in the future that would possibly be subject to constraints on the manipulated inputs and outputs, where the future behavior is computed according to a model of the plant. The model predictive controller uses the models and current plant measurements to calculate future moves in the independent variables that will result in operation that honors all independent and dependent variable constraints. The MPC then sends this set of independent variable moves to the corresponding regulatory controller set-points to be implemented in the process.

MPC uses the mathematical expressions of a process model to predict system behavior. These predictions are used to optimize the process over a defined time period. An MPC controller can operate according to the following algorithm.

1. Development of a process model by the control engineers.
2. At time t , previous process inputs and outputs are used, along with the process model, to predict future process outputs $u(f)$ over a "prediction horizon."
3. The control signals that produce the most desired behavior are selected.
4. The control signal is implemented over a pre-defined time interval.
5. Time advances to the next interval, and the procedure is repeated from step 2.

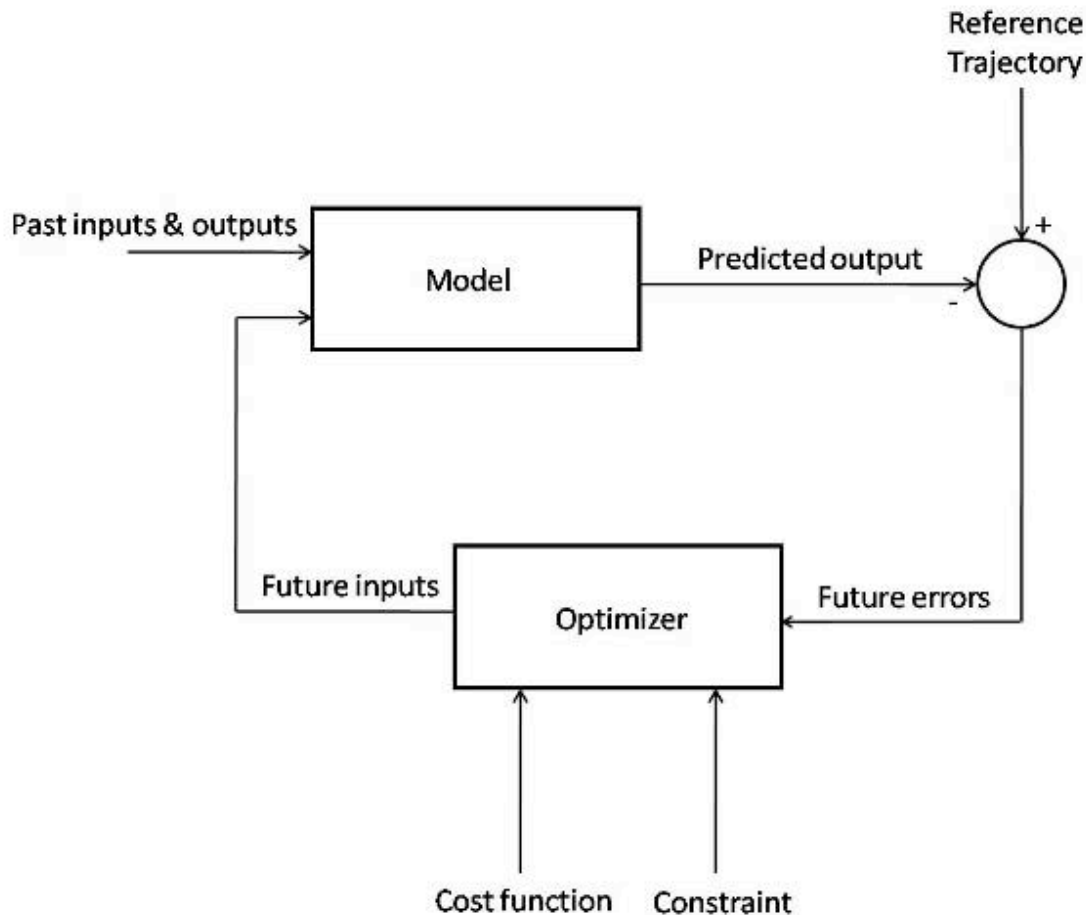
This is one of the many algorithm possibilities, which can be applied to systems with any number of inputs or outputs. The process model can be variable as well. Examples include physical models, input-output models, and state models which are all derived from the specific system being controlled.

When comparing predicted behavior to desired behavior, there are multiple techniques. A common procedure is to generate a second mathematical model that describes your desired behavior. When process behavior is predicted in step 2 of the MPC algorithm, the control signals which produce the predicted behavior that minimize deviations from your desired behavior over the $[t, t+h]$ interval, are selected. The generation of models and optimization process is repeated continuously as the algorithm is repeated.



As seen in the figure above, depending on the algorithm, MPC may generate possible outcomes given possible controller action. These generations are either based on past process outputs, or the process model. After many possible outcomes are generated, the controller can pick one based on the optimization goals. This generation and optimization process is repeated at every time step.

The flow diagram below depicts the flow of information used by the controller.



The figure above shows the basic structure of a Model Predictive Controller. The model takes data from past inputs and outputs, and combines it with the predicted future inputs, and gives a predicted output for the time step. This predicted output is combined with the reference trajectory, giving the predicted future errors of the system. These errors are fed into an optimizer, which enforces the constraints of the system (for instance, ensuring that a flow rate calculation for the model is not greater than the maximum flow) on the predicted outputs and minimizes the operating cost function. This gives the predicted future inputs, which are fed back into the main model, restarting the cycle.

3.2.1 Motivation

The motivation for the development and implementation of MPC controllers is compelling. MPC is very simple for sampled systems in which the control signal is constant over the interval $[t, t+h]$. The value of h can then be taken as the sampling interval, and the prediction horizon can become a small number of sampling intervals. This can reduce the computational power needed to implement a model predictive controller.

A highly desired feature of MPC is that constraints can be implemented in the controller. These constraints include heaters and valves that have a finite operating range, actuators

with finite states (on/off or low/high), and cost or energy limits for the process. MPC can incorporate these constraints and eliminate the possibility of variables exceeding their limits. This helps the process operate efficiently, prevents damage to equipment, and prevents the system from running away by continuously increasing a variable's setting when the limit for the equipment has already been reached. Another benefit of MPC controllers incorporating system constraints is the ability of the model to dynamically react to system changes. For example, if a valve is stuck open, it can be added as a constraint, and the model will compensate accordingly. This allows the controller to continue effectively controlling the system after an equipment malfunction. In a simpler control, such as PID control, this would not be possible.

MPC is a highly specific method for controlling a process. Each controller is specific to the system it was designed for and the model equations, constraints, and set points will change for different systems. This means that a controller developed for a tank reactor will not be able to control an evaporation unit as the process model will be very different. This weakness in MPC brings out its biggest strength. The specificity and customizable nature of the controller will empower you with the freedom to design for exactly what is desired.

MPC is a flexible control technique that uses discrete time segments and is the most commonly applied advanced control technique in the chemical process industry. MPC helps to simplify or completely eliminate controller design and instead works as a system modeling controller. With MPC the designer does not have to worry about optimizing control parameters such as with PID control. The ability of MPC controllers to handle constraints in an optimal fashion is also a contributor to its success.

3.2.2 Model Predictive Control Example

To demonstrate the concepts of MPC, a general example for the development of a sampled process and a first-order system will be shown.

General Model

Take equation 1 as our process model:

$$y(t) + a_1y(t-h) + \dots + a_ny(t-nh) = b_1u(t-h) + b_2u(t-2h) + \dots + b_nu(t-nh) \quad (1)$$

Where u is controller input, y is process output, and h is the time interval. This is a general equation that relates previous process output $y(t-h)$ and previous controller input $u(t-h)$. In some situations this equation may be created using fitted experimental data, but is most often a derivation using knowledge of your specific system and fundamentals of chemical engineering. At time t , total previous behavior y_p is shown as equation 2.

$$y_p = f(y(t), y(t - h), \dots, u(t - h), u(t - 2h), \dots) \quad (2)$$

Future process output y_f can be predicted using current and future control signals, $u(t)$ and $u(t + h)$ respectively:

$$y_f = f(u(t), u(t - h), \dots, u(t + Nh)) \quad (3)$$

Both y_p and y_f could possibly be created by fits of experimental data, but are more likely to be derived from specific equations related to your system. Deviations from the desired behavior y_d , either specified by another mathematical model or reference trajectory, produce an error function $e(t) = y(t) - y_d(t)$ for increments of control actions $\Delta u(t) = u(t) - u(t - h)$. The loss function J to be minimized is shown as equation 4.

$$J(u(t), u(t - h), \dots, u(t + Nh)) = \sum_{k=1}^{t+N} e(t + kh)^2 + \rho(\Delta u(t + (k - 1)h))^2 \quad (4)$$

The control inputs that minimize equation 4 are then applied to the system by the controller over the time interval, and the process is repeated. The control input function F in equation 5 is determined implicitly by the optimization.

$$u(t) = F(y(t), y(t - h), \dots, y(t - nh), u(t - h), y(t - 2h), \dots, u(t - nh)) \quad (5)$$

This general model is meant to be a guideline, and the equations listed representative, for the thought process required to create a model predictive controller.

First-Order System Example

Take the process model to be equation 6:

$$\Delta y(t + h) = -a\Delta y(t) + b\Delta u(t) \quad (6)$$

Let us define $\Delta y(t) = y(t) - y(t - h)$ and $\Delta u(t) = u(t) - u(t - h)$. Let us also define our desired system behavior y_d as a function which starts at $y(t)$ and exponentially approaches a set point y_{sp} with time constant T . Our desired behavior y_d then becomes equation 7:

$$y_d(t+h) = y(t) + (1 - e^{-\frac{h}{T}})(y_{sp} - y(t)) \quad (7)$$

Assuming that our controller can take as much action as needed to produce the desired behavior, the desired behavior can be realized in the next sampling period. This is done by setting $y(t+h)$ equal to $y_d(t+h)$, and can be seen in equation 8:

$$y(t+h) = y(t) + \Delta y(t+h) = y(t) - \alpha \Delta y(t) + b \Delta u(t) = y(t) + (1 - e^{-\frac{h}{T}})(y_{sp} - y(t)) \quad (8)$$

Solving equation 8 for $u(t)$ gives equation 9:

$$\Delta u(t) = \frac{a}{b} \Delta y(t) + \frac{1 - e^{-\frac{h}{T}}}{b} (y_{sp} - y(t)) \quad (9)$$

Upon examination of this result, you can see that we have produced a PI controller with

gains $k = \frac{a}{b}$ and $k_i = \frac{1 - e^{-\frac{h}{T}}}{b}$. It should be noted that the proportional gain k will only depend upon the developed process model, and the integral gain k_i depends on both the process model and the desired response rate T .

This process can be modified to include multiple inputs and outputs via the process model and desired behavior. We may also add system constraints to our MPC example by adding conditional statements limiting the maximum controller output discussed in the [logical programs](#) wiki. As discussed before, there are as many variations on the MPC process as you can think of. See the worked examples 1 and 2 for more MPC instances.

Question: is the above expression a PI control system or more of a PD control system? The first term is $k*(y(\text{present}) - y(\text{past}))$ which seems more like a derivative term. The second term is more like $k*(y(\text{set}) - y(\text{present}))$ which seems more like a P term.

3.3 Differences from Other Controllers Types

Model predictive control uses a mathematical model to simulate a process. This model then fits the inputs to predict the system behavior. In this way, MPC is a type of feed forward control. It uses system inputs as a basis of control. MPC is more complex than most other feed forward control types because of the way these predictions are used to optimize a process over a defined amount of time. Most feed forward control types do not take into account the process outputs much past a residence time. The MPC algorithm will compare predicted outputs to desired outputs and select signals that will minimize

this difference over the time selected. This control type can see ahead into multiple time steps in the future in order to optimize the process. Normal PID type controllers use mathematical expressions based on error from a set point. The governing equation for MPC controllers are based on set points, system properties, and desired outcomes and optimization.

MPC is very specific to the process it is modeling. Unlike ratio or cascade control set ups, where it is simple to implement and change set points in various situations, MPC will model one specific process and optimize it. As previously mentioned this can either be an advantage or disadvantage. MPC is great for selecting one type of operation on one system and perfecting it to the desired conditions. This also has a downside in that the model equation will work for one and only one situation.

3.4 Limitations of MPC

3.4.1 Advantages of MPC

1. MPC can be used to handle multivariable control programs.
2. MPC can consider actuator limitations.
3. MPC can increase profits by allowing for operation close to the system constraints.
4. MPC can perform online computations quickly.
5. MPC can be used for non-minimal phase and unstable processes.
6. MPC is easy to tune.
7. MPC is able to handle structural changes.

3.4.2 Disadvantages of MPC

1. Several MPC models are limited to only stable, open-loop processes.
2. MPC often requires a large number of model coefficients to describe a response.
3. Some MPC models are formulated for output disturbances, and they may not handle input disturbances well.
4. Some forms of MPC use a constant output disturbance assumption. This corrects for the fact that the output predicted by the model is not exactly equal to the actual measured output. This method assumes the correction term is constant in the future, which may not yield a good performance if there is a real disturbance at the plant input.

5. If the prediction horizon is not formulated correctly, control performance will be poor even if the model is correct.

6. Some systems have a wide range of operating conditions that change frequently. Some examples of this include exothermic reactors, batch processes, and any systems where different consumers have different product specifications. An MPC linear model will not be able to handle the dynamic behavior of these processes. A nonlinear model must be used for better control performance.

3.5 Industrial MPC Applications

There are many industrial applications that incorporate model predictive control in order to effectively control a multivariable system. In order to effectively do this, one needs to set up a working model by testing many different parameters in a plant. This is usually done by starting up a plant, varying many different parameters, and having the MPC program analyze the data.

In order to test the plant, one may vary parameters such as:

1. feed flow rate/composition
2. steam pressure
3. heat duty
4. recycle ratio
5. reactor temperatures

This is only a small sample of parameters that can be changed. Once these parameters have been changed, the data is analyzed, and downstream effects of these parameters are characterized as a function of these variables. This relationship can be a combination of many different relationships (linear, nonlinear, logarithmic, exponential, power, etc.).

By testing the plant thoroughly and coming up with a robust model, the engineers ensure that an MPC controller will be able to much more effectively run the plant. Barring any major process changes, this model should be accurate for normal use.

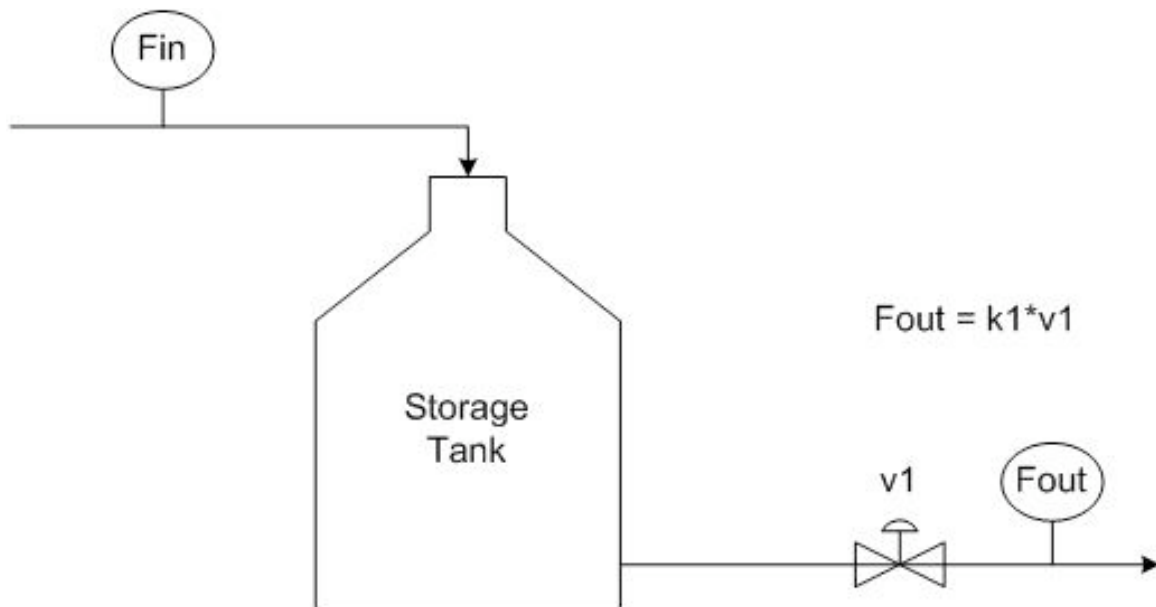
Some industrial MPC applications are:

1. Model Predictive Heuristic Control by Richard et al. 1976 (Adersa)
2. Dynamic Matrix Control (DMC) by Cutler and Ramaker 1979 (Shell Oil)
3. Quadratic-Program Dynamic Matrix (QDMC) Control by Cutler et al. 1983 (Shell Oil)

4. IDCOM-M by Setpoint, Inc (part of ASPEN Technology)
5. Generalized Predictive Control (GPC)

3.6 Implementing MPC using Excel

In MPC, values of the control variables will be optimized for a given time interval in order to best tell the system how it should act. The control variables will be optimized by optimizing some characteristic. Usually, this characteristic is simply the least squared error between an actual state and a "set" or desired state. This can easily be done using the Solver tool in Excel. See [MPC in Excel](#) for an example of implementing MPC to control the valve, v_1 , in the following system (keep reading to learn about everything in the Excel file).



To describe this system in words, there is a variable feed, F_{in} , with time that pours into a storage tank. The flow out of the tank, F_{out} , is controlled by the valve, v_1 , multiplied by a constant of proportionality, $k_1 = 50$. The tank volume is to be maintained at 150.

There are three scenarios contained in the example Excel file. In the first scenario, the valve is continuous and in the second, it is binary (can be open or closed only). In the third scenario, the valve is still binary; however, Solver cannot recognize this setup even though this setup may seem intuitive (this is discussed further below). As it turns out, it doesn't really matter if a binary or continuous valve is used. Both types of valves yield very similar results; however, the continuous valve yields slightly tighter control over the tank volume (see screenshot below).

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
19				MPC assuming continuous valve					MPC assuming binary valve								
20									Using MPC <i>correctly</i> (letting Solver think initially it can choose any values for v1)				Using MPC <i>incorrectly</i> (look how the Fout cells check to see if v1 is 1 or 0)				
21																	
22				sum of least squares: 408858					sum of least squares: 409588.2458				sum of least squares: 616273.152				
23				sum of least squares from the time the controller first acts until the end: 24.28831					sum of least squares from the time the controller first acts until the end: 754.5180095				sum of least squares from the time the controller first acts until the end: 207439.424				
24	time	Fin	V	Fout	v1 (MPC)	(V-Vset)^2		V	Fout	v1 (MPC)	(V-Vset)^2		V	Fout	v1 (MPC)	(V-Vset)^2	
99	7.4	31.609	150.056	26.6655	0.53331	0.003157		142.989	0	0	49.15103561		197.989	0	0	2302.96524	
100	7.5	25.8309	150.551	25.8154	0.51631	0.303087		146.15	0	0	14.82155646		201.15	0	0	2616.33504	
101	7.6	15.1411	150.552	25.0974	0.50195	0.304789		148.733	0	0	1.80475631		203.733	0	0	2887.25788	
102	7.7	29.7642	149.556	27.7989	0.55598	0.196739		150.247	50	1	0.061165848		205.247	0	0	3052.26607	
103	7.8	29.8362	149.753	29.7791	0.59558	0.06102		148.224	50	1	3.155098484		208.224	0	0	3390.00394	
104	7.9	34.5313	149.759	31.3583	0.62717	0.058232		146.207	50	1	14.38411759		211.207	0	0	3746.34093	
105	8	32.3695	150.076	31.2803	0.62561	0.005773		144.66	50	1	28.51040645		214.66	0	0	4180.97849	
106	8.1	23.6817	150.185	30.231	0.60462	0.034187		142.897	0	0	50.44642486		217.897	0	0	4610.06172	
107	8.2	36.8266	149.53	30.7764	0.61553	0.220927		145.266	0	0	22.41449205		220.266	0	0	4937.2553	
108	8.3	25.6309	150.135	28.8694	0.57739	0.018225		148.948	50	1	1.10614036		223.948	0	0	5468.34633	
109	8.4	30.0267	149.811	27.6976	0.55395	0.035666		146.511	50	1	12.17064756		226.511	0	0	5853.98736	
110	8.5	24.0554	150.044	25.6788	0.51358	0.001941		144.514	0	0	30.09588238		229.514	0	0	6322.48074	
111	8.6	24.8008	149.882	24.3336	0.49667	0.013992		146.92	0	0	9.489065109		231.92	0	0	6710.81552	
112	8.7	16.7253	149.928	23.1774	0.46365	0.005122		149.4	50	1	0.360425963		234.4	0	0	7123.3001	
113	8.8	32.4343	149.283	24.4854	0.48971	0.513764		146.072	0	0	15.42777862		236.072	0	0	7408.41998	
114	8.9	26.3788	150.078	23.4468	0.46894	0.006102		149.316	0	0	0.468396354		239.316	0	0	7977.27732	
115	9	18.7908	150.371	21.7067	0.43413	0.137879		151.953	50	1	3.816116295		241.953	0	0	8455.444	
116	9.1	20.1458	150.08	21.2798	0.4256	0.006357		148.833	0	0	1.362898635		243.833	0	0	8804.55072	
117	9.2	18.5492	149.966	21.535	0.4307	0.001133		150.847	0	0	0.717666524		245.847	0	0	9186.67655	
118	9.3	25.7376	149.668	22.8006	0.45601	0.110388		152.702	0	0	7.301175146		247.702	0	0	9545.69422	
119	9.4	22.3079	149.961	22.7419	0.45484	0.001486		155.276	50	1	27.83436294		250.276	0	0	10055.2417	
120	9.5	16.9677	149.918	22.0778	0.44156	0.006715		152.507	0	0	6.28312927		252.507	0	0	10507.6065	
121	9.6	23.1784	149.407	21.5435	0.43087	0.351595		154.203	50	1	17.66846993		254.203	0	0	10858.3461	
122	9.7	16.7697	149.571	19.9593	0.39919	0.184438		151.521	0	0	2.314139423		256.521	0	0	11346.7724	
123	9.8	24.4947	149.252	17.5396	0.35079	0.560147		153.198	50	1	10.22844946		258.198	0	0	11706.8493	
124	9.9	36.2061	149.947	10.9221	0.21844	0.0028		150.648	50	1	0.419471391		260.648	0	0	12242.906	
125	10	37.2061	152.475	50	1	6.128025		149.268	0	0	0.535425704		264.268	0	0	13057.238	

As you can see from this screen shot, the sum of the least squares between the actual volume and the set volume (Row 22) is lowest for the 1st scenario, when the valve is continuous. This measure of deviation from the set value is only slightly lower than in the 2nd scenario, when the valve is binary. In the 3rd scenario, Solver didn't work properly, resulting in all of the v1 variables (Column P) to be set to 0.

At the start of the simulation, the volume of the tank is 0, so v1 stays closed until time = 5.4 when the volume is very close to the set volume. If the deviations that occurred during the time v1 was closed (which is the same time length for all 3 scenarios) is removed from the sum of the least squares (Row 23) the 1st scenario suddenly looks much better at controlling the volume than the 2nd scenario.

There are a couple things to note while using Solver in Excel to perform MPC:

1) This note only applies if your system has a binary control variable. If you intend to use a conditional statement (such as an IF() function) that depends on the optimization of the control variable, you must leave open the possibility that this control variable can be any real number, whether it's binary or not. This may seem unnecessary because Solver will output only optimized discreet numbers. To put this in the context of the example Excel file, you might think you could have simply done the following to control Fout:

$$Fout = IF(v1 = 1, k1*V, 0)$$

(The variables "v1" and "k1" are not recognized by Excel. Instead of typing the variables into Excel, cells containing the variable values must be referenced.)

This statement says that if the valve is open, allow a flow of $k1$ (or 50), otherwise, the flow is 0. This would not allow Solver to work properly. If Solver chose a value of $v1 = 0.1$, measured the target cell, and then it chose $v1 = 0.2$, it wouldn't see any difference because in both cases the flow would be 0. Solver needs to be able to see a change in the system, whether it's practical or not, to determine the actual gradient of your system. This gradient cannot be determined if an IF() statement turns the continuous output to discrete output.

The proper way to handle this is to program a constraint into solver that allows only binary outputs of $v1$ values (select bin from the pull down menu when adding the constraint). Fout can then be programmed as:

- $Fout = v1 * k1$

Using this method, Solver can calculate the gradient of the system to define how it would react if $v1$ changed to a non-binary value. By using this method, Solver will output only binary values for the valve state as is desired.

2) Solver can only handle manipulating 200 variables at a time, so if your model requires looking at more than 200 time steps, you will have to optimize your system in sections.

3.7 Worked out Example 1

You have a tank outside your home used to supply water for various household functions (i.e. flushing the toilet). The optimal water pressure from the tank is achieved when the height of water in the tank is at 15, and the tank can hold water up to a height of 30, because when it rains, it pours. When it does rain, the level of water in this tank exceeds 15 and a model predictive controller and valve is in place to release water so the height will drop back down to this value (don't worry, this water is not wasted, but used as drinking water on your llama farm). At time $t=25$, there is a downpour that increases the flow into the tank by 150 and lasts for 100 time steps. Will this tank overflow, and how long will it take for the tank to return to the desired set point? Your controller output is 25 maximum.

Other key pieces of info:

$$H(0) = 15$$

$$A = 100$$

$$B = 1$$

$$T = 15$$

$$H_{set} = 15$$

h= 1

Solution:

To obtain the required information, we will produce a model predictive controller for the water tank system, and simulate how the system will behave during the downpour. The first step is to generate a mathematical model that describes the relevant parameters. Equation 10 below relates the fluid height in the tank H to the flow in, and controller signal u .

$$A \frac{dH}{dt} = F_{in} - Bu\sqrt{H(t)} \quad (10)$$

Where A and B are physical constants of the system. Next we will define the way we wish the height of fluid in the tank to act in equation 11.

$$H(t + h) = H(t) + (1 - e^{-h/T})(H_{set} - H(t)) \quad (11)$$

Where h is the time interval, T is an exponential time constant, and H_{set} is the desired liquid set point of 15. It can be seen by examining equation 11 that as time proceeds, the exponential term will reduce to zero, resulting in $H(t + h) = H_{set}$. The next step is to figure out how to produce a controller input that will give the desired behavior. This may be done by calculating the error between process model and desired behavior, and optimizing for u . Fortunately for us, this is a relatively simple set of equations that can be solved for u explicitly. By expanding equation 10 using the fundamental theorem of calculus to produce equation 12, and plugging equation 11 in for $H(t + h)$, equation 13 results solved for u .

$$A \frac{H(t + h) - H(t)}{h} = F_{in} - Bu\sqrt{H(t)} \quad (12)$$

$$u = \frac{(-AH_{set} + AH(t) + Ae^{-\frac{h}{T}} * H_{set} - Ae^{-\frac{h}{T}} H(t) + F_{in}h)}{(B\sqrt{H_{set}}h)} \quad (13)$$

These equations can be implemented in a spreadsheet to model the behavior of the height of liquid in the tank, as well as the actions taken by the controller to restore the set point. Keep in mind the 0 to 25 output restriction on your controller.

This spreadsheet has been made with the relevant equations and can be used to solve this problem and model tank behavior. This spreadsheet can be found here: [MPC example 1](#)

So yes, the tank will overflow, and will return to its set point after 200 time points.

3.8 Worked out Example 2

What happens if the actuator on the valve breaks and must be replaced with an older one you happened to have in your basement? This new (although old) actuator cannot operate the valve fast enough, and B is decreased from 1 to 0.8. How does the graph from example 1 change? What does this tell you about the physical meaning of parameter B?

Solution:

This B can easily be changed in the spreadsheet used in example 1. With this different actuator, and hence different B, we can see that the tank acquires more volume, and it takes longer for the tank to return to its optimal height of 15. This is because the valve on the tank cannot be opened as fast. Parameter B represents the physical properties/limitations of the valve, and pipe properties.

3.9 Sage's Corner

<http://www.youtube.com/v/XNccO4neVfc>

<http://www.youtube.com/v/2HkpKgX1yfE>

3.10 Multiple Choice Question 1

Which of the following is a highly desired feature for model predictive control?

- A) It is ideal in determining short-term behavior.
- B) It is the simplest of all feed forward controller types.
- C) It accounts for system constraints.
- D) Controllers of this type are universal and can be used without modification for any process.

3.11 Multiple Choice Question 2

Will a model predictive controller developed for a tank reactor be able to control an evaporation unit?

- A) Yes, as they are both standard pieces of chemical engineering equipment.
- B) Maybe, it depends if the reaction taking place in the reactor is exothermic or endothermic.

C) No, the governing equations will be very different.

D) Yes, because evaporation units and tank reactors can both use steam to supply heat.

3.12 Multiple Choice Question 3

Which of the following statements about MPC is false?

A) MPC uses a defined time interval.

B) MPC utilizes feed forward control.

C) MPC requires a certain number of inputs and outputs.

D) MPC can generate more than one possible outcome.

3.13 Answers to the multiple choice questions

1 - C

2 - C

3 - C

3.14 References

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Section 4. Neural Networks for automatic model construction

Title: MIMO Using Neural Networks

Authors: Group E - Ardemis Boghossian, James Brown, Sara Zak

Date Presented: November 2, 2006

Date Revised:

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

4.1 Introduction

Multiple Input Multiple Output (MIMOs) are systems that require multiple inputs and generate multiple outputs. MIMOs are controlled by controllers that combine multiple input readings in an algorithm to generate multiple output signals. MIMOs can be used with a variety of algorithms. The most versatile algorithm used to date is the neural network. Neural networks, which were initially designed to imitate human neurons, work to store, analyze, and identify patterns in input readings to generate output signals. In chemical engineering, neural networks are used to predict the outputs of systems such as distillation columns and CSTRs. This article will discuss how neural networks work, the advantages and disadvantages of neural networks, and some common applications of the networks.

4.2 MIMOs

As mentioned, Multiple Inputs Multiple Outputs (MIMOs) are systems that require multiple inputs and generate multiple outputs, as shown schematically in Figure 1.



Figure 1. Schematic diagram of MIMOs

As shown in the figure, MIMOs are controlled by controllers that combine multiple input readings in an algorithm to generate multiple output signals. Typically, MIMOs do not require that the the number of inputs and outputs be the same. Instead, any number of input readings could be used to generate any number of output signals.

4.3 Neural Networks

Various types of controllers can be used to control MIMOs. One of the most accurate and versatile controllers used for MIMOs is the neural network. Neural networks are controllers that crudely imitate the human neuron. Initially, these networks were designed to model neural brain activity. However, as people began to recognize the advantages of neural networks, these networks were applied to controller algorithm design. Like a human neuron, neural networks work to store, analyze, and identify patterns in data by performing learning tasks. The ability of these networks to "learn" parallels the human neuron's ability to learn, making these automatic controllers the closest analog to a human controller.

4.3.1 Neurons

Like neurons in the body, network neurons receive inputs, store this data, and transmit outputs to either another neuron or directly to the MIMO. In order to transmit this data, the neuron must relate the multiple inputs to the multiple outputs. A simple mathematical representation of this relationship is shown below.

$$y = f(w_1a_1 + w_2a_2 + w_3a_3 + \dots + w_na_n) = f\left(\sum_{i=1}^n w_i a_i\right)$$

w_i = weight

a_i = input

y = output

f = sigmoid function (any nonlinear function)

According to this relationship, the multiple input parameters are each multiplied by the corresponding weight factor, w_i . These weight factors "weigh" the significance of each input, scaling each input proportionally to the effect it will have on the output. These weighted inputs are then added and the sum is input into the sigmoid function to generate an output. This output can then be sent to multiple neurons that, in turn, each generate its own output.

The sigmoid function in this relationship is a nonlinear, empirical function that relates the input readings to the output signals. This empirical function can take on many forms depending on the data set. The equation that is best able to predict the outputs for the given system will be used (polynomial, sine, logarithmic, etc.). For example, one form this function may take is the hyperbolic sine function, where

$$f(x) = \sinh(\alpha x)$$

$$x = \text{sum of weighted inputs} = \sum_{i=1}^n w_i a_i$$

α = empirical parameter

In this sigmoid function, α is an empirical parameter that adjusts the function outputs. The effect of α on this sigmoid function is shown in Figure 2.

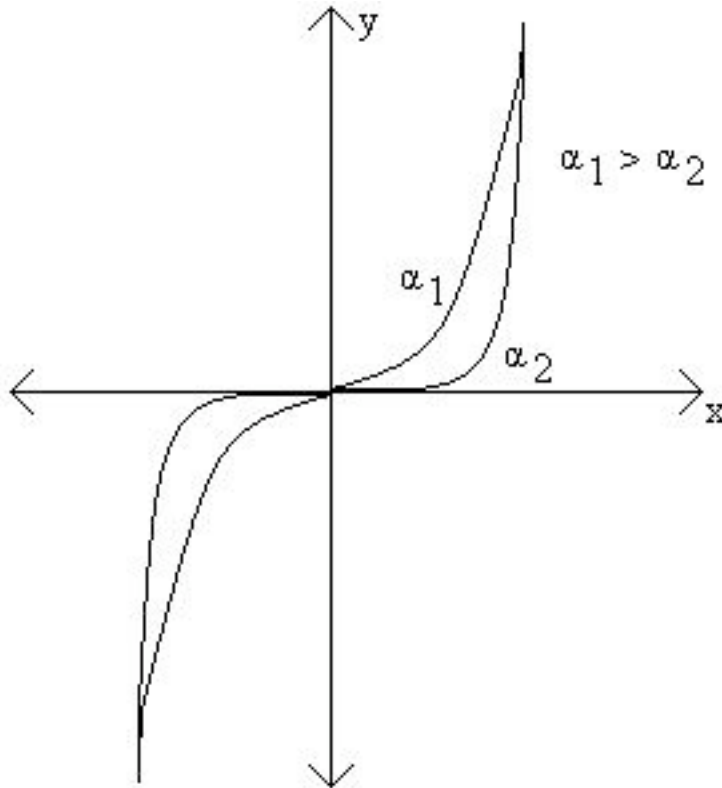


Figure 2. Plot of hyperbolic sine sigmoid function with varying αx

As shown in Figure 2, increasing α increases the output for this particular sigmoid function. Like most empirical functions, the hyperbolic sine sigmoid function can only be used within a specified range of values (x values between the vertical asymptotes). In this case, the range would depend on the value of α .

4.3.2 Combining Neurons into Neural Networks

Once neurons have been programmed to correlate input and output data, they can be connected in a feedforward series to produce a neural network, or neural net (NN). A schematic diagram of a neural network is shown in Figure 3.

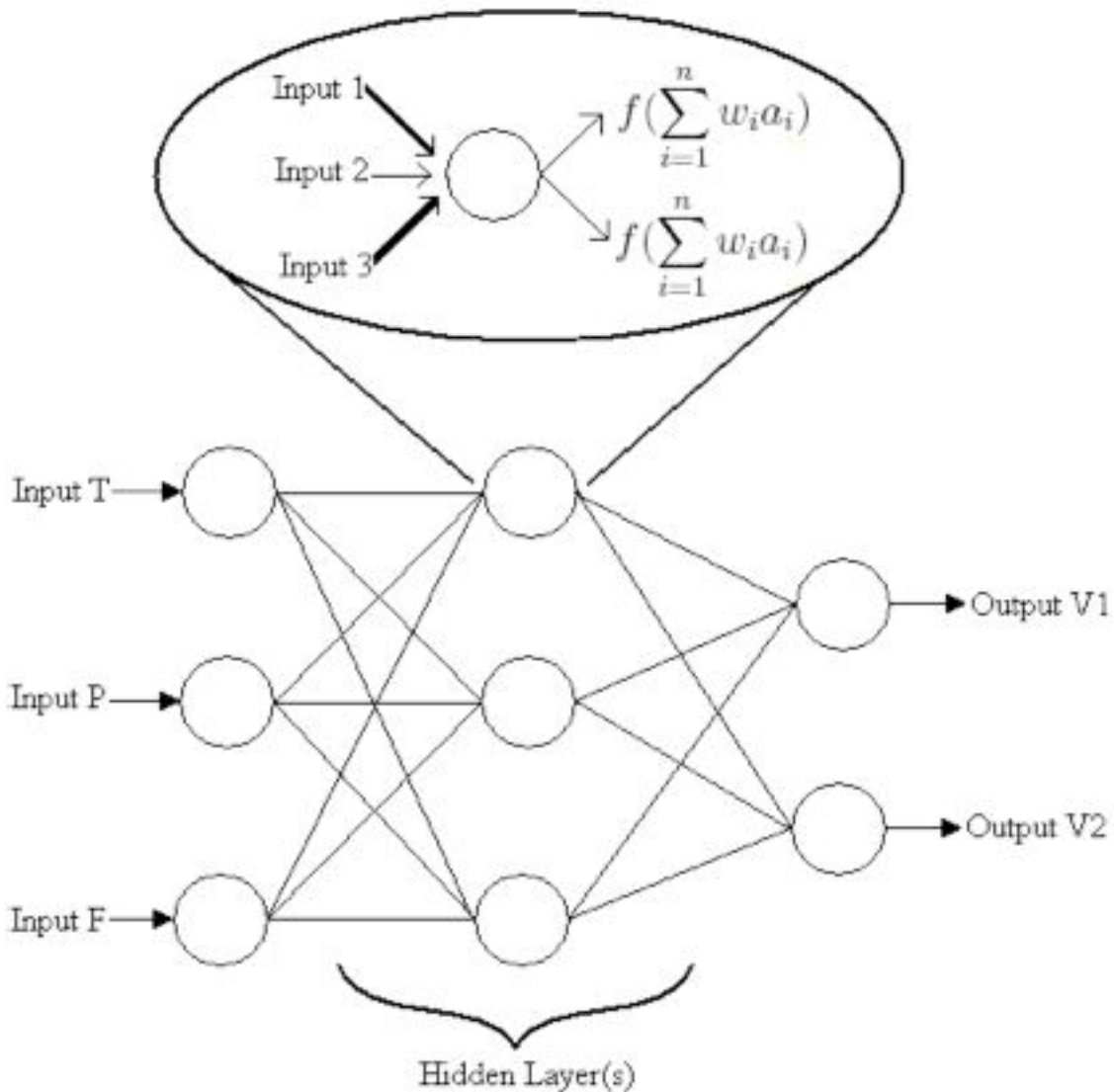


Figure 3. Schematic diagram of a neural network.

Figure 3 shows MIMO parameters, such as temperature, pressure, and flow readings, are first processed in the first layer of neurons. The outputs of the first layer of neurons then serve as the inputs to the second layer. The outputs of the second layer then become the inputs to the third layer, and so on, until the final output of the network is used to directly affect MIMO controls such as valves. The layers of neurons between the initial and final layers are known as hidden layers.

The way neurons within hidden layers correlate the inputs and outputs is analogous to the way individual neurons correlate these variables. As shown in the flowchart inset of the diagram, a neuron within the network receives multiple inputs. Each of these input parameters are then weighted, having the most effective parameters weighted more heavily. These weighted input values are added and input into the particular sigmoid function the neuron is programmed to follow. The output of this function is then sent to

other neurons as input. These input values are then reweighed for that particular neuron. This process is continued until the final output of the neuron network is used to adjust the desired controls. Although the diagram shows only one hidden layer, these neuron networks can consist of multiple layers. Although almost all continuous functions can be approximated by a single hidden layer, incorporating multiple hidden layers decreases the numbers of weights used. Since more layers will result in more parameters, each of these individual parameters will be weighted less. With more parameters and less weights, the system becomes more sensitive to parameter change (a greater "rippling" effect within the network).

The "rippling" effect of a neuron network makes the system difficult to model analytically. A small change in a single input variable would result in multiple changes throughout the the entire network. Although modelling these complex networks is beyond the scope of the class, only a basic, qualitative understanding of how neural networks function is necessary to analyze neural network controllers and their effects on input and output parameters.

4.3.3 Learning Process

The ability of neural networks to learn distinguishes them from most automatic controllers. Like humans, neural networks learn by example, and thus need to be trained. Neural networks are usually configured to specific applications and have the ability to process large amounts of data. Complex trends and patterns can be detected by neural networks that would otherwise be imperceptible to humans or other computing programs. Within neural networks, there are learning procedures that allow the device to recognize a certain pattern and carry out a specific task. These learning procedures consist of an algorithm that enables the network to determine the weighting parameters in order to match the given data (inputs and outputs) with a function. In this iterative procedure, the initial input values are used to generate initial output values. Based on these input and output values, the weights within the network are adjusted to match the data. These adjusted weights are then used to correlate the next pair of input and output values. Again, these values are used to adjust weights. This process continues until the network obtains a good fit for the data. A flow chart summarizing this iterative process is shown in Figure 4.

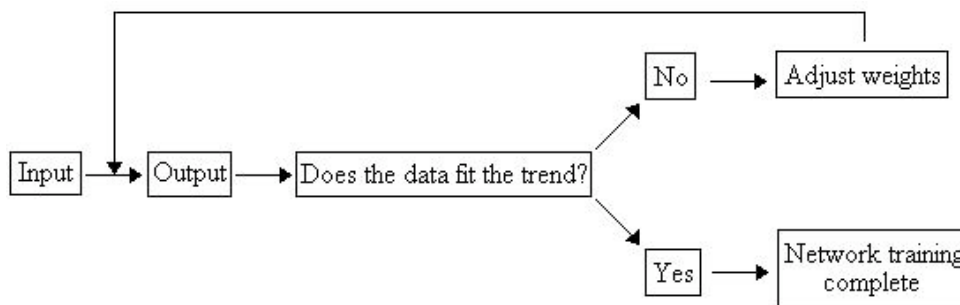


Figure 4. Flowchart for training a network.

A visual example of the learning process that takes place in a neural network is shown in the link below.

<http://tralvex.com/pub/nap/video/jn-learn.mpg>

As illustrated in the video, the neural network learns by tracing the path of an object over a specific area and sequence. For this application, inputs for the neural network included the position, velocity, and direction. Once the the neural network has completed its training, it will use what it learned to predict trajectories. A visual example of this is shown in the link below.

<http://tralvex.com/pub/nap/video/jn-pred.mpg>

As illustrated in this video, the neural network can predict where the object will move given the position, velocity, and direction of the object.

The trajectories shown in these videos demonstrate an important characteristic of neural networks. In these videos, the neural network can only predict outputs for objects that behave similar to the output it encountered during training. For instance, if a person was to start running forward, then stop, spin in a circle, and start running backwards, the neural network output would be unpredictable.

Once the neural network becomes capable of predicting system outputs, it is run like any other controller. In real-time, this often entails the chemical process and a computer system of some sort. Often, such as in LabVIEW, the chemical engineer is presented with a user-friendly data acquisition program that allows the user to set desired temperatures, flowrates, etc. and displays the system's input and outputs. Although the neural network continually sends signals to the system controllers (such as valves), the network algorithm is embedded in the acquisition program. Therefore, once the system is up and running, the user does not directly see the algorithm working.

4.4 Advantages and Disadvantages

Given the interesting, human-like behavior of neural networks, one would expect all process applications to be controlled by neural networks. However, the advantages and disadvantages of neural networks limit their use in applications. The following lists summarize these advantages and disadvantages.

Advantages

- Neural networks are very general and can capture a variety of patterns very accurately
- The static, non-linear function used by neural networks provide a method to fit the parameters of a particular function to a given set of data.
- A wide variety of functions can be used to fit a given set of data

- Neural networks do not require excessive statistical training
- There is no need to assume an underlying input data distribution when programming a neural network
- Neural networks can detect all possible, complex nonlinear relationships between input and outputs
- Neural networks are the closest thing to having an actual human operate a system (i.e. they can "learn")

Disadvantages

- Neural networks are difficult to design. One must determine the optimal number of nodes, hidden layers, sigmoid function, etc.
- Neural networks are difficult to model analytically because a small change in a single input will affect the entire network
- The operation of neural networks is limited to the training process. If the network is trained poorly, then it will operate poorly and the outputs cannot be guaranteed.
- There is a great computational burden associated with neural networks
- Neural networks require a large sample size in order to empirically fit data
- Neural networks have a "black box" nature. Therefore, errors within the complex network are difficult to target.
- Outside of their data training range, neural networks are unpredictable. This occurs because neural networks may "overfit" data. For instance, during training, a neural network may fit a 10th order polynomial to only 5 data points. When using this model to make predictions of values outside this 5-point range, the neural network behaves unpredictably.

4.5 Applications of Neural Networks

Each neural network will generate a different algorithm based on the inputs and outputs to the system. Because neural networks fit a specific function to the given data, they can be used in a variety of applications. Within chemical engineering, neural networks are frequently used to predict how changing one input (such as pressure, temperature, etc.) on a distillation column will influence the compositions and flow rates of the streams exiting the column. The network training is performed on various inputs to the column, and thus can predict how changing one input will affect the product streams. Within a CSTR, neural networks can be used to determine the effect of one input parameter such as temperature or pressure on the products.

In addition to its applications to chemical equipment, neural networks can also be applied to model material responses as a function of various loads under various conditions. These models can then be used in product development to create a device for a particular application, or to improve an existing device. For example, by modeling the corrosion of steel under different temperature and pH conditions, implanted biomedical devices can be manufactured or improved.

Neural networks are also often used in biology and biological applications to predict the outcome of a certain event. For example, neural networks can be used to predict the growth of cells and bacteria in cell culture labs, given a set of varying conditions, such as temperature and pH. In addition, neural network models have been used to predict the mortality rate in intensive care units in hospitals. Data was collected from different patients, and a neural network model was created to predict the mortality of future patients given a set of specified conditions. Neural networks have also been used to diagnose breast cancer in patients by predicting the effects of a tumor provided specified input conditions of the patient.

Neural networks are also used in applications beyond the chemical aspect of controllers. For instance, neural networks are used to predict travel time based on different travel conditions. Signs on the highways that give estimated travel times are examples of neural networks. They predict the amount of time required to reach a certain destination given the varying traffic volume, road conditions, and weather conditions.

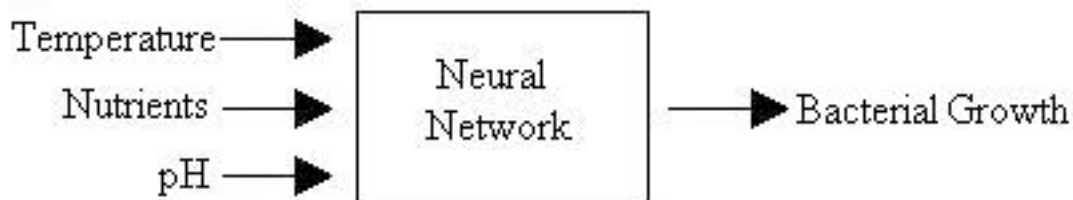
Neural networks are not limited to the applications listed above. They can be used to model most predictable events, and the complexity of the network will increase depending on the situation. For more information on the uses listed above, refer to the journal articles listed in the references section of this wiki.

4.6 Worked out Example 1

Hypothetical Industries has expanded to now include a biology lab! As an employee, you are working on developing a new antibiotic, and thus have been assigned to predict the growth of bacteria. Your boss wants to know how the growth of the bacteria is affected by different conditions, such as temperatures, pH, and provided nutrients. You don't really feel like manipulating all these conditions, and then sitting and watching bacteria grow on a petri dish, so you decide to come up with a way to predict the how the bacteria will grow. Using the information presented in the wiki, determine what the inputs and outputs to this neural network are.

SOLUTION:

The inputs to the neural network are each of the parameters that may affect the growth of the bacteria. In this situation, the inputs are the temperature, pH, and nutrients provided (such as sugars, amino acids, and antibiotics). The outputs from this system include the growth of the bacteria.



4.7 Worked out Example 2

As seen in the example above, a neural network can be used to predict bacterial growth. Given the information presented in the wiki, explain the advantages and disadvantages of using a neural network to model bacterial growth.

SOLUTION:

Advantages

- Because there are so many inputs (temperature, pH, etc.), a neural network fits a function to this data that is able to predict how future conditions would affect the bacterial growth.
- Neural networks provide a mechanical method of modeling the system of bacterial growth that is extremely similar to have an actual human predict the growth of bacteria.
- Someone monitoring the system does not need much statistical training to use the neural network.

Disadvantages

- You must first run a large number of samples with varying conditions in order to obtain a good fit for the neural network. Based on how well you would like your network to predict bacterial growth, the number of samples that must be run in order to create the network changes. The network will only function as well as it is trained, so if a high degree of accuracy is desired, then more data inputs will be required. This becomes time consuming and expensive.
- Because of the black box nature of the neural networks, it is difficult to determine how the individual parameters such as temperature or pH will affect the bacterial growth.
- Neural networks cannot be used to predict the growth patterns of the bacteria outside of the given data ranges.

4.8 Multiple Choice Question 1

Why would someone want to increase the number of hidden layers when combining neurons into a neural network?

- a.) To decrease the amount of programming needed
- b.) To decrease the number of weights required

- c.) To increase the cost associated with the system
- d.) To increase the aesthetic structure of the system

4.9 Multiple Choice Question 2

What does the neural network output if its inputs are outside its training range?

- a.) Zero
- b.) Input^2
- c.) $\text{sqrt}(\text{input})$
- d.) The outputs outside of range are unpredictable

4.10 References

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Section 5. Understanding MIMO Control Through Two Tanks Interaction

Written by: Erin Baragar, Omar Ismail, Yuan Chen

5.1 Introduction

We have been familiar with the models of single surge tank manipulated by first order process and two tanks in series manipulated by second order process, both of which are typical examples of Single Input Single Output (SISO) control. However, in the real chemical processes, there are always interactions between the reactors. The following page will discuss the two tanks model by taking into consideration the interaction between the two tanks. To manipulate this model, we need to use Multiple Input Multiple Output (MIMO) control, which will add more complexity in understanding the overall process.

5.2 Two Tanks Interaction Model

The following figure, Figure 1, demonstrates how two tanks model works to interact each other. From Figure 1, we can see that the input of Tank1, x_1 , not only affects the level in Tank1, but also affects that in Tank2. The same goes for the input of Tank2, x_2 . We use the resistance, R_3 , to account for the interaction between the two tanks.

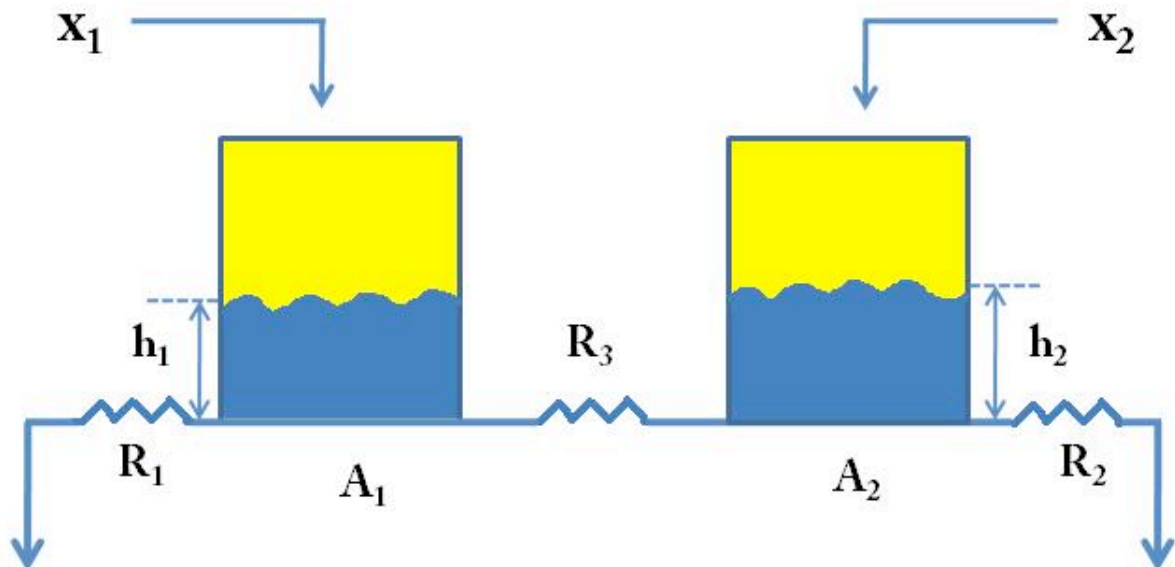


Figure 1: Two tanks interaction model

In the above figure,

x_1 = Input of Tank1
 x_2 = Input of Tank2
 A_1 = Cross section area of Tank1
 A_2 = Cross section area of Tank2
 h_1 = Level of Tank1
 h_2 = Level of Tank2
 R_1 = Resistance of Tank1
 R_2 = Resistance of Tank2
 R_3 = Interaction Resistance

5.2.1 Mathematical Equations for the Process

Now, we will derive the mathematical equations to describe the process, now we assume the direction of the flow goes from Tank1 to Tank2:

To begin with, we write down the governing equation for each of the tanks, taking into consideration the interaction term:

$$\begin{aligned}
 A_1 \frac{dh_1}{dt} &= x_1 - \frac{h_1}{R_1} dt - \frac{(h_1 - h_2)}{R_3} = x_1 + h_1 \left(-\frac{1}{R_1} - \frac{1}{R_3} \right) + h_2 \left(\frac{1}{R_3} \right) \\
 A_2 \frac{dh_2}{dt} &= x_2 - \frac{h_2}{R_2} dt + \frac{(h_1 - h_2)}{R_3} = x_2 + h_2 \left(-\frac{1}{R_2} - \frac{1}{R_3} \right) + h_1 \left(\frac{1}{R_3} \right)
 \end{aligned}$$

Under steady state, the time derivatives, i.e. the left hand side of the above equations, go to zero:

$$\begin{aligned}
 0 &= x_1(0) + h_1(0) \left(-\frac{1}{R_1} - \frac{1}{R_3} \right) + h_2(0) \left(\frac{1}{R_3} \right) \\
 0 &= x_2(0) + h_1(0) \left(\frac{1}{R_3} - \frac{1}{R_3} \right) + h_2(0) \left(-\frac{1}{R_2} - \frac{1}{R_3} \right)
 \end{aligned}$$

Now, we define the deviation variables as follows:

$$\begin{aligned}
 X_1 &= x_1 - x_1(0), Y_1 = h_1 - h_1(0) \\
 X_2 &= x_2 - x_2(0), Y_2 = h_2 - h_2(0)
 \end{aligned}$$

Set $y_1=h_1$, $y_2=h_2$, we can obtain the following equations:

$$A_1 \frac{dy_1}{dt} = \frac{x_1}{A_1} + y_1 \left(-\frac{1}{A_1 R_1} - \frac{1}{A_1 R_3} \right) + y_2 \left(\frac{1}{A_1 R_3} \right)$$

$$A_2 \frac{dy_2}{dt} = \frac{x_2}{A_1} + y_1 \left(\frac{1}{A_2 R_3} \right) + y_2 \left(-\frac{1}{A_2 R_2} - \frac{1}{A_2 R_3} \right)$$

It will be more general if we write down the above equations into a form of Matrix:

$$\begin{bmatrix} \dot{y}_1 \\ \dot{y}_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{A_1} & 0 \\ 0 & \frac{1}{A_2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} -\frac{1}{A_1 R_1} - \frac{1}{A_1 R_2} & \frac{1}{A_1 R_3} \\ \frac{1}{A_2 R_3} & -\frac{1}{A_2 R_2} - \frac{1}{A_2 R_3} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

We can represent the above equation using the following equation:

$$\begin{aligned} \vec{\dot{y}} &= \vec{\overline{B}} \vec{x} + \vec{\overline{A}} \vec{y} \\ \vec{\dot{y}} - \vec{\overline{A}} \vec{y} &= \vec{\overline{B}} \vec{x} \\ \vec{x} &= (\vec{\overline{B}}^{-1}) \left(\frac{\partial}{\partial t} - \vec{\overline{A}} \right) \vec{y} = \vec{\overline{G}}_p^{-1} \vec{y} \end{aligned}$$

Invert the above equation:

$$\vec{y} = \vec{\overline{G}}_p \vec{x}$$

Now, set

$$\vec{\overline{G}}_p = \begin{bmatrix} \hat{G}_{p1,1} & \hat{G}_{p1,2} \\ \hat{G}_{p2,1} & \hat{G}_{p2,2} \end{bmatrix}$$

We get the following equation:

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} \hat{G}_{p1,1} & \hat{G}_{p1,2} \\ \hat{G}_{p2,1} & \hat{G}_{p2,2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

5.2.2 Control Diagram

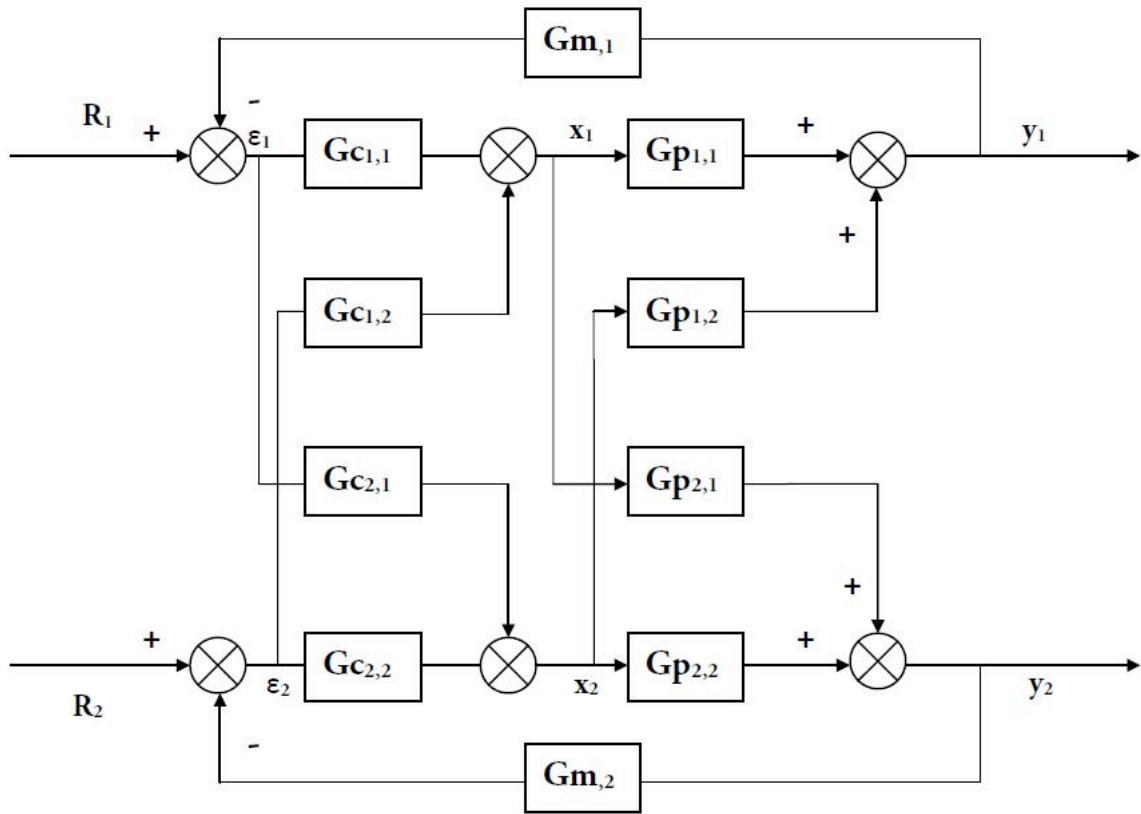


Figure 2: Control Diagram for Two tanks interaction model.

5.2.3 Decouple the process

$$E_1 = R_1 + \widehat{G}_{m1} \cdot Y_1$$

$$E_2 = R_2 + \widehat{G}_{m2} \cdot Y_2$$

$$\begin{bmatrix} E_1 \\ E_2 \end{bmatrix} = \begin{bmatrix} R_1 \\ R_2 \end{bmatrix} + \begin{bmatrix} \widehat{G}_{m1} & 0 \\ 0 & \widehat{G}_{m2} \end{bmatrix} \begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix}$$

$$\vec{E} = \vec{R} - \widehat{G}_m \cdot \vec{Y}$$

Summarizing All Equations

$$\left. \begin{array}{l} \vec{Y} = \widehat{G}_p \cdot \vec{X} \\ \vec{X} = \widehat{G}_c \cdot \vec{E} \\ \vec{E} = \vec{R} - \widehat{G}_m \cdot \vec{Y} \end{array} \right\} \vec{Y} = \widehat{G}_c \widehat{G}_p \widehat{G}_c \left(\vec{R} - \widehat{G}_m \cdot \vec{Y} \right)$$

$$\vec{Y} + \widehat{G}_c \widehat{G}_p \widehat{G}_c \vec{Y} = \widehat{G}_p \widehat{G}_c \vec{R}$$

$$\left(\vec{I} + \widehat{G}_c \widehat{G}_p \widehat{G}_c \right) \vec{Y} = \widehat{G}_p \widehat{G}_c \vec{R}$$

$$\vec{Y} = \left(\vec{I} + \widehat{G}_c \widehat{G}_p \widehat{G}_c \right)^{-1} \widehat{G}_p \widehat{G}_c \vec{R}$$

If $\widehat{G}_p \widehat{G}_c$ is diagonal, i.e. $\begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}$

Then $\vec{Y} = [\text{Diagonal}] \vec{R}$

$$\begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \begin{bmatrix} R_1 \\ R_2 \end{bmatrix}$$

$$Y_1 = aR_1$$

$$Y_2 = bR_2$$

$$\begin{aligned} \ddot{G}_p \ddot{G}_c &= \begin{bmatrix} G_{p1,1} & G_{p1,2} \\ G_{p2,1} & G_{p2,2} \end{bmatrix} \cdot \begin{bmatrix} G_{c1,1} & G_{c1,2} \\ G_{c2,1} & G_{c2,2} \end{bmatrix} = \begin{bmatrix} G_{p1,1} \cdot G_{c1,1} + G_{p1,2} \cdot G_{c2,1} & G_{p1,1} \cdot G_{c1,2} + G_{p1,2} \cdot G_{c2,2} \\ G_{p2,1} \cdot G_{c1,1} + G_{p2,2} \cdot G_{c2,1} & G_{p2,1} \cdot G_{c1,2} + G_{p2,2} \cdot G_{c2,2} \end{bmatrix} \\ &= \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \end{aligned}$$

Using this identity, $G_{c1,2}$ & $G_{c2,1}$ can be calculated.

5.3 Reference


- http://controls.engin.umich.edu/wiki/index.php/Second-order_differential_equations

Part III
Statistical Analysis for
Chemical Process Control

Chapter 13. Statistics and Probability

Background

Section 1. Basic statistics: mean, median, average, standard deviation, z-scores, and p-value

Note:  [Video lecture](#) available for this section!

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Date Presented: 11/21/06; Revised: 11/5/07

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

1.1 Introduction

Statistics is a field of mathematics that pertains to data analysis. Statistical methods and equations can be applied to a data set in order to analyze and interpret results, explain variations in the data, or predict future data. A few examples of statistical information we can calculate are:

- Average value (mean)
- Most frequently occurring value (mode)
- On average, how much each measurement deviates from the mean (standard deviation of the mean)
- Span of values over which your data set occurs (range), and
- Midpoint between the lowest and highest value of the set (median)

Statistics is important in the field of engineering by it provides tools to analyze collected data. For example, a chemical engineer may wish to analyze temperature measurements from a mixing tank. Statistical methods can be used to determine how reliable and reproducible the temperature measurements are, how much the temperature varies within the data set, what future temperatures of the tank may be, and how confident the engineer can be in the temperature measurements made. This article will cover the basic statistical functions of mean, median, mode, standard deviation of the mean, weighted averages and standard deviations, correlation coefficients, z-scores, and p-values.

1.2 What is a Statistic?

In the mind of a statistician, the world consists of populations and samples. An example of a population is all 7th graders in the United States. A related example of a sample

would be a group of 7th graders in the United States. In this particular example, a federal health care administrator would like to know the average weight of 7th graders and how that compares to other countries. Unfortunately, it is too expensive to measure the weight of every 7th grader in the United States. Instead statistical methodologies can be used to estimate the average weight of 7th graders in the United States by measure the weights of a sample (or multiple samples) of 7th graders.

Parameters are to populations as statistics are to samples.

A parameter is a property of a population. As illustrated in the example above, most of the time it is infeasible to directly measure a population parameter. Instead a sample must be taken and statistic for the sample is calculated. This statistic can be used to estimate the population parameter. (A branch of statistics know as Inferential Statistics involves using samples to infer information about a populations.) In the example about the population parameter is the average weight of all 7th graders in the United States and the sample statistic is the average weight of a group of 7th graders.

A large number of statistical inference techniques require samples to be a single random sample and independently gathers. In short, this allows statistics to be treated as random variables. A in-depth discussion of these consequences is beyond the scope of this text. It is also important to note that statistics can be flawed due to large variance, bias, inconsistency and other errors that may arise during sampling. Whenever performing over reviewing statistical analysis, a skeptical eye is always valuable.

Statistics take on many forms. Examples of statistics can be seen below.

1.3 Basic Statistics

When performing statistical analysis on a set of data, the mean, median, mode, and standard deviation are all helpful values to calculate. The mean, median and mode are all estimates of where the "middle" of a set of data is. These values are useful when creating groups or bins to organize larger sets of data. The standard deviation is the average distance between the actual data and the mean.

1.3.1 Mean and Weighted Average

The mean (also know as average), is obtained by dividing the sum of observed values by the number of observations, n . Although data points fall above, below, or on the mean, it can be considered a good estimate for predicting subsequent data points. The formula for the mean is given below as equation (1). The excel syntax for the mean is AVERAGE(starting cell: ending cell).

$$\bar{X} = \frac{\sum_{i=1}^n X_i}{n} \quad (1)$$

However, equation (1) can only be used when the error associated with each measurement is the same or unknown. Otherwise, the weighted average, which incorporates the standard deviation, should be calculated using equation (2) below.

$$X_{wav} = \frac{\sum w_i x_i}{\sum w_i} \quad (2)$$

where $w_i = \frac{1}{\sigma_i^2}$ and x_i is the data value.

1.3.2 Median

The median is the middle value of a set of data containing an odd number of values, or the average of the two middle values of a set of data with an even number of values. The median is especially helpful when separating data into two equal sized bins. The excel syntax to find the median is MEDIAN(starting cell: ending cell).

1.3.3 Mode

The mode of a set of data is the value which occurs most frequently. The excel syntax for the mode is MODE(starting cell: ending cell).

1.3.4 Considerations

Now that we've discussed some different ways in which you can describe a data set, you might be wondering when to use each way. Well, if all the data points are relatively close together, the average gives you a good idea as to what the points are closest to. If on the other hand, almost all the points fall close to one, or a group of close values, but occassionally a value that differs greatly can be seen, then the mode might be more accurate for describing this system, whereas the mean would incorporate the occassional outlying data. The median is useful if you are interested in the range of values your system could be operating in. Half the values should be above and half the values should be below, so you have an idea of where the middle operating point is.

1.3.5 Standard Deviation and Weighted Standard Deviation

The standard deviation gives an idea of how close the entire set of data is to the average value. Data sets with a small standard deviation have tightly grouped, precise data. Data sets with large standard deviations have data spread out over a wide range of values. The formula for standard deviation is given below as equation (3). The excel syntax for the standard deviation is STDEV(starting cell: ending cell).

$$\sigma = \sqrt{\frac{1}{n-1} \sum_{i=1}^{i=n} (X_i - \bar{X})^2} \quad (3)$$

Side Note: Bias Estimate of Population Variance

The standard deviation (the square root of variance) of a sample can be used to estimate a population's true variance. Equation (3) above is an unbiased estimate of population variance. Equation (3.1) below is another common method for calculating sample standard deviation, although it is a biased estimate. Although the estimate is biased, it is advantageous in certain situations because the estimate has a lower variance. (This relates to the bias-variance trade-off for estimators.)

$$\sigma_n = \sqrt{\frac{1}{n} \sum_{i=1}^{i=n} (X_i - \bar{X})^2} \quad (3.1)$$

When calculated standard deviation values associated with weighted averages, equation (4) below should be used.

$$\sigma_{wav} = \frac{1}{\sqrt{\sum w_i}} \quad (4)$$

1.3.6 The Sampling Distribution and Standard Deviation of the Mean

Population parameters follow all types of distributions, some are normal, others are skewed like the F-distribution and some don't even have defined moments (mean, variance, etc.) like the Cauchy distribution. However, many statistical methodologies, like a z-test (discussed later in this article), are based off of the normal distribution. How does this work? Most sample data are not normally distributed.

This highlights a common misunderstanding of those new to statistical inference. The distribution of the population parameter of interest and the *sampling distribution* are not the same. *Sampling distribution?!?* What is that?

Imagine an engineering is estimating the mean weight of widgets produced in a large batch. The engineer measures the weight of N widgets and calculates the mean. So far, one sample has been taken. The engineer then takes another sample, and another and another continues until a very larger number of samples and thus a larger number of mean sample weights (assume the batch of widgets being sampled from is near infinite for simplicity) have been gathered. The engineer has generated a sample distribution.

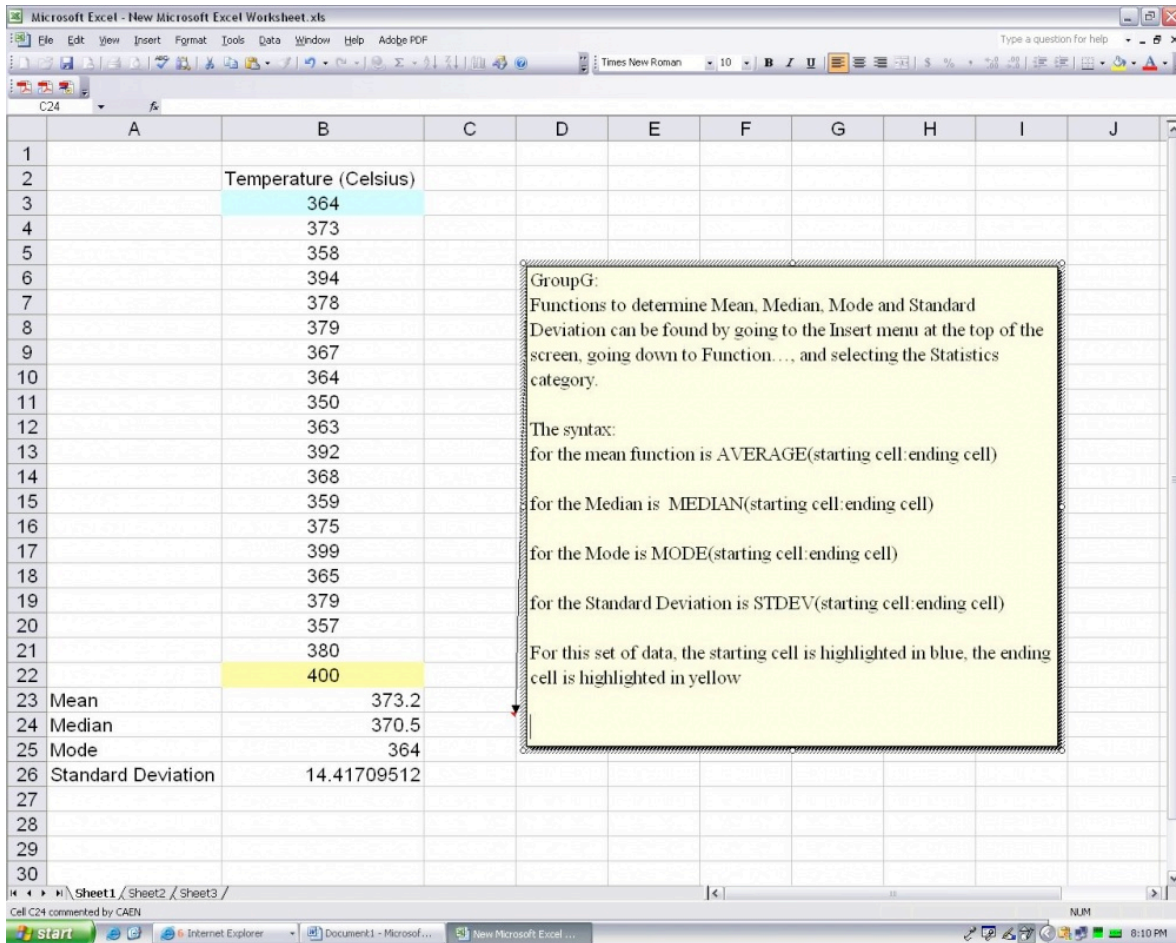
As the name suggested, a sample distribution is simply a distribution of a particular statistic (calculated for a sample with a set size) for a particular population. In this example, the statistic is mean widget weight and the sample size is N. If the engineer were to plot a histogram of the mean widget weights, he/she would see a bell-shaped distribution. This is because the Central Limit Theorem guarantees that as the sample size approaches infinity, the sampling distributions of statistics calculated from said samples approach the normal distribution.

Conveniently, there is a relationship between sample standard deviation (σ) and the standard deviation of the sampling distribution ($\sigma_{\bar{X}}$ - also know as the *standard deviation of the mean* or *standard error* deviation). This relationship is shown in equation (5) below:

$$\sigma_{\bar{X}} = \frac{\sigma_X}{\sqrt{N}} \quad (5)$$

An important feature of the standard deviation of the mean, $\sigma_{\bar{X}}$ is the factor \sqrt{N} in the denominator. As sample size increases, the standard deviation of the mean decrease while the standard deviation, σ does not change appreciably.

Microsoft Excel has built in functions to analyze a set of data for all of these values. Please see the screen shot below of how a set of data could be analyzed using Excel to retrieve these values.



1.3.7 Example by Hand

You obtain the following data points and want to analyze them using basic statistical methods. {1,2,2,3,5}

Calculate the average: Count the number of data points to obtain $n = 5$

$$mean = \frac{1 + 2 + 2 + 3 + 5}{5} = 2.6$$

Obtain the mode: Either using the excel syntax of the previous tutorial, or by looking at the data set, one can notice that there are two 2's, and no multiples of other data points, meaning the 2 is the mode.

Obtain the median: Knowing the $n=5$, the halfway point should be the third (middle) number in a list of the data points listed in ascending or descending order. Seeing as how the numbers are already listed in ascending order, the third number is 2, so the median is 2.

Calculate the standard deviation: Using the equation shown above,

$$\sigma = \sqrt{\frac{1}{5-1}((1-2.6)^2 + (2-2.6)^2 + (2-2.6)^2 + (3-2.6)^2 + (5-2.6)^2)} = 1.52$$

1.3.8 Example by Hand (Weighted)

Three University of Michigan students measured the attendance in the same Process Controls class several times. Their three answers were (all in units people):

Student 1: $A = 100 \pm 3$

Student 2: $A = 105 \pm 4$

Student 3: $A = 102 \pm 2$

What is the best estimate for the attendance A ?

$$w_i = \frac{1}{\sigma_i^2}, \quad w_1 = \frac{1}{9}, \quad w_2 = \frac{1}{16}, \quad w_3 = \frac{1}{4}$$

$$A_{wav} = \frac{\sum w_i A_i}{\sum w_i} = \frac{\frac{1}{9} * 100 + \frac{1}{16} * 105 + \frac{1}{4} * 102}{\frac{1}{9} + \frac{1}{16} + \frac{1}{4}} = 101.92 \text{ students}$$

$$\sigma_{wav} = \frac{1}{\sqrt{\sum w_i}} = \frac{1}{\sqrt{\frac{1}{9} + \frac{1}{16} + \frac{1}{4}}} = .65$$

Therefore,

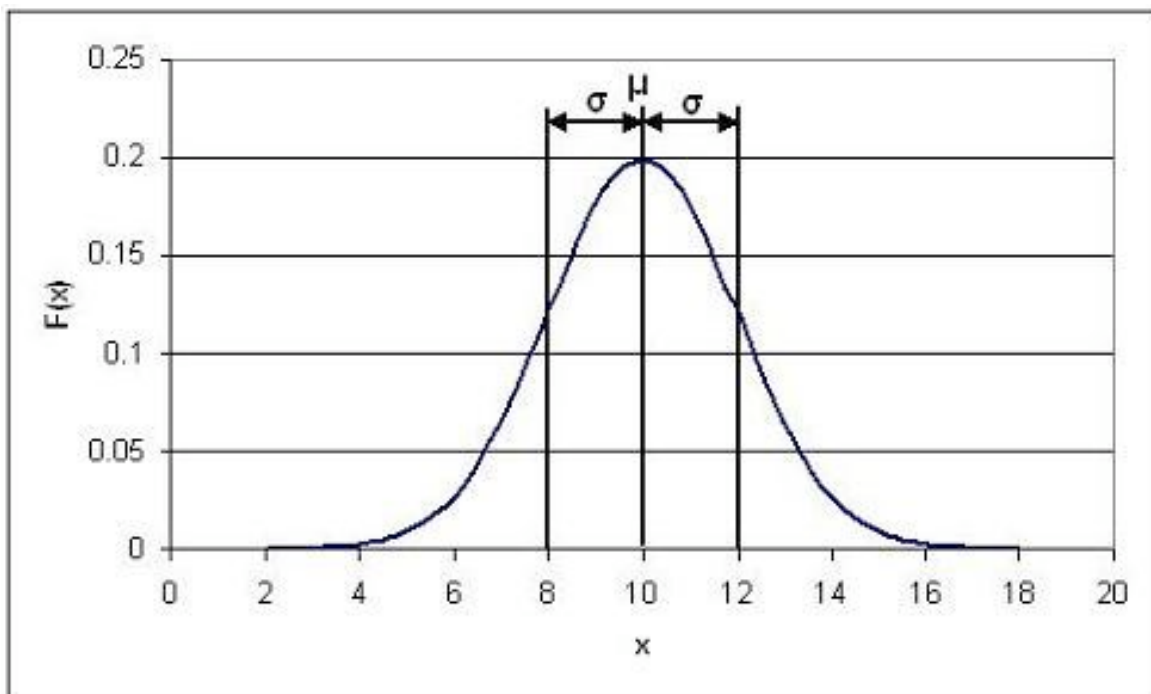
$A = 101.92 \pm .65$ students

1.3.9 Gaussian Distribution

Gaussian distribution, also known as normal distribution, is represented by the following probability density function:

$$PDF_{\mu,\sigma}(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

where μ is the mean and σ is the standard deviation of a very large data set. The Gaussian distribution is a bell-shaped curve, symmetric about the mean value. An example of a Gaussian distribution is shown below.



In this specific example, $\mu = 10$ and $\sigma = 2$.

Probability density functions represent the spread of data set. Integrating the function from some value x to $x + a$ where a is some real value gives the probability that a value falls within that range. The total integral of the probability density function is 1, since every value will fall within the total range. The shaded area in the image below gives the probability that a value will fall between 8 and 10, and is represented by the expression:

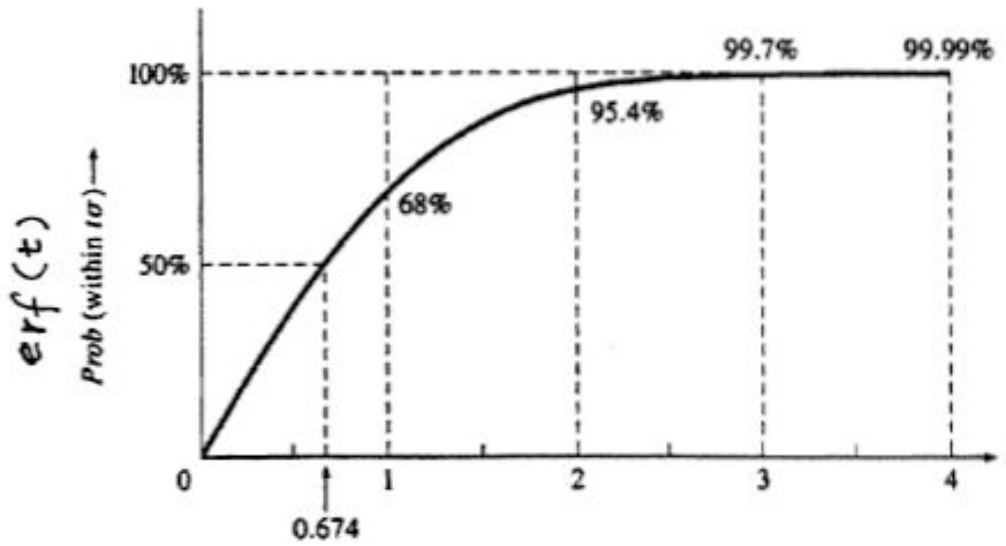
Gaussian distribution is important for statistical quality control, six sigma, and quality engineering in general. For more information see [What is 6 sigma?](#).

1.3.10 Error Function

A normal or Gaussian distribution can also be estimated with a error fuction as shown in the equation below.

$$P(8 \leq x \leq 10) = \int_8^{10} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx = erf(t)$$

Here, erf(t) is called "error function" because of its role in the theory of normal random variable. The graph below shows the probability of a data point falling within t*σ of the mean.



t	0	0.25	0.5	0.75	1.0	1.25	1.5	1.75	2.0	2.5	3.0	3.5	4.0
Prob (%)	0	20	38	55	68	79	87	92	95.4	98.8	99.7	99.95	99.99

For example if you wanted to know the probability of a point falling within 2 standard deviations of the mean you can easily look at this table and find that it is 95.4%. This table is very useful to quickly look up what probability a value will fall into x standard deviations of the mean.

1.3.11 Correlation Coefficient (r value)

The linear correlation coefficient is a test that can be used to see if there is a linear relationship between two variables. For example, it is useful if a linear equation is compared to experimental points. The following equation is used:

$$r = \frac{\sum(X_i - X_{mean})(Y_i - Y_{mean})}{\sqrt{\sum(X_i - X_{mean})^2}\sqrt{\sum(Y_i - Y_{mean})^2}}$$

The range of r is from -1 to 1. If the r value is close to -1 then the relationship is considered anti-correlated, or has a negative slope. If the value is close to 1 then the relationship is considered correlated, or to have a positive slope. As the r value deviates from either of these values and approaches zero, the points are considered to become less correlated and eventually are uncorrelated.

There are also probability tables that can be used to show the significant of linearity based on the number of measurements. If the probability is less than 5% the correlation is considered significant.

1.3.12 Linear Regression

The correlation coefficient is used to determine whether or not there is a correlation within your data set. Once a correlation has been established, the actual relationship can be determined by carrying out a linear regression. The first step in performing a linear regression is calculating the slope and intercept:

$$\text{Slope} = \frac{n \sum_i X_i Y_i - \sum_i X_i \sum_j Y_j}{n \sum_i X_i^2 - (\sum_i X_i)^2}$$

$$\text{Intercept} = \frac{(\sum_i X_i^2) \sum_i (Y_i) - \sum_i X_i \sum_i X_i Y_i}{n(\sum_i X_i^2) - (\sum_i X_i)^2}$$

Once the slope and intercept are calculated, the uncertainty within the linear regression needs to be applied. To calculate the uncertainty, the standard error for the regression line needs to be calculated.

$$S = \sqrt{\frac{1}{n-2} \left(\sum_i Y_i^2 - \text{intercept} \sum Y_i - \text{slope} \left(\sum_i Y_i X_i \right) \right)}$$

The standard error can then be used to find the specific error associated with the slope and intercept:

$$S_{slope} = S \sqrt{\frac{n}{n \sum_i X_i^2 - (\sum_i X_i)^2}}$$

$$S_{intercept} = S \sqrt{\frac{\sum(X_i^2)}{n(\sum X_i^2) - (\sum_i X_i Y_i)^2}}$$

Once the error associated with the slope and intercept are determined a confidence interval needs to be applied to the error. A confidence interval indicates the likelihood of any given data point, in the set of data points, falling inside the boundaries of the uncertainty. For a table of confidence interval values, see [student's t-distribution](#) Wikipedia page.

$$\beta = slope \pm \Delta slope \simeq slope \pm t^* S_{slope}$$

$$\alpha = intercept \pm \Delta intercept \simeq intercept \pm t^* S_{intercept}$$

Now that the slope, intercept, and their respective uncertainties have been calculated, the equation for the linear regression can be determined.

$$Y = \beta X + \alpha$$

1.3.13 Z-Scores

A z-score (also known as z-value, standard score, or normal score) is a measure of the divergence of an individual experimental result from the most probable result, the mean. Z is expressed in terms of the number of standard deviations from the mean value.

$$z = \frac{X - \mu}{\sigma} \quad (6)$$

$X = ExperimentalValue$

$\mu = Mean$

$\sigma = StandardDeviation$

Z-scores assuming the sampling distribution of the test statistic (mean in most cases) is normal and transform the sampling distribution into a standard normal distribution. As explained above in the section on sampling distributions, the standard deviation of a

sampling distribution depends on the number of samples. Equation (6) is to be used to compare results to one another, whereas equation (7) is to be used when performing inference about the population.

Whenever using z-scores it is important to remember a few things:

- Z-scores normalize the sampling distribution for meaningful comparison.
- Z-scores require a large amount of data.
- Z-scores require independent, random data.

$$z_{obs} = \frac{X - \mu}{\frac{\sigma}{\sqrt{n}}} \quad (7)$$

$n = \text{SampleNumber}$

1.3.14 P-Value

A p-value is a statistical value that details how much evidence there is to reject the most common explanation for the data set. It can be considered to be the probability of obtaining a result at least as extreme as the one observed, given that the null hypothesis is true. In chemical engineering, the p-value is often used to analyze marginal conditions of a system, in which case the p-value is the probability that the null hypothesis is true.

The null hypothesis is considered to be the most plausible scenario that can explain a set of data. The most common null hypothesis is that the data is completely random, that there is no relationship between two system results. The null hypothesis is always assumed to be true unless proven otherwise. An alternative hypothesis predicts the opposite of the null hypothesis and is said to be true if the null hypothesis is proven to be false.

The following is an example of these two hypotheses:

4 students who sat at the same table during in an exam all got perfect scores.

Null Hypothesis: The lack of a score deviation happened by chance.

Alternative Hypothesis: There is some other reason that they all received the same score.

If it is found that the null hypothesis is true then the Honor Council will not need to be involved. However, if the alternative hypothesis is found to be true then more studies will need to be done in order to prove this hypothesis and learn more about the situation.

As mentioned previously, the p-value can be used to analyze marginal conditions. In this case, the null hypothesis is that there is no relationship between the variables controlling the data set. For example:

- Runny feed has no impact on product quality
- Points on a control chart are all drawn from the same distribution
- Two shipments of feed are statistically the same

The p-value proves or disproves the null hypothesis based on its significance. A p-value is said to be significant if it is less than the level of significance, which is commonly 5%, 1% or .1%, depending on how accurate the data must be or stringent the standards are. For example, a health care company may have a lower level of significance because they have strict standards. If the p-value is considered significant (is less than the specified level of significance), the null hypothesis is false and more tests must be done to prove the alternative hypothesis.

Upon finding the p-value and subsequently coming to a conclusion to reject the *Null Hypothesis* or fail to reject the *Null Hypothesis*, there is also a possibility that the wrong decision can be made. If the decision is to reject the *Null Hypothesis* and in fact the *Null Hypothesis* is true, a type 1 error has occurred. The probability of a type one error is the same as the level of significance, so if the level of significance is 5%, "the probability of a type 1 error" is .05 or 5%. If the decision is to fail to reject the *Null Hypothesis* and in fact the *Alternative Hypothesis* is true, a type 2 error has just occurred. With respect to the type 2 error, if the *Alternative Hypothesis* is really true, another probability that is important to researchers is that of actually being able to detect this and reject the *Null Hypothesis*. This probability is known as the [power](#) (of the test) and it is defined as 1 - "probability of making a type 2 error."

If an error occurs in the previously mentioned example testing whether there is a relationship between the variables controlling the data set, either a type 1 or type 2 error could lead to a great deal of wasted product, or even a wildly out-of-control process. Therefore, when designing the parameters for hypothesis testing, researchers must heavily weigh their options for level of significance and power of the test. The sensitivity of the process, product, and standards for the product can all be sensitive to the smallest error.

Important Note About Significant P-values

If a P-value is greater than the applied level of significance, and the null hypothesis should not just be blindly accepted. Other tests should be performed in order to determine the true relationship between the variables which are being tested. More information on

this and other misunderstandings related to P-values can be found at [P-values: Frequent misunderstandings](#).

Calculation

There are two ways to calculate a p-value. The first method is used when the z-score has been calculated. The second method is used with the Fisher's exact method and is used when analyzing marginal conditions.

First Method: Z-Score

The method for finding the P-Value is actually rather simple. First calculate the z-score and then look up its corresponding p-value using the standard normal table.

This table can be found here: [Media:Group G Z-Table.xls](#)

This value represents the likelihood that the results are not occurring because of random errors but rather an actual difference in data sets.

To read the standard normal table, first find the row corresponding to the leading significant digit of the z-value in the column on the lefthand side of the table. After locating the appropriate row move to the column which matches the next significant digit.

Example:

If your z-score = 1.13

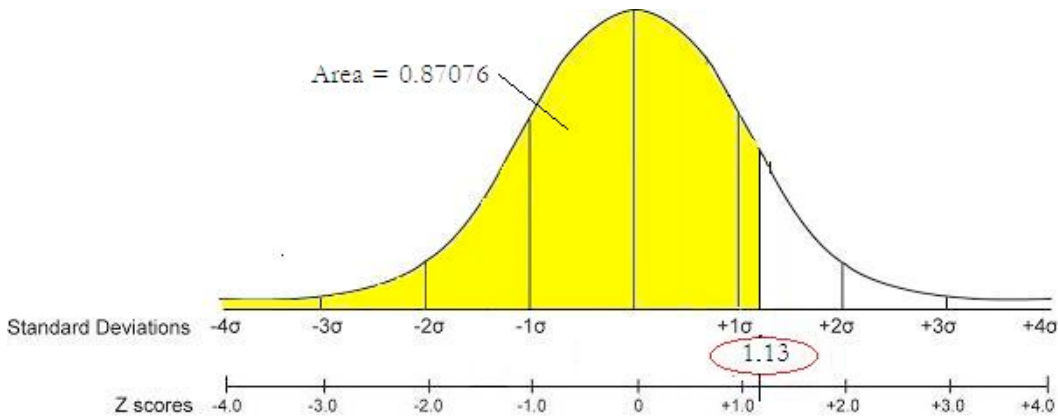
Follow the rows down to 1.1 and then across the columns to 0.03. The P-value is the highlighted box with a value of 0.87076.

z	0	0.01	0.02	0.03	0.04	0.05
0	0.5	0.50399	0.50798	0.51197	0.51595	0.51994
0.1	0.53983	0.5438	0.54776	0.55172	0.55567	0.55962
0.2	0.57926	0.58317	0.58706	0.59095	0.59483	0.59871
0.3	0.61791	0.62172	0.62552	0.6293	0.63307	0.63683
0.4	0.65542	0.6591	0.66276	0.6664	0.67003	0.67364
0.5	0.69146	0.69497	0.69847	0.70194	0.7054	0.70884
0.6	0.72575	0.72907	0.73237	0.73565	0.73891	0.74215
0.7	0.75804	0.76115	0.76424	0.7673	0.77035	0.77337
0.8	0.78814	0.79103	0.79389	0.79673	0.79955	0.80234
0.9	0.81594	0.81859	0.82121	0.82381	0.82639	0.82894
1	0.84134	0.84375	0.84614	0.84849	0.85083	0.85314
1.1	0.86433	0.8665	0.86864	0.87076	0.87286	0.87493
1.2	0.88493	0.88686	0.88877	0.89065	0.89251	0.89435
1.3	0.9032	0.9049	0.90658	0.90824	0.90988	0.91149
1.4	0.91924	0.92073	0.9222	0.92364	0.92507	0.92647
1.5	0.93319	0.93448	0.93574	0.93699	0.93822	0.93943

Values in the table represent area under the standard normal distribution curve to the left of the z-score.

Using the previous example:

Z-score = 1.13, P-value = 0.87076 is graphically represented below.



Second Method: Fisher's Exact

In the case of analyzing marginal conditions, the P-value can be found by summing the Fisher's exact values for the current marginal configuration and each more extreme case using the same marginals. For information about how to calculate Fisher's exact click the following

link: [Discrete Distributions: hypergeometric, binomial, and poisson#Fisher.27s exact](#)

1.3.15 Chi-Squared Test

A Chi-Squared test gives an estimate on the agreement between a set of observed data and a random set of data that you expected the measurements to fit. Since the observed values are continuous, the data must be broken down into bins that each contain some observed data. Bins can be chosen to have some sort of natural separation in the data. If none of these divisions exist, then the intervals can be chosen to be equally sized or some other criteria.

The calculated chi squared value can then be correlated to a probability using excel or published charts. Similar to the Fisher's exact, if this probability is greater than 0.05, the null hypothesis is true and the observed data is not significantly different than the random.

Calculating Chi Squared

The Chi squared calculation involves summing the distances between the observed and random data. Since this distance depends on the magnitude of the values, it is normalized by dividing by the random value

$$\chi^2 = \sum_{k=1}^N \frac{(\textit{observed} - \textit{random})^2}{\textit{random}}$$

or if the error on the observed value (sigma) is known or can be calculated:

$$\chi^2 = \sum_{k=1}^N \left(\frac{\textit{observed} - \textit{theoretical}}{\textit{sigma}} \right)^2$$

Detailed Steps to **Calculate** Chi Squared by Hand

Calculating Chi squared is very simple when defined in depth, and in step-by-step form can be readily utilized for the estimate on the agreement between a set of observed data and a random set of data that you expected the measurements to fit. Given the data:

	1	2	3	4	5	6	7
x _i	12	14	17	28	26	40	45
y _i	9	18	23	31	47	51	53
σ _i	3	4	2	4	4	3	5

Step 1: Find χ_o^2

$$\chi_o^2 = \sum_i \frac{(y_i - A - Bx_i)^2}{\sigma_{yi}^2}$$

When:

$$A = \frac{S_{xx}S_y - S_xS_{xy}}{\Delta}$$

$$B = \frac{SS_{xy} - S_xS_y}{\Delta}$$

$$\Delta = SS_{xx} - (S_x)^2$$

$$S = \sum \frac{1}{\sigma_{yi}^2}$$

$$S_x = \sum \frac{x_i}{\sigma_{yi}^2}$$

$$S_y = \sum \frac{y_i}{\sigma_{yi}^2}$$

$$S_{xy} = \sum \frac{x_i y_i}{\sigma_{yi}^2}$$

$$S_{xx} = \sum \frac{x_i^2}{\sigma_{yi}^2}$$

The Excel function CHITEST(actual_range, expected_range) also calculates the value. The two inputs represent the range of data the actual and expected data, respectively. χ_o^2

Step 2: Find the Degrees of Freedom

$$df = n - k$$

When: df = Degrees of Freedom

n = number of observations

k = the number of constraints

Step 3: Find
$$\tilde{\chi}_o^2 = \frac{\chi_o^2}{df}$$

$\tilde{\chi}_o^2$ = the established value of $\tilde{\chi}^2$ obtained in an experiment with df degrees of freedom

Step 4: Find $P(\tilde{\chi}^2 \geq \tilde{\chi}_o^2)$ using Excel or published charts.

The Excel function CHIDIST(x,df) provides the p-value, where x is the value of the chi-squared statistic and df is the degrees of freedom. Note: Excel gives only the p-value and not the value of the chi-square statistic.

$P(\tilde{\chi}^2 \geq \tilde{\chi}_o^2)$ = the probability of getting a value of $\tilde{\chi}^2$ that is as large as the established $\tilde{\chi}_o^2$

Step 5: Compare the probability to the significance level (i.e. 5% or 0.05), if this probability is greater than 0.05, the null hypothesis is true and the observed data is not significantly different than the random. A probability smaller than 0.05 is an indicator of independence and a significant difference from the random.

Chi Squared Test versus Fisher's Exact

- For small sample sizes, the Chi Squared Test will not always produce an accurate probability. However, for a random null, the Fisher's exact, like its name, will always give an exact result.
 - Chi Squared will not be correct when:
 1. fewer than 20 samples are being used
 2. if an expected number is 5 or below and there are between 20 and 40 samples
- For large contingency tables and expected distributions that are not random, the p-value from Fisher's Exact can be a difficult to compute, and Chi Squared Test will be easier to carry out.

1.3.16 Binning in Chi Squared and Fisher's Exact Tests

When performing various statistical analyzes you will find that Chi-squared and Fisher's exact tests may require binning, whereas ANOVA does not. Although there is no optimal choice for the number of bins (k), there are several formulas which can be used to calculate this number based on the sample size (N). One such example is listed below:

$$k = 1 + \log_2 N$$

Another method involves grouping the data into intervals of equal probability or equal width. The first approach in which the data is grouped into intervals of equal probability is generally more acceptable since it handles peaked data much better. As a stipulation, each bin should contain at least 5 or more data points, so certain adjacent bins sometimes need to be joined together for this condition to be satisfied. Identifying the number the bins to use is important, but it is even more important to be able to note which situations call for binning. Some Chi-squared and Fisher's exact situations are listed below:

- **Analysis of a continuous variable:**

This situation will require binning. The idea is to divide the range of values of the variable into smaller intervals called bins.

- **Analysis of a discrete variable:**

Binning is unnecessary in this situation. For instance, a coin toss will result in two possible outcomes: heads or tails. In tossing ten coins, you can simply count the number of times you received each possible outcome. This approach is similar to choosing two bins, each containing one possible result.

- **Examples of when to bin, and when not to bin:**

- You have twenty measurements of the temperature inside a reactor: as temperature is a continuous variable, you should bin in this case. One approach might be to determine the mean (X) and the standard deviation (σ) and group the temperature data into four bins: $T < X - \sigma$, $X - \sigma < T < X$, $X < T < X + \sigma$, $T > X + \sigma$
- You have twenty data points of the heater setting of the reactor (high, medium, low): since the heater setting is discrete, you should not bin in this case.

1.4 Worked out Example 1

1.4.1 Question 1

Say we have a reactor with a mean pressure reading of 100 and standard deviation of 7 psig. Calculate the probability of measuring a pressure between 90 and 105 psig.

1.4.2 Solution 1

To do this we will make use of the z-scores.

$$Pr(a \leq z \leq b) = F(b) - F(a) = F\left(\frac{b - \mu}{\sigma}\right) - F\left(\frac{a - \mu}{\sigma}\right)$$

where:

a is the lower bound

b is the upper bound

Substitution of z-transformation equation (3)

$$z = \frac{X - \mu}{\sigma}$$

$$z_{upper} = \frac{b - \mu}{\sigma} = \frac{105 - 100}{7} = 0.714$$

$$z_{lower} = \frac{a - \mu}{\sigma} = \frac{90 - 100}{7} = -1.43$$

Look up z-score values in a standard normal table. [Media:Group G Z-Table.xls](#)

$$z_{upper} = 0.714 \rightarrow F(z_{upper}) = 0.76155$$

$$z_{lower} = -1.43 \rightarrow F(z_{lower}) = 0.07636$$

So:

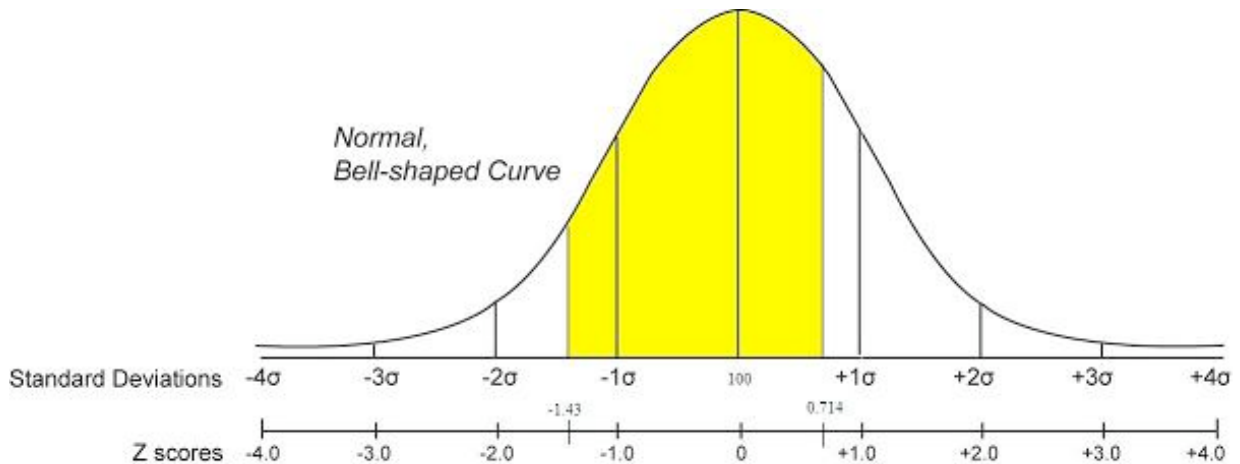
$$Pr(a \leq z \leq b) = F(.714) - F(-1.43)$$

$$= 0.76155 - 0.07636$$

$$= 0.68479.$$

The probability of measuring a pressure between 90 and 105 psig is **0.68479**.

A graphical representation of this is shown below. The shaded area is the probability



1.4.3 Alternate Solution

We can also solve this problem using the probability distribution function (PDF). This can be done easily in Mathematica as shown below. More information about the PDF is and how it is used can be found in the [Continuous Distribution](#) article

PDF is described by the following equation :

$$f(x) = \left(\frac{1}{\sigma \sqrt{2\pi}} \right) * \text{Exp} \left(\frac{-1}{2} * \left(\frac{x - \mu}{\sigma} \right)^2 \right)$$

Given $\mu = 100$ and $\sigma = 7$ we can plug these values in the equation to get :

$$f(x) = \left(\frac{1}{7 * \sqrt{2 * \pi}} \right) * e^{\left(\frac{-1}{2} * \left(\frac{x-100}{7} \right)^2 \right)}$$

To find the probability between the two points 90 and 105, we perform the following integration:

$$f(90 \leq x \leq 105) = \int_{90}^{105} \left(\frac{1}{7 * \sqrt{2 * \pi}} \right) * e^{\left(\frac{-1}{2} * \left(\frac{x-100}{7} \right)^2 \right)} dx$$

This results in the following expression :

$$\begin{aligned} f(90 \leq x \leq 105) &= \frac{1}{2} * \left(\text{Erf} \left[\frac{(105 - 100)}{7 * \sqrt{2}} \right] - \text{Erf} \left[\frac{(90 - 100)}{7 * \sqrt{2}} \right] \right) \\ &= \frac{1}{2} * \left(\text{Erf} \left[\frac{5}{7 * \sqrt{2}} \right] + \text{Erf} \left[\frac{5 * \sqrt{2}}{7} \right] \right) \end{aligned}$$

Or Simply entered in mathematica as

$$\text{In}[3]:= f = \left(\frac{1}{7 * \sqrt{2 * \pi}} \right) * e^{\left(\frac{-1}{2} * \left(\frac{x-100}{7} \right)^2 \right)}$$

`NIntegrate[f, {x, 90, 105}]`

$$\text{Out}[3]= \frac{e^{-\frac{1}{98} (-100+x)^2}}{7 \sqrt{2 \pi}}$$

`Out[4]= 0.685911`

As you can see the the outcome is approximately the same value found using the z-scores.

1.5 Worked out Example 2

1.5.1 Question 2

You are a quality engineer for the pharmaceutical company “Headache-b-gone.” You are in charge of the mass production of their children’s headache medication. The average weight of acetaminophen in this medication is supposed to be 80 mg, however when you run the required tests you find that the average weight of 50 random samples is 79.95 mg with a standard deviation of .18.

- Identify the null and alternative hypothesis.
- Under what conditions is the null hypothesis accepted?

c) Determine if these differences in average weight are significant.

1.5.2 Solution 2

a)

- Null hypothesis: This is the claimed average weight where $H_0=80$ mg
- Alternative hypothesis: This is anything other than the claimed average weight (in this case $H_a<80$)

b) The null hypothesis is accepted when the p-value is greater than .05.

c) We first need to find Z_{obs} using the equation below:

$$z_{obs} = \frac{X - \mu}{\frac{\sigma}{\sqrt{n}}}$$

Where n is the number of samples taken.

$$z_{obs} = \frac{79.95 - 80}{\frac{.18}{\sqrt{50}}} = -1.96$$

Using the z-score table provided in earlier sections we get a p-value of .025. Since this value is less than the value of significance (.05) we reject the null hypothesis and determine that the product does not reach our standards.

1.6 Worked out Example 3

1.6.1 Question 3

15 students in a controls class are surveyed to see if homework impacts exam grades. The following distribution is observed.

	High Homework Grades	Low Homework Grades	Totals
High Exam Grades	6	3	9
Low Exam Grades	2	4	6
Totals	8	7	15

Determine the p-value and if the null hypothesis (Homework does not impact Exams) is significant by a 5% significance level using the P-fisher method.

1.6.2 Solution 3

To find the p-value using the p-fisher method, we must first find the p-fisher for the original distribution. Then, we must find the p-fisher for each more extreme case. The p-fisher for the original distribution is as follows.

$$p_{fisher} = \frac{9!6!8!7!}{15!6!3!2!4!} = 0.195804$$

To find the more extreme case, we will gradually decrease the smallest number to zero. Thus, our next distribution would look like the following.

	High Homework Grades	Low Homework Grades	Totals
High Exam Grades	7	2	9
Low Exam Grades	1	5	6
Totals	8	7	15

The p-fisher for this distribution will be as follows.

$$p_{fisher} = \frac{9!6!8!7!}{15!7!2!1!5!} = 0.0335664$$

The final extreme case will look like this.

	High Homework Grades	Low Homework Grades	Totals
High Exam Grades	8	1	9
Low Exam Grades	0	6	6
Totals	8	7	15

The p-fisher for this distribution will be as follows.

$$p_{fisher} = \frac{9!6!8!7!}{15!8!1!0!6!} = 0.0013986$$

Since we have a 0 now in the distribution, there are no more extreme cases possible. To find the p-value we will sum the p-fisher values from the 3 different distributions.

$$p_{value} = 0.195804 + 0.0335664 + 0.0013986 = 0.230769$$

Because p-value=0.230769 we cannot reject the null hypothesis on a 5% significance level.

1.7 Application: What do p-values tell us?

1.7.1 Population Example

Out of a random sample of 400 students living in the dormitory (group A), 134 students caught a cold during the academic school year. Out of a random sample of 1000 students living off campus (group B), 178 students caught a cold during this same time period.

Population table

	Group A	Group B	
Sick	a=134	b=178	a+b=312
Not Sick	c=266	d=822	c+d=1088
	a+c=400	b+d=1000	a+b+c+d=1400

Fisher's Exact:

$$p_f = \frac{(a + b)!(c + d)!(a + c)!(b + d)!}{(a + b + c + d)!a!b!c!d!}$$

Solve:

$$p_f = \frac{(312)!(1088)!(400)!(1000)!}{(1400)!134!178!266!822!}$$

$$p_f = 2.28292 * 10^{-10}$$

Comparison and interpretation of p-value at the 95% confidence level

This value is very close to zero which is much less than 0.05. Therefore, the number of students getting sick in the dormitory is significantly higher than the number of students getting sick off campus. There is more than a 95% chance that this significant difference is not random. Statistically, it is shown that this dormitory is more conducive for the spreading of viruses. With the knowledge gained from this analysis, making changes to the dormitory may be justified. Perhaps installing sanitary dispensers at common locations throughout the dormitory would lower this higher prevalence of illness among dormitory students. Further research may determine more specific areas of viral spreading by marking off several smaller populations of students living in different areas of the dormitory. This model of significance testing is very useful and is often applied to a multitude of data to determine if discrepancies are due to chance or actual differences between compared samples of data. As you can see, purely mathematical analyses such as these often lead to physical action being taken, which is necessary in the field of Medicine, Engineering, and other scientific and non-scientific venues.

1.8 Multiple Choice Question 1

you are given the following set of data: {1,2,3,5,5,6,7,7,7,9,12} What is the mean, median and mode for this set of data? And then the z value of a data point of 7?

- a) 5.82, 6, 7, 0.373
- b) 6, 7, 5.82, 6.82
- c) 7, 6, 5, 0.373

d) 7, 6, 5.82, 3.16

Answer: a

1.9 Multiple Choice Question 2

What is n and the standard deviation for the above set of data {1,2,3,5,5,6,7,7,7,9,12}?
And then consulting the table from above, what is the p-value for the data "12"?

a) 12, 3.16, 5.82

b) 7, 3.16, 0.83

c) 11, 3.16, 0.97

d) 11, 5.82, 0

Answer: c


1.10 Sage's Corner

http://www.youtube.com/v/_3ZJeSrysf

1.11 References

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Setion 2. SPC: Basic Control Charts: Theory and Construction, Sample Size, X-Bar, R charts, S charts

Note:  [Video lecture](#) available for this section!

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- [First round reviews for this page](#)
- [Rebuttal for this page](#)

2.1 Introduction

Control charts are one of the most commonly used methods of [Statistical Process Control](#) (SPC), which monitors the stability of a process. The main features of a control chart include the data points, a centerline (mean value), and upper and lower limits (bounds to indicate where a process output is considered "out of control"). They visually display the fluctuations of a particular process variable, such as temperature, in a way that lets the engineer easily determine whether these variations fall within the specified process limits. Control charts are also known as Shewhart charts after Walter Shewhart, who developed them in the early 1900's.

2.2 Control Chart Background

A process may either be classified as in control or out of control. The boundaries for these classifications are set by calculating the mean, standard deviation, and range of a set of process data collected when the process is under stable operation. Then, subsequent data can be compared to this already calculated mean, standard deviation and range to determine whether the new data fall within acceptable bounds. For good and safe control, subsequent data collected should fall within three standard deviations of the mean. Control charts build on this basic idea of statistical analysis by plotting the mean or range of subsequent data against time. For example, if an engineer knows the mean (grand average) value, standard deviation, and range of a process, this information can be displayed as a bell curve, or population density function (PDF). The image below shows the control chart for a data set with the PDF overlay.

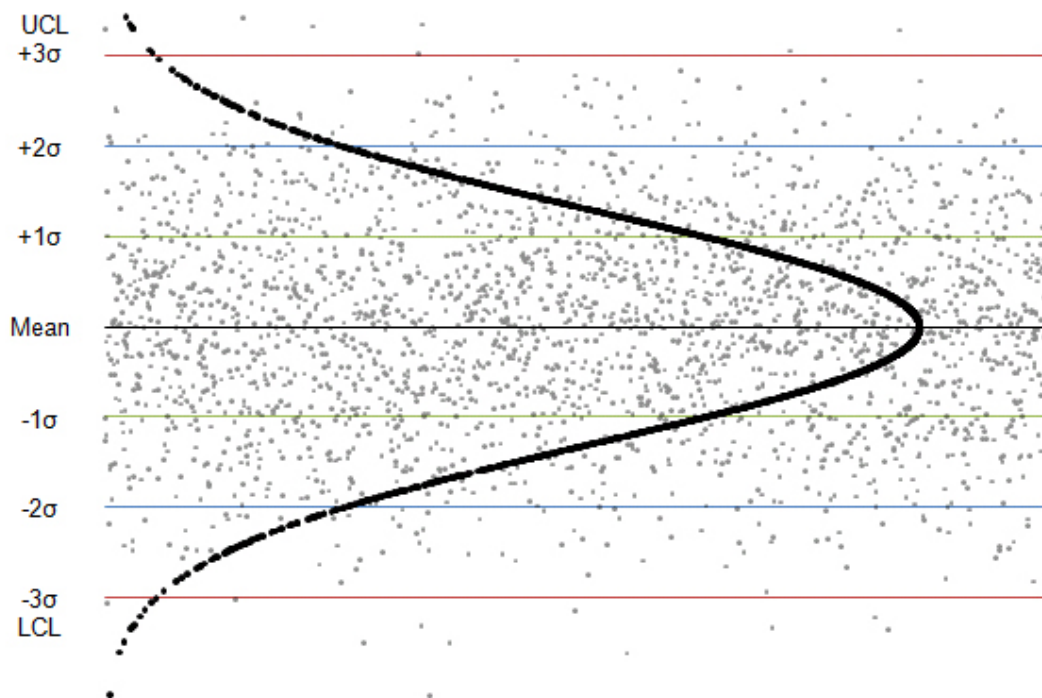


Figure I. Control chart showing PDF for a data set

The centerline is the mean value of the data set and the green, blue and red lines represent one, two, and three standard deviations from the mean value. In generalized terms, if data points fall within three standard deviations of the mean (within the red lines), the process is considered to be in control. These rules are discussed in greater detail later in this section.

Control Charts are commonly used in six sigma control today, as a means of overall process improvement. For more on six-sigma control, see [six sigma](#).

2.3 Control Chart Functions

The main purpose of using a control chart is to monitor, control, and improve process performance over time by studying variation and its source. There are several functions of a control chart:

1. It centers attention on detecting and monitoring process variation over time.
2. It provides a tool for ongoing control of a process.

3. It differentiates special from common causes of variation in order to be a guide for local or management action.
4. It helps improve a process to perform consistently and predictably to achieve higher quality, lower cost, and higher effective capacity.
5. It serves as a common language for discussing process performance.

2.4 Sample Size and Subgrouping

There are a few key conditions that must be met when constructing control charts:

- The initial predictions for the process must be made while the process is assumed to be stable. Because future process quality will be compared to these predictions, they must be based off of a data set that is taken while the operation is running properly.
- Multiple subsets of data must be collected, where a subset is simply a set of n measurements taken over a specific time range. The number of subsets is represented as k . A subset average, subset standard deviation, and subset range will be computed for each subset.
- From these subsets, a grand average, an average standard deviation, and an average range are calculated. The grand average is the average of all subset averages. The average standard deviation is simply the average of subset standard deviations. The average range is simply the average of subset ranges.

The upper and lower control limits for the process can then be determined from this data.

- Future data taken to determine process stability can be of any size. This is because any point taken should fall within the statistical predictions. It is assumed that the first occurrence of a point not falling within the predicted limits shows that the system must be unstable since it has changed from the predictive model.
- The subsets are defined, based on the data and the process. For example, if you were using a pH sensor, the sensor would most likely output pages of data daily. If you know that your sensor has the tendency to drift every day, you might select a 30 minute subset of data. If it drifts monthly you might set your subset to be 24 hours or 12 hours.
- Finally, the population size, N is assumed to be infinite. Alternatively, if the population is finite but the sample size is less than 5% of the population size, we can still approximate the population to be near infinite. That is, $n/N \leq 0.05$ where n is the sample size and N is the population size. [5]

2.5 X-Bar, R-Charts, and S-Charts

There are three types of control charts used to determine if data is out of control, x-bar charts, r-charts and s-charts. An x-bar chart is often paired with either an r-chart or an s-chart to give a complete picture of the same set of data.

Pairing X-Bar with R-Charts

X-Bar (average) charts and R (range) -charts are often paired together. The X-Bar chart displays the centerline, which is calculated using the grand average, and the upper and lower control limits, which are calculated using the average range. Future experimental subsets are plotted compared to these values. This demonstrates the centering of the subset values. The R-chart plots the average range and the limits of the range. Again, the future experimental subsets are plotted relative to these values. The R-chart displays the dispersion of the subsets. X-Bar/R-Chart plot a subgroup average. Note that they should only be used when subgroups really make sense. For example, in a Gage R&R study, when operators are testing in duplicates or more, subgrouping really represents the same group.

Pairing X-Bar with S-Charts

Alternatively, X-Bar charts can be paired with S-charts (standard deviation). This is typically done when the size of the subsets are large. For larger subsets, the range is a poor statistic to estimate the distributions of the subsets, and instead, standard deviation is used. In this case, the X-Bar chart will display control limits that are calculated using the average standard deviation. The S-Charts are similar to the R-charts; however, instead of the range, they track the standard deviation of multiple subsets.

Smoothing Data with a Moving Average

If it is desired to have smooth data, the moving average method is one option. This method involves taking the average of a number of points, and using that average for the middle data point. From this point on, the data is treated the same as any normal group of k subsets. Though this method will produce a smoother curve, it has a lag in detecting points, which may be problematic if the points are out of the acceptable range. This time lag would keep the control system from reacting to the problem until after the average is found. For this reason, moving average charts are appropriate mainly for slower processes that can handle the lag.

For example, let us calculate a value for a set of data which takes samples every second. We will use an average of 10 points to find this, however, in practice there is no set number of data points that should be used. For the point $t = 50$, we must wait until data has been collected through $t = 54$. The points are then averaged for $t = 45-54$ and used as the function value. For the next point, $t = 51$, the average of the points for $t = 46-55$ are used, and so on. If this is still confusing, please see [moving average](#) for a more detailed explanation.

Reading Control Charts

Control charts can determine whether a process is behaving in an "unusual" way.

Note: The upper and lower control limits are calculated using the grand average and either the average range and average sigma. Example calculations are shown in the Creating Control Charts Section.

The quality of the individual points of a subset is determined unstable if any of the following occurs:

Rule 1: Any point falls beyond 3σ from the centerline (this is represented by the upper and lower control limits).

Rule 2: Two out of three consecutive points fall beyond 2σ on the same side of the centerline.

Rule 3: Four out of five consecutive points fall beyond 1σ on the same side of the centerline.

Rule 4: Nine or more consecutive points fall on the same side of the centerline.

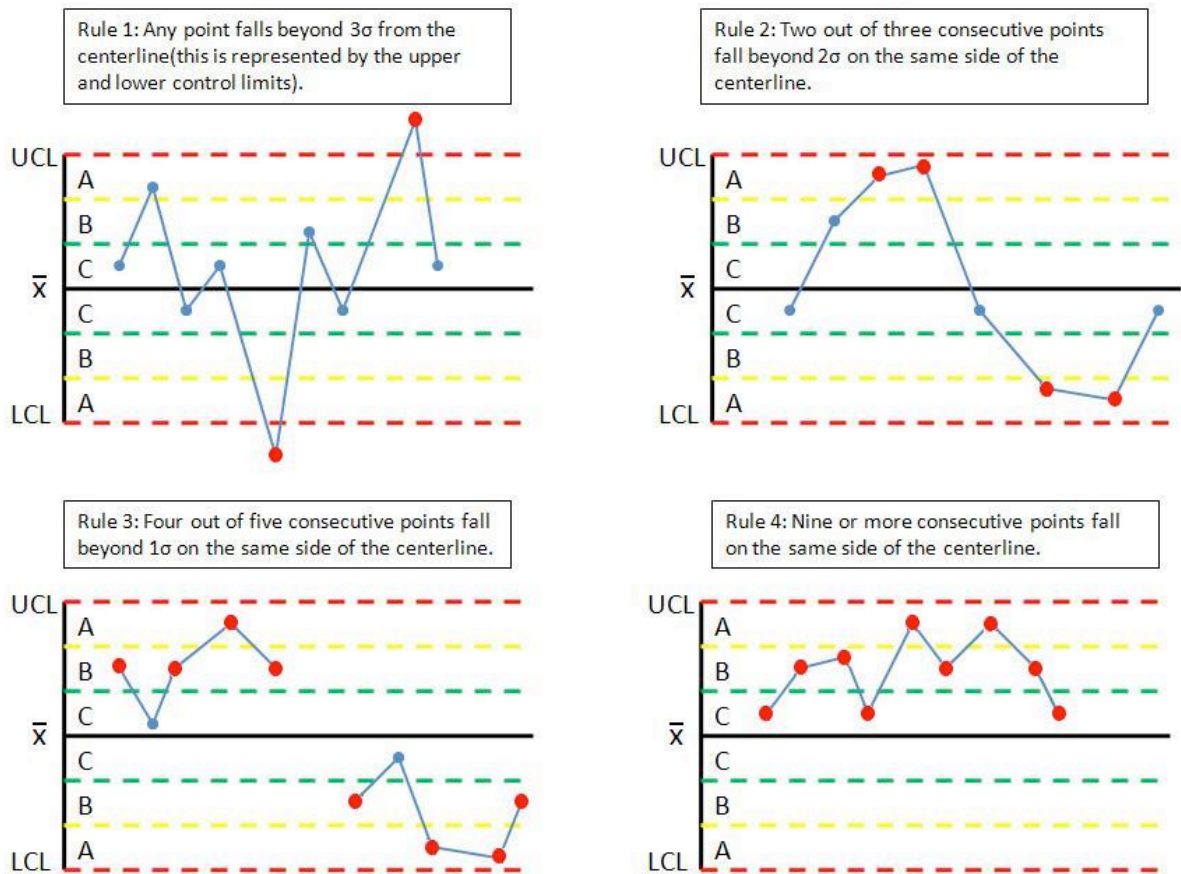


Figure III. Quality control rules.

The quality of a subset is determined unstable according to the following rules:

1. Any subset value is more than three standard deviations from the centerline.
2. Two consecutive subset values are more than two standard deviations from the centerline and are on the same side of the centerline.
3. Three consecutive subset values are more than one standard deviation from the centerline and are on the same side of the centerline.

Creating Control Charts

To establish upper and lower control limits on control charts, there are a number of methods. We will discuss the method for the number of components in a subset, n , less than 15. For methods involving $n > 15$ and other techniques, see Process Control and Optimization, Liptak, 2.34. Here, the table of constants for computing limits, and the limit equations are presented below.

Please note that Table A below does NOT contain data for a sample problem. Any time you make a control chart, you refer to this table. The values in the table are used in the equations for the upper control limit (UCL), lower control limit (LCL), etc. This will be explained in the examples below. If you are interested in how these constants were derived, there is a more detailed explanation in [Control Chart Constants](#).

Subgroup n	X-bar chart		S-chart		R-chart	
	Using R_a A2	Using S_a A3	B3	B4	D3	D4
2	1.886	2.659	0	3.267	0	3.268
3	1.023	1.954	0	2.568	0	2.574
4	0.729	1.628	0	2.266	0	2.282
5	0.577	1.427	0	2.089	0	2.114
6	0.483	1.287	0.03	1.97	0	2.004
7	0.419	1.182	0.118	1.882	0.076	1.924
8	0.373	1.099	0.185	1.815	0.136	1.864
9	0.337	1.032	0.239	1.761	0.184	1.816
10	0.308	0.975	0.284	1.716	0.223	1.777
11	0.285	0.927	0.322	1.678	0.256	1.744
12	0.266	0.886	0.354	1.646	0.283	1.717
13	0.249	0.85	0.382	1.619	0.307	1.693
14	0.235	0.817	0.407	1.593	0.328	1.672
15	0.223	0.789	0.428	1.572	0.347	1.653

Table A: Table of Constants

To determine the value for n , the number of subgroups

In order to determine the upper (UCL) and lower (LCL) limits for the x-bar charts, you need to know how many subgroups (n) there are in your data. Once you know the value of n , you can obtain the correct constants (A2, A3, etc.) to complete your control chart. This can be confusing when you first attend to create a x-bar control chart. The value of n is the number of subgroups within each data point. For example, if you are taking temperature measurements every min and there are three temperature readings per

minute, then the value of **n** would be **3**. And if this same experiment was taking four temperature readings per minute, then the value of **n** would be **4**. Here are some examples with different tables of data to help you further in determining **n**:

Subset #	Values (kg)
1 (control)	1.02, 1.03, 0.98, 0.99
2 (control)	0.96, 1.01, 1.02, 1.01
3 (control)	0.99, 1.02, 1.03, 0.98
4 (control)	0.96, 0.97, 1.02, 0.98
5 (control)	1.03, 1.04, 0.95, 1.00
6 (control)	0.99, 0.99, 1.00, 0.97
7 (control)	1.02, 0.98, 1.01, 1.02
8 (experimental)	1.02, 0.99, 1.01, 0.99
9 (experimental)	1.01, 0.99, 0.97, 1.03
10 (experimental)	1.02, 0.98, 0.99, 1.00
11 (experimental)	0.98, 0.97, 1.02, 1.03

Example 1:

n= 4 since there are four readings of kg.

Example 2:

time (hours)	pH			
1	7.00	7.30	6.99	7.00
2	7.12	7.25	7.12	7.20
3	7.20	7.16	7.20	7.16
4	6.98	7.00	6.94	7.00
5	6.99	6.99	6.99	6.98
6	7.00	6.93	7.02	6.93
7	6.92	7.00	6.92	7.02
8	6.88	6.82	6.94	6.99
9	7.10	7.00	7.00	7.00
10	7.21	7.02	7.21	7.04
11	7.01	6.86	7.01	6.90
12	6.86	6.98	6.90	6.98
13	6.90	7.00	6.87	7.00
14	7.01	7.04	7.01	7.05
15	7.00	6.95	7.00	6.99
16	7.09	7.20	7.03	7.20
17	6.89	7.14	6.87	7.15
18	6.98	6.80	6.98	6.89
19	7.00	6.90	7.00	6.90
20	7.20	7.00	7.23	7.00
21	7.04	7.03	7.08	7.00
22	6.90	6.92	6.98	6.92
23	7.00	7.00	7.00	7.00
24	7.00	6.97	7.01	6.98

$n = 4$ since there are four readings of pH.

time (min)	T1	T2	T3
0	305.1578	311.1926	303.0032
1	308.6441	299.2898	307.9012
2	304.4789	308.7662	312.273
3	303.2384	303.7872	308.4915
4	316.6728	303.9563	303.3419
5	297.3459	308.0937	306.353
6	310.0358	304.9309	304.5568
7	302.2579	304.0973	317.315
8	305.5338	308.5081	308.1174
9	311.6743	302.4106	305.5727
10	303.535	312.9508	305.1281
11	307.5137	312.0491	307.6593
12	310.6001	305.5229	311.1861
13	307.6121	313.0331	313.4924
14	313.2346	312.1953	297.2964
15	306.0061	301.9239	298.6282
16	310.8455	308.7776	300.404
17	306.6952	299.0904	304.7548
18	305.2398	307.3239	297.1759
19	303.3781	305.8241	306.5276
20	309.3113	316.0451	309.9065

Example 3:

$n=3$ since there are three readings of temperature.

After creating multiple control charts, determining the value of n will become quite easy.

Calculating UCL and LCL

For the X-Bar chart the following equations can be used to establish limits, where X_{GA} is the grand average, R_A is the average range, and S_A is the average standard deviation.

Calculating Grand Average, Average Range and Average Standard Deviation

To calculate the grand average, first find the average of the n readings at each time point. The grand average is the average of the averages at each time point.

To calculate the grand range, first determine the range of the n readings at each time point. The grand range is the average of the ranges at each time point.

To calculate the average standard deviation, first determine the standard deviation of the n readings at each time point. The average standard deviation is the average of the standard deviations at each time point.

Note: You will need to calculate either the grand range or the average standard deviation, not both.

For X-bar charts, the UCL and LCL may be determined as follows:

$$\text{Upper Control Limit (UCL)} = X_{GA} + A_2 R_A$$

$$\text{Lower Control Limit (LCL)} = X_{GA} - A_2 R_A$$

Alternatively, S_A can be used as well to calculate UCL and LCL:

$$\text{Upper Control Limit (UCL)} = X_{GA} + A_3 S_A$$

$$\text{Lower Control Limit (LCL)} = X_{GA} - A_3 S_A$$

The centerline is simply X_{GA} .

For R-charts, the UCL and LCL may be determined as follows:

$$\text{UCL} = D_4 R_A$$

$$\text{LCL} = D_3 R_A$$

The centerline is the value R_A .

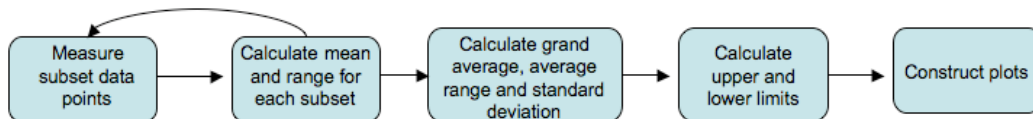
For S-charts, the UCL and LCL may be determined as follows:

$$UCL = B_4 S_A$$

$$LCL = B_3 S_A$$

The centerline is S_A .

The following flow chart demonstrates the general method for constructing an X-bar chart, R-chart, or S-chart:



Calculating Region Boundaries

To determine if your system is out of control, you will need to section your data into regions A, B, and C, below and above the grand average. These regions are shown in Figure III. To calculate the boundaries between these regions, you must first calculate the UCL and LCL. The boundaries are evenly spaced between the UCL and LCL. One way to calculate the boundaries is shown below.

$$\text{Boundary between A and B above } X_{GA} = X_{GA} + (UCL - X_{GA}) * 2 / 3$$

$$\text{Boundary Between B and C above } X_{GA} = X_{GA} + (UCL - X_{GA}) * 1 / 3$$

$$\text{Boundary Between A and B below } X_{GA} = LCL + (X_{GA} - LCL) * 2 / 3$$

$$\text{Boundary Between B and C below } X_{GA} = LCL + (X_{GA} - LCL) * 1 / 3$$

2.6 Example 1

Assume that in the manufacture of 1 kg Mischmetal ingots, the product weight varies with the batch. Below are a number of subsets taken at normal operating conditions (subsets 1-7), with the weight values given in kg. Construct the X-Bar, R-charts, and S-charts for the experimental data (subsets 8-11). Measurements are taken sequentially in increasing subset number.

Subset #	Values (kg)
1 (control)	1.02, 1.03, 0.98, 0.99
2 (control)	0.96, 1.01, 1.02, 1.01
3 (control)	0.99, 1.02, 1.03, 0.98
4 (control)	0.96, 0.97, 1.02, 0.98
5 (control)	1.03, 1.04, 0.95, 1.00
6 (control)	0.99, 0.99, 1.00, 0.97
7 (control)	1.02, 0.98, 1.01, 1.02
8 (experimental)	1.02, 0.99, 1.01, 0.99
9 (experimental)	1.01, 0.99, 0.97, 1.03
10 (experimental)	1.02, 0.98, 0.99, 1.00
11 (experimental)	0.98, 0.97, 1.02, 1.03

Solution:

First, the average, range, and standard deviation are calculated for each subset.

Subset #	Values (kg)	Average (\bar{X})	Range (R)	Standard Deviation (s)
1 (control)	1.02, 1.03, 0.98, 0.99	1.0050	0.05	0.023805
2 (control)	0.96, 1.01, 1.02, 1.01	1.0000	0.06	0.027080
3 (control)	0.99, 1.02, 1.03, 0.98	1.0050	0.05	0.023805
4 (control)	0.96, 0.97, 1.02, 0.98	0.9825	0.06	0.026300
5 (control)	1.03, 1.04, 0.95, 1.04	1.0150	0.09	0.043589
6 (control)	0.99, 0.99, 1.00, 0.97	0.9875	0.03	0.012583
7 (control)	1.02, 0.98, 1.01, 1.02	1.0075	0.04	0.018930
8 (experimental)	1.02, 0.99, 1.01, 0.99	1.0025	0.03	0.015000
9 (experimental)	1.01, 0.99, 0.97, 1.03	1.0000	0.06	0.025820
10 (experimental)	1.02, 0.98, 0.99, 1.00	0.9975	0.04	0.017078
11 (experimental)	0.98, 0.97, 1.02, 1.03	1.0000	0.06	0.029439

Next, the grand average X_{GA} , average range R_A , and average standard deviation S_A are computed for the subsets taken under normal operating conditions, and thus the centerlines are known. Here $n=4$.

$$X_{GA} = 1.0004$$

$$R_A = 0.05428$$

$$S_A = 0.023948$$

X-Bar limits are computed (using R_A).

$$UCL = X_{GA} + A_2R_A = 1.0004 + 0.729(0.05428) = 1.04$$

$$LCL = X_{GA} - A_2R_A = 1.0004 - 0.729(0.05428) = 0.96$$

X-Bar limits are computed (using S_A).

$$UCL = X_{GA} + A_3S_A = 1.0004 + 1.628(0.023948) = 1.04$$

$$LCL = X_{GA} - A_3S_A = 1.0004 - 1.628(0.023948) = 0.96$$

Note: Since $n=4$ (a relatively small subset size), both R_A and S_A can be used to accurately calculate the UCL and LCL.

R-chart limits are computed.

$$UCL = D_4R_A = 2.282(0.05428) = 0.12$$

$$LCL = D_3R_A = 0(0.05428) = 0$$

S-chart limits are computed.

$$UCL = B_4S_A = 2.266(0.023948) = 0.054266$$

$$LCL = B_3S_A = 0(0.023948) = 0$$

The individual points in subsets 8-11 are plotted below to demonstrate how they vary with in comparison with the control limits.

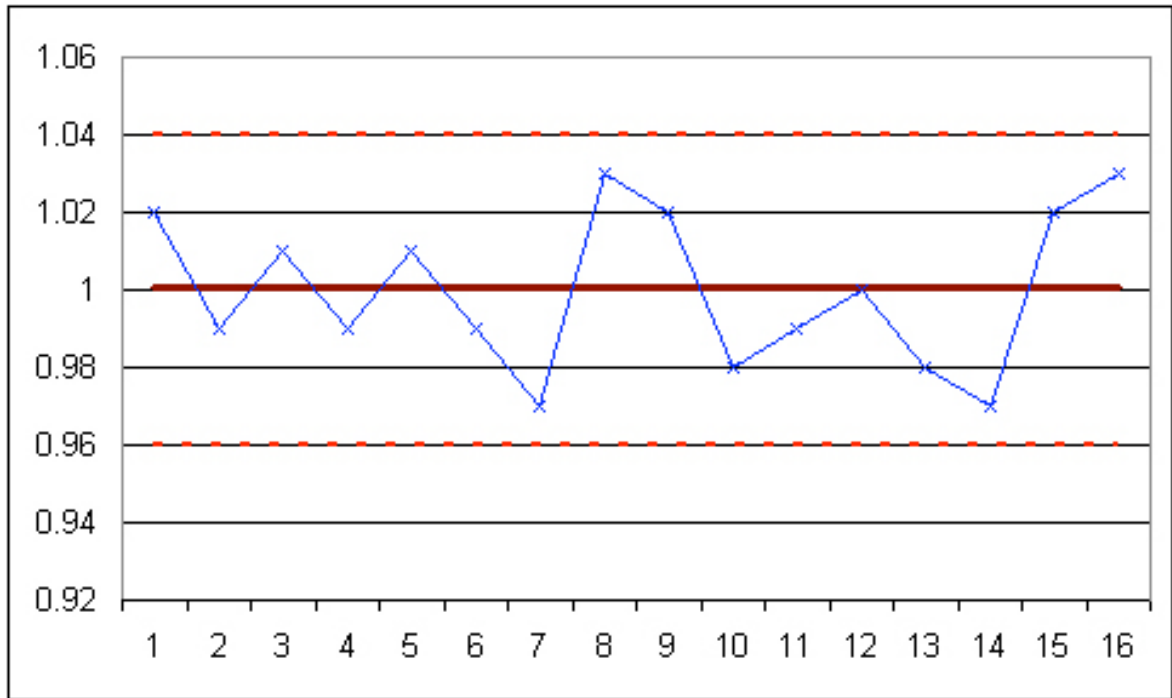


Figure E-1: Chart of individual points in subsets 8-11.

The subgroup averages are shown in the following X-Bar chart:

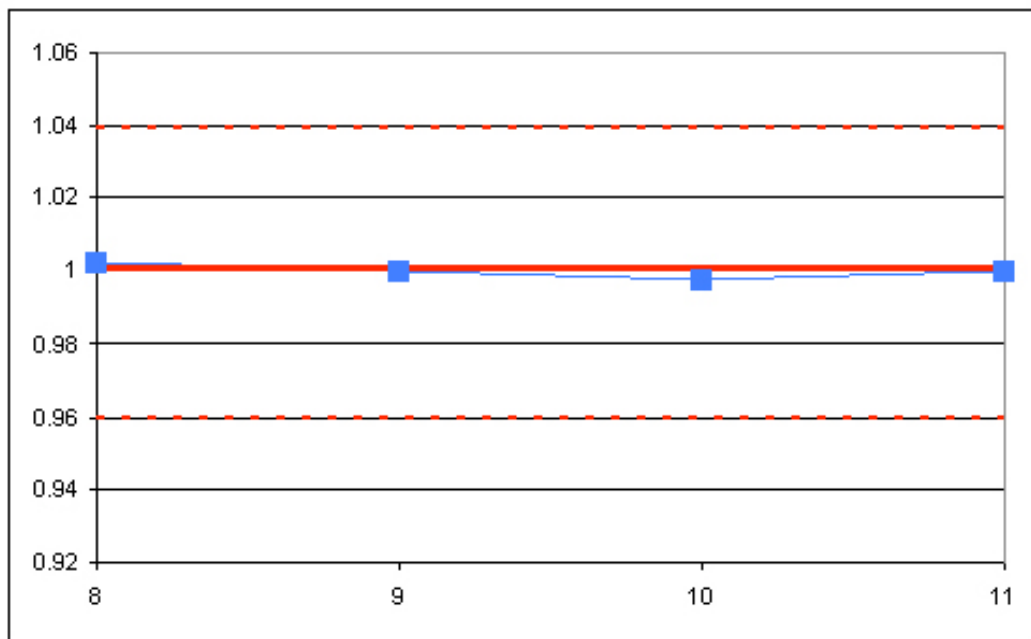


Figure E-2: X-Bar chart for subsets 8-11.

The R-chart is shown below:

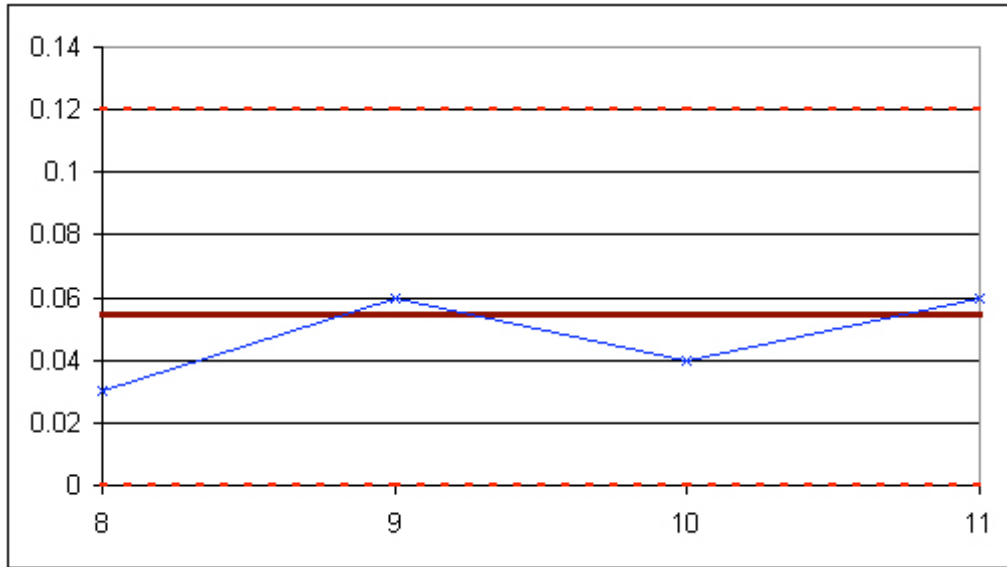


Figure E-3: R-chart for subsets 8-11.

The S-chart is shown below:

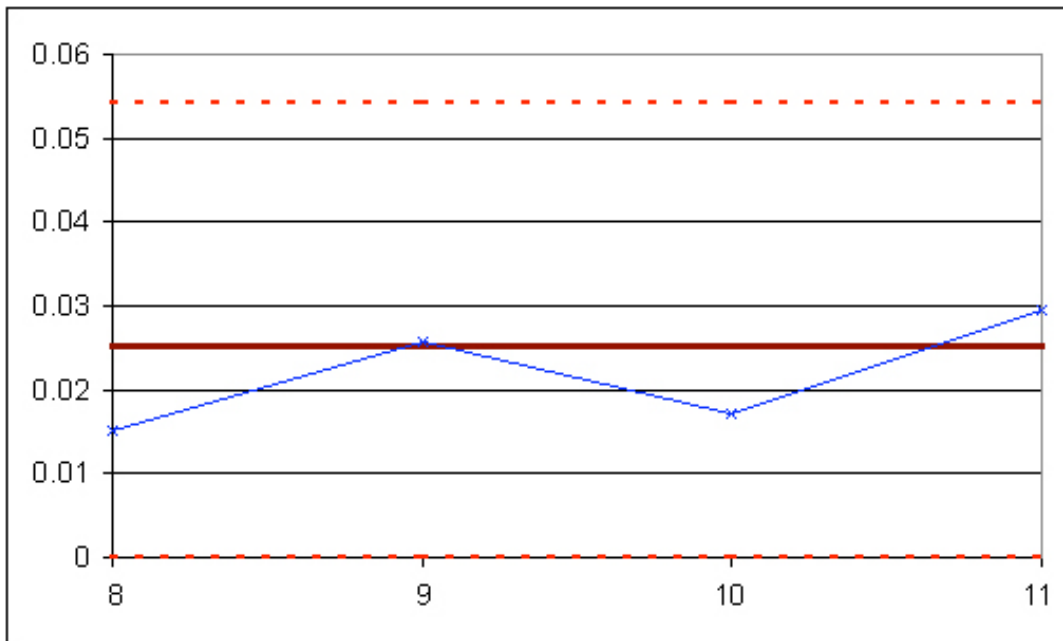


Figure E-4: S-chart for subsets 8-11.

The experimental data is shown to be in control, as it obeys all of the rules given above.

2.7 Example 2

It's your first day on the job as a chemical engineer in a plant, and one of your responsibilities is to monitor the pH of a particular process. You are asked by your boss to monitor the stability of the system. She gives you some baseline data for the process, and you collect data for the process during your first day. Construct X-bar and R-Charts to report your results.

Table 1: Baseline data

time (hours)	pH			
1	7.00	7.30	6.99	7.00
2	7.12	7.25	7.12	7.20
3	7.20	7.16	7.20	7.16
4	6.98	7.00	6.94	7.00
5	6.99	6.99	6.99	6.98
6	7.00	6.93	7.02	6.93
7	6.92	7.00	6.92	7.02
8	6.88	6.82	6.94	6.99
9	7.10	7.00	7.00	7.00
10	7.21	7.02	7.21	7.04
11	7.01	6.86	7.01	6.90
12	6.86	6.98	6.90	6.98
13	6.90	7.00	6.87	7.00
14	7.01	7.04	7.01	7.05
15	7.00	6.95	7.00	6.99
16	7.09	7.20	7.03	7.20
17	6.89	7.14	6.87	7.15
18	6.98	6.80	6.98	6.89
19	7.00	6.90	7.00	6.90
20	7.20	7.00	7.23	7.00
21	7.04	7.03	7.08	7.00
22	6.90	6.92	6.98	6.92
23	7.00	7.00	7.00	7.00
24	7.00	6.97	7.01	6.98

To be consistent with the baseline data, each hour you take four pH readings. The data you collect is displayed below.

Table 2: Experimental data

time (hours)	pH	pH	pH	pH
1	6.99	6.99	7.00	6.89
2	6.98	7.12	7.05	6.96
3	7.00	7.18	7.08	7.04
4	7.01	6.94	6.98	7.00
5	6.90	6.99	6.93	7.01
6	6.96	7.01	7.00	7.14
7	7.04	6.92	6.82	7.01
8	7.00	6.93	7.00	6.90
9	7.01	7.00	7.02	6.92
10	7.04	7.18	6.99	6.93
11	6.91	7.01	6.90	7.00
12	7.00	6.97	6.98	7.18
13	7.00	6.89	7.00	7.03
14	7.03	7.01	7.05	6.87
15	6.97	7.00	7.00	6.98
16	7.03	6.97	7.02	6.98
17	6.99	6.89	6.87	6.99
18	6.89	6.98	6.98	6.98
19	6.98	7.00	7.00	7.02
20	7.02	7.15	6.97	6.98
21	7.02	7.08	7.08	7.00
22	6.97	7.01	6.98	7.05
23	7.01	7.04	6.99	7.08
24	6.97	7.00	6.98	6.98

Solution

For this situation, there are $k=24$ subsets because there are 24 data sets. For each subset, $n=4$ because there are four pH measurements taken each hour. The first thing you do is calculate the mean and range of each subset. The means are calculated using the

AVERAGE() Excel function and the ranges are calculated using MAX() – MIN(). Once these values are calculated, the Grand Average X_{GA} and average range R_A are calculated. These values are simply the means of each subset's mean and range. This data is displayed below.

Table 3: Data used to calculate and grand average and Range.

Control Data						
time (hours)	pH				x_ave	range
1	7.00	7.30	6.99	7.00	7.07	0.31
2	7.12	7.25	7.12	7.20	7.17	0.13
3	7.20	7.16	7.20	7.16	7.18	0.04
4	6.98	7.00	6.94	7.00	6.98	0.06
5	6.99	6.99	6.99	6.98	6.99	0.01
6	7.00	6.93	7.02	6.93	6.97	0.09
7	6.92	7.00	6.92	7.02	6.97	0.10
8	6.88	6.82	6.94	6.99	6.91	0.17
9	7.10	7.00	7.00	7.00	7.03	0.10
10	7.21	7.02	7.21	7.04	7.12	0.19
11	7.01	6.86	7.01	6.90	6.95	0.15
12	6.86	6.98	6.90	6.98	6.93	0.12
13	6.90	7.00	6.87	7.00	6.94	0.13
14	7.01	7.04	7.01	7.05	7.03	0.04
15	7.00	6.95	7.00	6.99	6.99	0.05
16	7.09	7.20	7.03	7.20	7.13	0.17
17	6.89	7.14	6.87	7.15	7.01	0.28
18	6.98	6.80	6.98	6.89	6.91	0.18
19	7.00	6.90	7.00	6.90	6.95	0.10
20	7.20	7.00	7.23	7.00	7.11	0.23
21	7.04	7.03	7.08	7.00	7.04	0.08
22	6.90	6.92	6.98	6.92	6.93	0.08
23	7.00	7.00	7.00	7.00	7.00	0.00
24	7.00	6.97	7.01	6.98	6.99	0.04
Means:					7.01	0.12

Now that you know $X_{GA} = 7.01$ and $R_A = 0.12$, you can calculate the upper control limit, UCL, and lower control limit, LCL, for the X-bar control chart.

From Table A, $A_2 = 0.729$ when $n=4$. Using equations UCL and LCL for X-bar charts listed above:

$$UCL = 7.01 + 0.729(0.12) = 7.0982$$

$$LCL = 7.01 - 0.729(0.12) = 6.9251$$

Then the $UCL = 7.0982$, $LCL = 6.9251$ and $X_{GA} = 7.01$ are plotted in Excel along with the average values of each subset from the experimental data to produce the X-bar control chart.

Experimental Data						
time (hours)	ph				x ave	range
1	6.99	6.99	7.00	6.89	6.97	0.11
2	6.98	7.12	7.05	6.96	7.03	0.16
3	7.00	7.18	7.08	7.04	7.08	0.18
4	7.01	6.94	6.98	7.00	6.98	0.07
5	6.90	6.99	6.93	7.01	6.96	0.11
6	6.96	7.01	7.00	7.14	7.03	0.18
7	7.04	6.92	6.82	7.01	6.95	0.22
8	7.00	6.93	7.00	6.90	6.96	0.10
9	7.01	7.00	7.02	6.92	6.99	0.10
10	7.04	7.18	6.99	6.93	7.04	0.25
11	6.91	7.01	6.90	7.00	6.96	0.11
12	7.00	6.97	6.98	7.18	7.03	0.21
13	7.00	6.89	7.00	7.03	6.98	0.14
14	7.03	7.01	7.05	6.87	6.99	0.18
15	6.97	7.00	7.00	6.98	6.99	0.03
16	7.03	6.97	7.02	6.98	7.00	0.06
17	6.99	6.89	6.87	6.99	6.94	0.12
18	6.89	6.98	6.98	6.98	6.96	0.09
19	6.98	7.00	7.00	7.02	7.00	0.04
20	7.02	7.15	6.97	6.98	7.03	0.18
21	7.02	7.08	7.08	7.00	7.05	0.08
22	6.97	7.01	6.98	7.05	7.00	0.08
23	7.01	7.04	6.99	7.08	7.03	0.09
24	6.97	7.00	6.98	6.98	6.98	0.03

Table 4: Average subset values and ranges plotted on the X-bar and R-chart

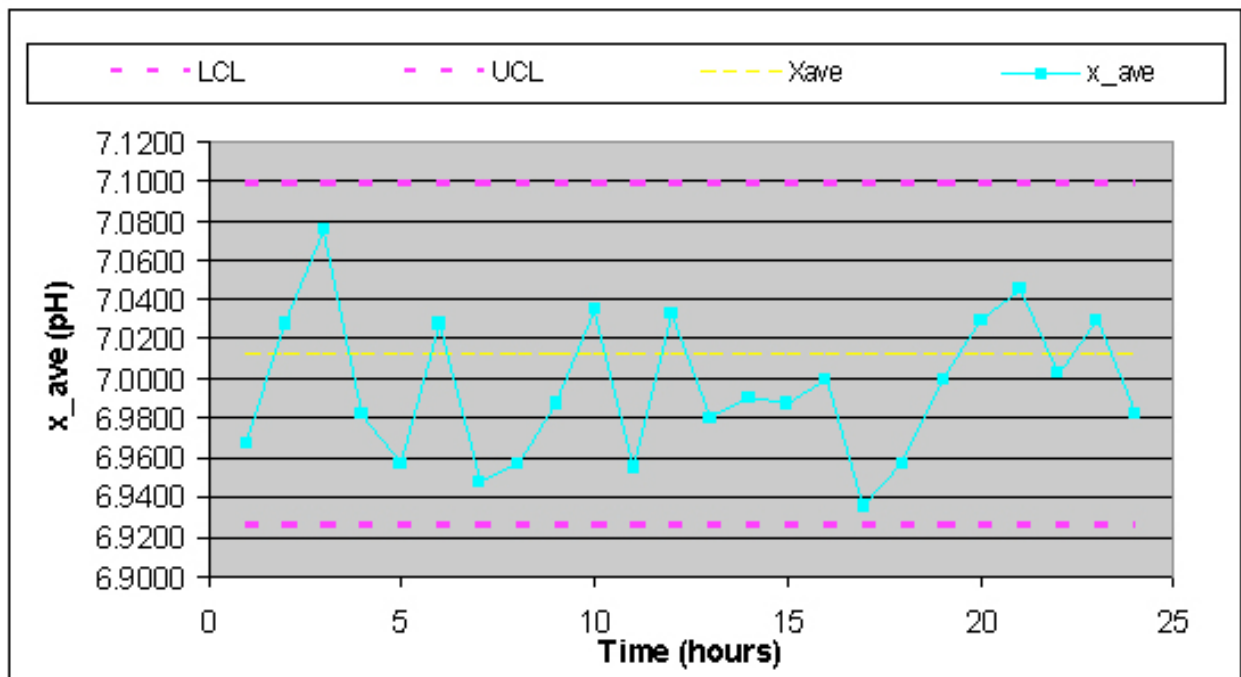


Figure E-5: X-bar control chart

Then, to construct the Range charts, the upper and lower control limits were found. For $n=4$, $D_3 = 0$ and $D_4 = 2.282$ so then:

$$LCL = D_3 R_A = 0(0.12) = 0$$

$$UCL = D_4 R_A = 2.282(0.12) = 0.2710$$

Then, $UCL = 0.2710$, $LCL = 0$, $R_A = 0.12$, and the ranges for each subset were plotted vs. time in Excel (Figure E-6).

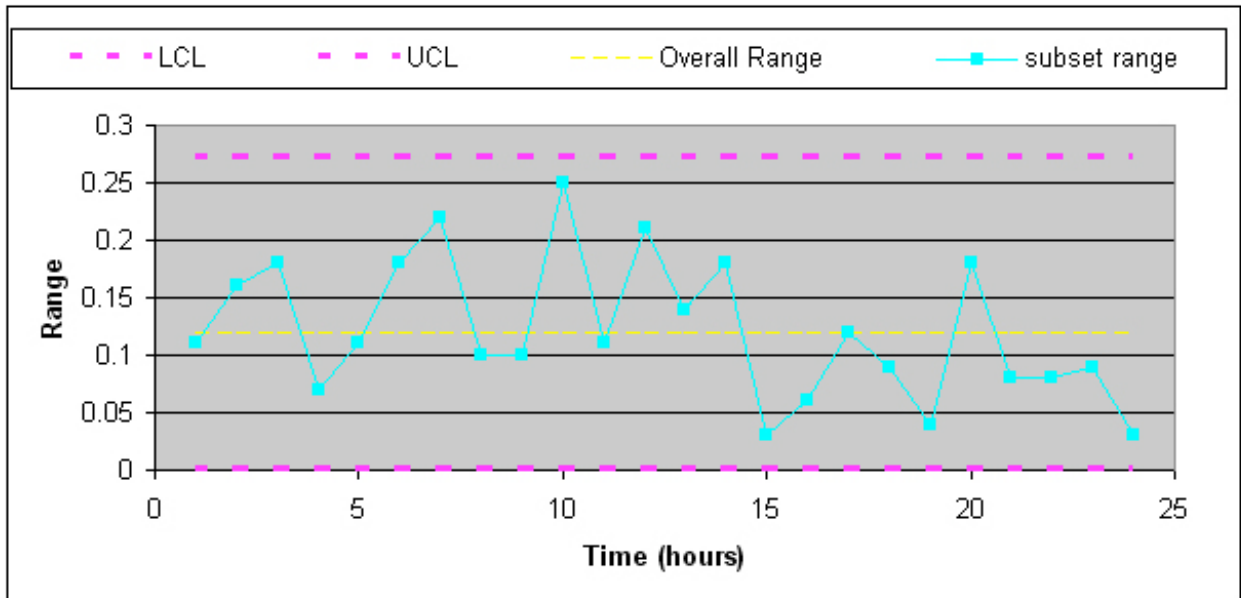


Figure E-6: Range control chart

From both of these charts, the process is in control because all rules for stability are met.

Rule 1: No point falls beyond the UCL and LCL.

Rule 2: Two out of three consecutive points do not fall beyond 2σ on the same side of the centerline.

Rule 3: Four out of five consecutive points do not fall beyond 1σ on the same side of the centerline.

Rule 4: Nine or more consecutive points do not fall on the same side of the centerline.

It's important that both of these charts be used for a given set of data because it is possible that a point could be beyond the control band in the Range chart while nothing is out of control on the X-bar chart.

Another issue worth noting is that if the control charts for this pH data did show some points beyond the LCL or UCL, this does not necessarily mean that the process itself is out of control. It probably just means that the pH sensor needs to be recalibrated.

2.8 Example 3

A simple out-of-control example with a sample constructed control chart.

You have been analyzing the odd operation of a temperature sensor in one of the plant's CSTR reactors. This particular CSTR's temperature sensor consists of three small thermocouples spaced around the reactor: T1, T2, and T3. The CSTR is jacketed and cooled with industrial water. The reaction taking place in the reactor is moderately exothermic. You know the thermocouples are working fine; you just tested them, but a technician suggests the CSTR has been operating out of control for the last 10 days. There have been daily samples taken and there is a control chart created from the CSTR's grand average and standard deviation from the year's operation.

You are assigned to see if the CSTR is operating out of control. The grand average is 307.47 units of temperature and the grand standard deviation is 4.67 units of temperature. The data is provided for construction of the control chart in Table 1 and the data from the last 10 troublesome days is shown in Table 2. You decide to plot the troublesome data onto the control chart to see if it violates any stability rules.

	<i>Value</i>	<i>Calculate</i>
<i>Upper Control Limit</i>	316.60	$\mu + R_3\sigma$
<i>Upper Zone A Threshold</i>	313.56	$\mu + (2/3)*R_3\sigma$
<i>Upper Zone B Threshold</i>	310.51	$\mu + (1/3)*R_3\sigma$
<i>Grand Average Value</i>	307.47	μ
<i>Lower Zone B Threshold</i>	304.42	$\mu - (1/3)*R_3\sigma$
<i>Lower Zone A Threshold</i>	301.38	$\mu - (2/3)*R_3\sigma$
<i>Lower Control Limit</i>	298.33	$\mu - R_3\sigma$

μ	307.47
σ	4.67
R_3	1.954

Table 3-1. Data for Construction of Control Chart

The way I found A_3 or in this case, R_3 , I used the control charts constants table which is found on this wiki page. I decided to use the x-bar using the standard deviations) but you can also use the range). I found that the value for n(number of subgroups) is three since the CSTR's temperature sensor consists of **three small thermocouples** (T1,T2,T3). Therefore by looking at the constant chart, I get A_3 (or R_3 in this case) to be 1.954. Here's the table below:

Subgroup	X-bar chart	
	Using Ra	Using Sa
<i>n</i>	A2	A3
2	1.886	2.659
3	1.023	1.954
4	0.729	1.628
5	0.577	1.427
6	0.483	1.287

Also, you will notice if you used the range instead of the standard deviation to determine the UCL,LCL, etc. that the values will be roughly the same. Here's the table in comparing the values of UCL and LCL using either A_2 (range) or A_3(stdev):

	A3 (stdev)	A2 (range)
	1.954	1.023
	Using Sdev	Using Range
UCL	316.5997379	316.473784
LCL	298.3347317	298.460686

Note: These values were using the same grand average (307.47), the grand standard deviation (4.67) and the grand range (8.80)

Sample Day	T1	T2	T3
1	299.82	310.26	306.60
2	311.68	307.04	300.90
3	310.94	311.68	306.83
4	325.00	308.82	304.97
5	321.43	300.98	311.23
6	320.74	308.97	305.26
7	314.77	313.25	303.36
8	332.75	302.76	306.11
9	319.87	296.81	305.95
10	315.21	314.99	309.60

Table 3-2. Sample Data from Past 10 Troublesome Days

Solution

When the sample data was graphed onto the control chart, the image below was seen.

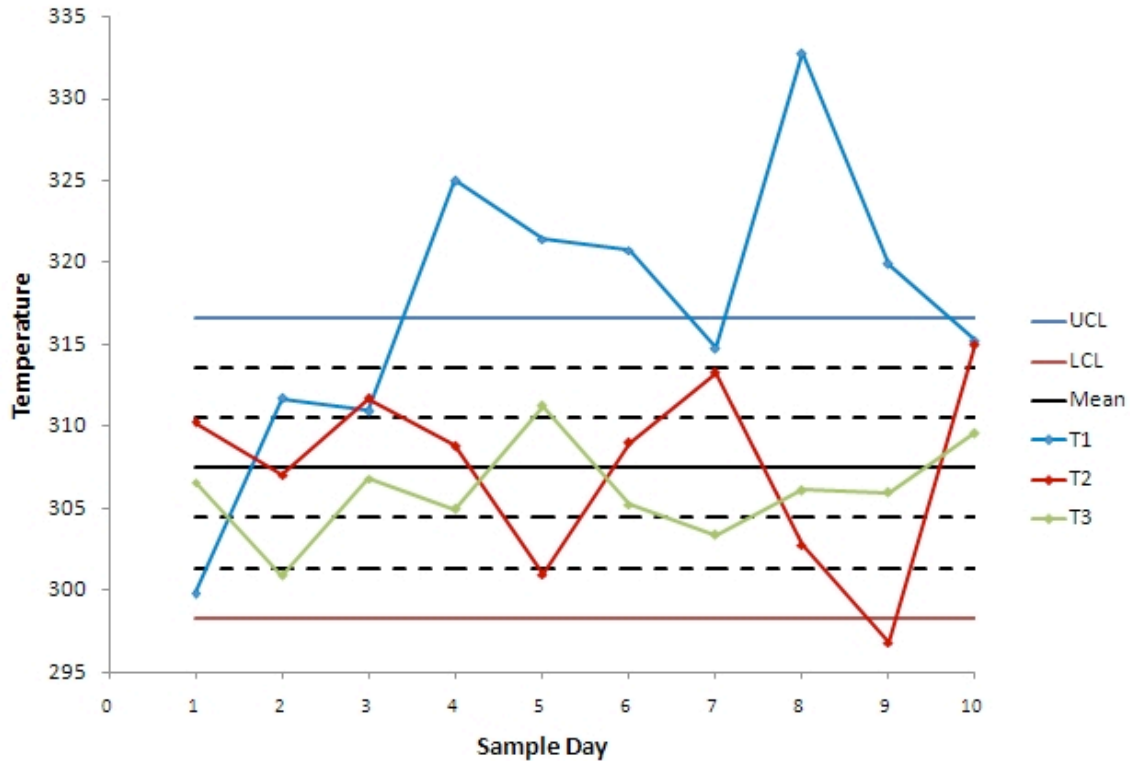


Figure 3-1. 10-Day Data Graphed Onto Control Chart

We can see from the control chart that the CSTR system is clearly out of control. Each thermocouple was tested to see which stability rules it violates.

The first thermocouple (**T1**) violates every stability rule.

- *Rule 1* - Several points from the T1 data fall above the upper control line.
- *Rule 2* - There are many instances where at least two out of three consecutive points fall above the zone AB threshold.
- *Rule 3* - There are eight consecutive points falling above the BC threshold.
- *Rule 4* - Nine consecutive points fall above the mean value.

Judging on this thermocouple's performance, we can say that the system is out of control, but we will analyze the other thermocouples' performance for good measure.

The second thermocouple (**T2**) violates stability rule 1, 2, and 3.

- *Rule 1* - One point falls below the lower control line.

- *Rule 2* - Two consecutive points (samples 9 and 10) fall beyond the AB threshold.
- *Rule 3* - Of the last five samples from T2, four are beyond the BC threshold.

The third thermocouple (**T3**) does not violate any stability rules and the results it displays are within control.

This system is **out of control** because the data from the thermocouples falls beyond the threshold rules for the unit's control chart. This could be explained with many potential situations. One is explained below.

If the CSTR's agitator is knocked loose, the agitation could become erratic. The erratic agitation could create eddy currents and hot spots in the CSTR.

The entire system is out of control because you know that the thermocouples are operating fine and more than one thermocouple violates the stability rules.

2.9 Multiple Choice Question 1

When is it useful to use a moving average data set?

- A. Never
- B. When instant response to process is desired
- C. When you have a process that changes slowly
- D. Always, as it is a far superior method

2.10 Multiple Choice Question 2

What does n signify?

- A. The number of subsets in collected data
- B. The number of data points in a subset
- C. The upper control limit for an X-bar chart
- D. The centerline for an R-chart

2.11 Multiple Choice Question 3

Of the four stability rules for reading control charts, how many must occur in order for a subset to be determined unstable?

- A. 1
- B. 2
- C. 3
- D. 4

2.12 Multiple Choice Answers

Question 1: C

Question 2: B

Question 3: A

2.13 Sage's Corner

SPC Control Presentation


<http://video.google.com/googleplayer.swf?docId=1396803583755378767>

[Slides without narration SPC control](#)

2.14 References

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Section 3. Six Sigma: What is it and what does it mean?

Note:  [Video lecture](#) available for this section!

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The often-used six sigma symbol.

3.1 Introduction

Every generation of business strives for a new level of quality. The quality program that is currently in vogue and being widely used and recognized by industry is the Six Sigma program. Six Sigma is a relatively new program, and was only started in 1986. It was first put into implementation at Motorola, but is now in use by most large corporations. Some of these other large companies include GE, Honeywell, and Bank of America. The Six Sigma program is in place to eliminate any abnormalities, failures, or defects that occur within a given process. These are problems that already exist. DFSS (Design for six sigma) starts earlier, to develop or redesign the process itself, so fewer wrinkles show up in the first place, thus systematically preventing downstream errors. Six Sigma is also used in developing new processes. The Six Sigma program strives to achieve six standard deviations between the mean and the closest specification limit on a short term study. Studies run to obtain this goal are short term capability studies, which include common cause or random variation, such as operator control, and long term studies, which include random and special types of variation. Both of these studies are evaluated on a Z-scale. The short term data variability which makes up long term variability tends to cause the mean to shift. This shift of the mean is by 1.5 standard deviations. Most companies are looking on a long term scale, because they would rather have a good/safe product in the long run/for a long time rather than for a short amount of time. Using this idea, the goal for the Six Sigma program is to have fewer than 3.4 failures per one million opportunities when the data is evaluated to include the shifted mean from process variability (6 standard deviations - 1.5 standard deviations = 4.5 standard deviations). The 4.5 vs 6 standard deviations is the same goal, but the 4.5 represents data variation in the long run, which is used in most processes. We will be using the shifted mean scenario for the rest of this article when referring to opportunity goals. This leaves very slight room for error on a process and leads to a very high level of quality in the products.

To reiterate, the term "Six Sigma" comes from the standard deviation and the Gaussian distribution. 3.4 failures per one million opportunities represents 4.5 standard deviations (sigma) away from the median value, either up or down, under a bell curve. This will be discussed further below along with what the Six Sigma program represents, what mathematically this means, and finally what a Gaussian distribution is. After the basics have been covered we will move onto Statistical Process Control. Statistical Process Control is different ways to analyze the data that you have obtained. Finally, we will relate Six Sigma to process control and explain how you can tell if something is in Six Sigma control or not.

3.2 The Six Sigma Program

Six Sigma is defined as a measure of quality that organizations strive to achieve. It is a disciplined, data-driven approach used to eliminate defects in any process – from manufacturing to transactional and from product to service. Six Sigma does not refer to a process operating within 6 or 4.5 standard deviations of the desired state. To achieve Six Sigma, a process must not produce more than 3.4 defects per million opportunities, where a defect is defined as anything outside of the customer specification. One million opportunities, and only 3.4 defects? Sounds like an efficient process. Here is an example that will help demonstrate. Let's say a surgeon at the top of his field has a 5.51 sigma ranking. Sounds pretty good, right? That means that if he operates on 1,000,000 patients per year he loses 30 of them. When a process is operating at Six Sigma, it is seen that there are essentially zero defects within a process.

In chemical engineering, many different processes require strict, robust control. For example, a reactor may need to be maintained between a specified temperature range to keep the plant safe. However, there is also an optimum temperature at which the reaction will occur. Engineers will want to keep a tight control around this temperature to make the system more efficient, while also closely watching the variable and keeping track of how close it gets to the control limits. Crossing the control limits is not the only problem. In order for a system to be in statistical control as stated by the Six Sigma program, the data points must not frequently approach the same control limit. The Six Sigma program helps engineers monitor processes to keep them within their desirable ranges. Many industries employ the Six Sigma system as well as its hierarchy of positions to champion data-driven problem solving.

Originally invented by Motorola, the Six Sigma system contains belt rankings that represent a person's achievements utilizing Six Sigma methodologies and associated roles and responsibilities. These rankings are modeled after the martial arts system, as detailed below.

Yellow Belts (YB)

Yellow belt is the first level in the Six Sigma program. To get yellow belt status one must go through a training course in Six Sigma and pass an online certification. Yellow belt

team members do not lead projects on their own, but they are usually a core team member with special knowledge on a project. Yellow belts are responsible for:

- The development of process maps to support Six Sigma projects.
- Running smaller process improvement projects using the Plan, Do, Check, Act (PDCA) method
- Being a subject matter expert on the Six Sigma project

Yellow Belt Projects

- usually limited to identifying small projects that could benefit from improvement

Green Belts (GB)

Green belts are new team members that achieve certification after completing training in a Six Sigma course. To complete green belt training, new members must complete a relevant project that utilizes the DMAIC model outlined below. To maintain green belt certification, green belts generally complete DMAIC projects once every twelve months. Green belts are also responsible for:

- Recommending Six Sigma projects
- Participating on Six Sigma project teams
- Leading Six Sigma teams in local improvement projects

Green Belt Projects

Green belts complete six sigma projects while still holding their current job duties. Therefore, a six sigma project undertaken by a green belt could include:

- Statistical analysis to improve reliability on a reactor within the green belt's current responsibility
- Root cause analysis and elimination of quality control problems that chronically affect the green belt's department

Black Belts (BB)

Black belts are intermediate team members that employ in-depth technical expertise to achieve Six Sigma objectives. Furthermore, black belts can become temporary, full-time change agents for a moderate period of time (two-three years) to produce change using Six Sigma methods. Black belts are also responsible for:

- Demonstrating mastery of black belt knowledge
- Demonstrating proficiency at achieving results through the application of the Six Sigma approach
- Consultation for functional area Internal Process Improvement

- Coaching, Mentoring, and Recommending green belts

Black Belt Projects

Black belts complete six sigma projects outside of their previous job duties. Therefore, a six sigma project undertaken by a black belt could include:

- Plant-level process controls improvement at a facility that greatly affects the finished product at a facility
- Assessment of total warranty/quality control issues at a facility through large scale statistical data analysis and improvement

Master Black Belts (MBB)

The major duty of master black belts include acting as project leaders, as well as:

- Training and mentoring Black Belts and Green Belts
- Helping to decide large-scale Six Sigma projects
- Maintaining the quality of Six Sigma measurements
- Developing Six Sigma training

Master Black Belt Projects

Most master black belts would only be involved with directing black and/or green belts in their projects. Their effect on process would generally be limited to pointing out and suggesting large projects for appointed black belts to undertake.

To complete Six Sigma projects, belt candidates utilize the DMAIC model. DMAIC (Define, Measure, Analyze, Improve, Control) is an improvement system for existing processes falling below specification and looking for incremental improvement. DMADV (Define, Measure, Analyze, Design, Verify) is an improvement system used to develop new processes at Six Sigma quality level. Below, the steps for DMAIC and DMADV are outlined.

Table 1 - Outline of the steps used in DMAIC (improve an existing process)

D	<p>Define the goals of the improvement activity. The most important goals are obtained from customers. At the top level the goals will be the strategic objectives of the organization, such as greater customer loyalty, increased market share, or greater employee satisfaction.</p> <p>At the operations level, a goal might be to increase the throughput of a production department.</p> <p>At the project level goals might be to reduce the defect level and increase throughput for a particular process. Obtain goals from direct communication with customers, shareholders, and employees.</p>
M	<p>Measure the existing system. Establish valid and reliable metrics to help monitor progress towards the goal(s) defined at the previous step. Begin by determining the current baseline. Use exploratory and descriptive data analysis to help you understand the data.</p>
A	<p>Analyze the system to identify ways to eliminate the gap between the current performance of the system or process and the desired goal. Use statistical tools to guide the analysis.</p>
I	<p>Improve the system. Be creative in finding new ways to do things better, cheaper, or faster. Use project management and other planning and management tools to implement the new approach. Use statistical methods to validate the improvement.</p>
C	<p>Control the new system. Institutionalize the improved system by modifying compensation and incentive systems, policies, procedures, budgets, operating instructions and other management systems. You may wish to utilize standardization such as ISO 9000 to assure that documentation is correct. Use statistical tools to monitor stability of the new systems.</p>

Table 2 - Outline of the steps used in DMADV (develop a new process)

D	Define the goals of the design activity. What is being designed? Why? Use QFD or Analytic Hierarchical Process to assure that the goals are consistent with customer demands and enterprise strategy.
M	Measure. Determine Critical to Stakeholder metrics. Translate customer requirements into project goals.
A	Analyze the options available for meeting the goals. Determine the performance of similar best-in-class designs.
D	Design the new product, service or process. Use predictive models, simulation, prototypes, pilot runs, etc. to validate the design concept's effectiveness in meeting goals.
V	Verify the design's effectiveness in the real-world.

All charts and descriptions referenced from Pyzdek, Thomas, "DMAIC and DMADV Explained" <http://www.pyzdek.com/DMAICDMADV.htm> , 2003

3.3 Statistics and Six Sigma

You are probably already familiar with the concepts of average, standard deviation, and Gaussian distribution. However, they are very important concepts in Six Sigma, so they are reviewed in this section. This section also discusses analysis methods used in Six Sigma.

3.3.1 Average

The equation for calculating an **average** is shown below.

$$\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i = \frac{x_1 + x_2 + \dots + x_N}{N}$$

where

\bar{x} = average

x_i = measurement for trial i

N = number of measurements

This equation relates to Six Sigma because it is the value that you aim for when you are creating your product. After millions of products made, you will have a very good idea of what your exact average product specification is. The average is combined with the specification limits, which are the limits that determine if your product is in or out of spec. The wider the specification limits are, the more room for deviation from the average there is for your product. A product specification would be written like this:

10 ± 2 mm

Where the first number (10) represents the average and the second number (2) represents the amount of error allowable from the average without violating 4.5 standard deviations (on a long term scale). Thus, your product can range from 8 to 12 mm for this example.

The average is a good representation of the a set of data. However, the main problem it experiences is the how it is strongly influenced by outlier values. For example, say a town had a population of 50 people with an average income of \$30,000 per person. Now say that a person moves into the town with an income of \$1,000,000. This would move the average up to approximately \$50,000 per person. However, this is not a good representation of the average income of the town. Hence, outlier values must be taken into account when analyzing data. In contrast to the mean, sometimes the median can be a good representation of a set of data. The median is defined as the middle value of a set of data are arranged in order. The median is immune to outlier values as it basically one value and is not calculated it any way so it cannot be influenced by a wide range of numbers. Both the mean and median can be taken into account when analyzing a set of data points.

3.3.2 Standard Deviation

The equation for **standard deviation** is shown below.

$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})^2}$$

where σ = standard deviation, and the other variables are as defined for the average.

For each measurement, the difference between the measured value and the average is calculated. This difference is called the residual. The sum of the squared residuals is calculated and divided by the number of samples minus 1. Finally, the square root is taken.

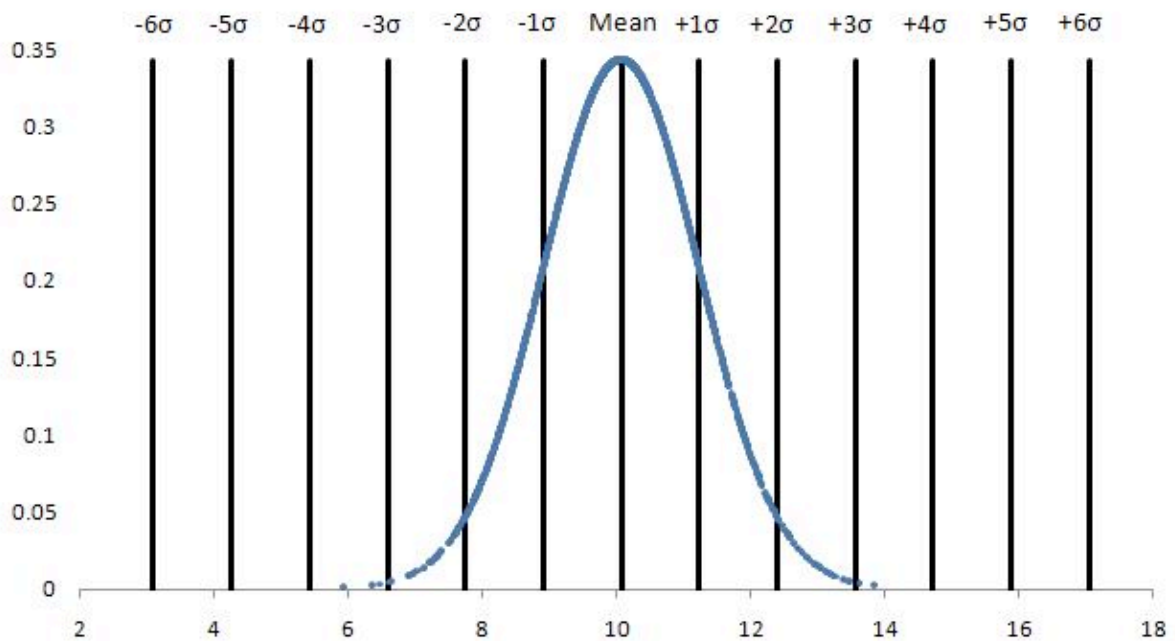
The standard deviation is the basis of Six Sigma. The number of standard deviations that can fit within the boundaries set by your process represent Six Sigma. If you can fit 4.5 standard deviations within your process specifications then you have obtained a Six Sigma process for a long term scale. However, the number of errors that you can have for your process as you move out each standard deviation continues to decrease. The table below shows the percentage of data that falls within the standard deviations and the amount of defects per sigma, in terms of "Defects Per Million Opportunities" or DPMO. The percentage of errors that you are allowed is one minus the percentage encompassed by the percent of the total.

# of Standard Deviations	% of Total	DPMO
1	68.27	690,000

2	95.45	308,537
3	99.73	66,807
4	99.9937	6,210
5	99.99994	233
6	99.9999998	3.4

Data from: <http://www.isixsigma.com/library/content/c020813a.asp>

The image below shows an example data set (see [#Gaussian Distribution](#) below) with lines marking 1 to 6 standard deviations from the mean. In this example, the mean is approximately 10 and the standard deviation is 1.16.



3.3.3 Gaussian Distribution

The normal, or Gaussian, distribution is a family of continuous probability distributions. The normal distribution function was first introduced in 1733, and since has become the most widely used family of distribution functions in statistical analysis. These distribution functions are defined by two parameters: a location (most commonly the "mean", μ), and a scale (most commonly the "variance", σ^2). The use of normal distributions in statistics can be seen as advantageous due to its ability to maximize information entropy around a given mean and variance. Information entropy is the measure of uncertainty associated with a random variable.

For the purposes of this class and Chemical Engineering applications, you can model a given set of data using the [probability density function](#) which is shown below.

$$\varphi = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right)$$

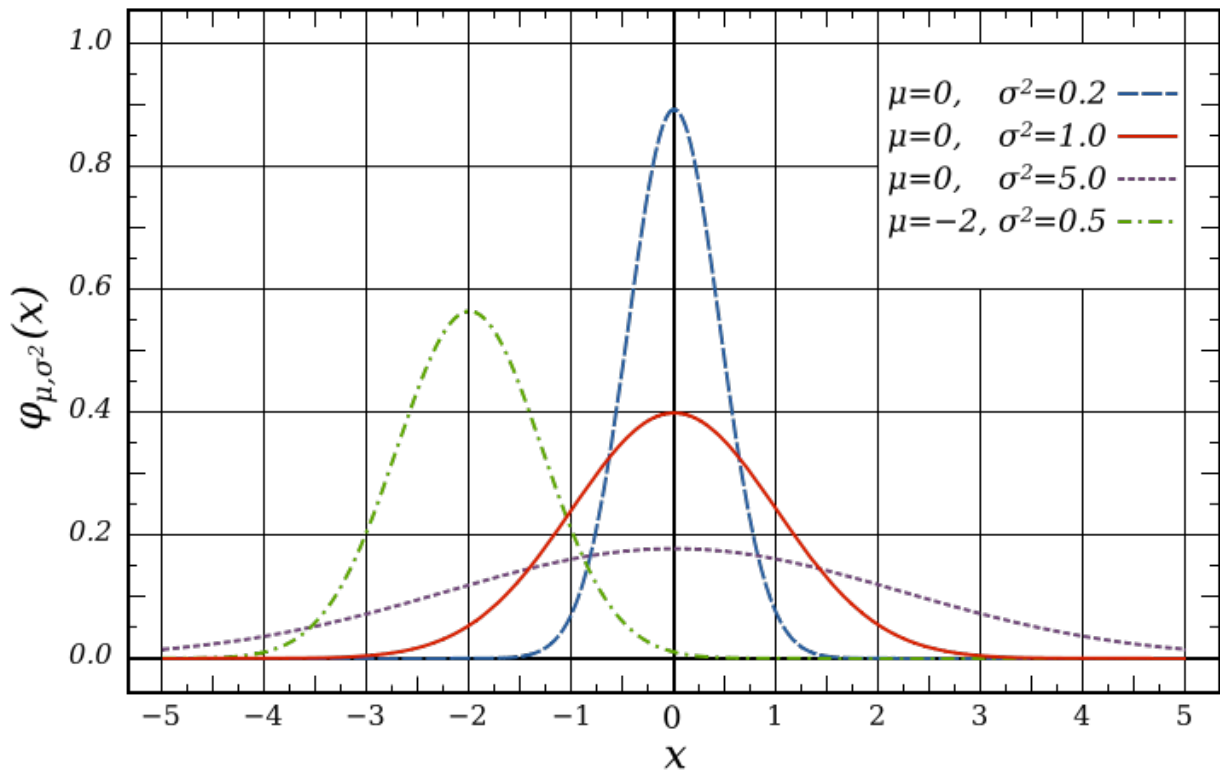
where

φ = probability density

μ = average

and the other variables are as defined in the above two sections.

The above PDF equation gives graphs, depending on mean and variance, similar to those below.

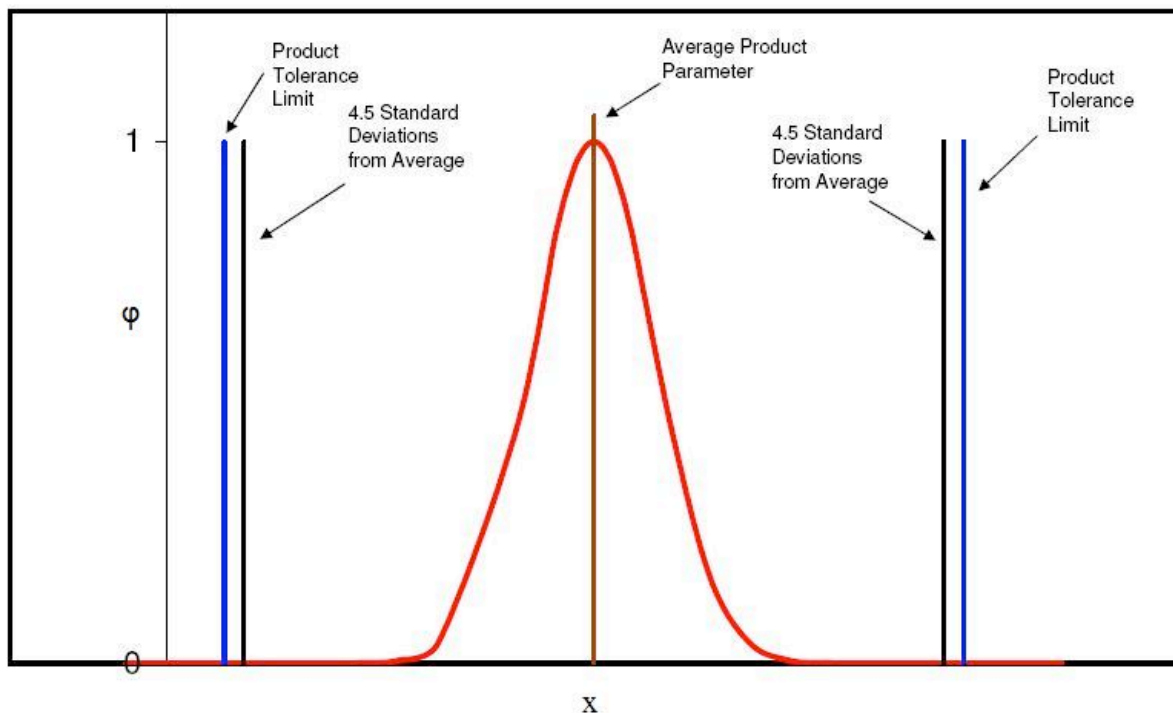


Above are 4 examples of different distributions given different values for mean and standard deviation. An important case is the standard normal distribution shown as the red line. The standard normal distribution is the normal distribution with a mean of 0 and a variance of 1. It is also important to note some special properties of probability density functions:

- symmetry about the mean, μ

- the mode and mean are both equal to the mean
- the inflection points always occur one standard deviation away from the mean, at $\mu - \sigma$ and $\mu + \sigma$

Suppose we have a process where we make a product of a certain concentration and we have good control over the process. After analyzing a set of data from a time period we see that we have a standard deviation of only 0.01 and our product concentration is required to be within 0.05. In order to say our product is essentially defect-free, 4.5 standard deviations away from the average must be less than our required product tolerance (± 0.05). In this case 4.5 standard deviations is equal to 0.045 and our product tolerance is 0.05. This is more easily seen graphically, as seen in the figure below.



As you can see 4.5 standard deviations on either side of the averages falls just slightly inside of the required tolerances for our product. This means that 99.997% of our product will fall inside of our product tolerances.

3.3.4 Analysis Methods

Two ways to analyze data for similarities (percent confidence) would be running a regression analysis or an analysis of variance (ANOVA). The difference between these two methods of analysis is that the ANOVA is for comparing independent groups such as 4 different reactor compositions that are supposed to make the same product (in reality this doesn't happen). A linear regression would be used for data that is dependent on each other, such as looking at the difference between slurry product permeabilities when a

one-reactant composition in the process is changed. The percent confidence is the same as the student's t-test, where you would want a t value (error) that is less than 0.05 to have statistically similar data.

One statistical program that is widely used in Six Sigma projects is MINITAB. MINITAB is similar to Microsoft Excel but has much greater statistical analysis capabilities. This program allows you to run linear regressions and ANOVAs by the click of an option. It also graphs not only in 2-D but 3-D as well and runs statistical analysis methods that are more in depth than those offered in Excel. MINITAB graphical and analytical tools can provide insight and information throughout the DMAIC process. MINITAB can be used to:

- **Identify** - visualize sources of variation and relationships among variables
- **Verify** - having statistical confidence behind conclusions

3.3.5 Key Tool Bar Descriptions on MINITAB

- File - typical of most programs - save, open, print, etc.
- Data - can subset data easily (stratification), transpose data, stack and unstack, convert text to numeric and back, code data
- Calc - calculator function - one time calc (doesn't update as you update your data)
- Stat - t-tests, regression, ANOVA, DOE, control charts, quality tools (Pareto and Gage R&R)
- Graph - plots, histogram, matrix plot
- Editor - find/replace (if you need to find items)
- Tools - options and links to some external tools
- Window - session window shows details on what you have open

MINITAB is a powerful tool to help us understand the language of measurement and the different uses of measurement system. Some unique features of MINITAB include: Measurement System Analysis (MSA) and the Gage Reproducibility and Repeatability Study (Gage R&R). These two complicated Six Sigma analysis can be accomplished within steps using MINITAB.

3.4 Statistical Process Control

Statistical process control (SPC) is an effective method of determining whether a system has deviated from its normal statistical behavior by the use of control charts. Walter Shewhart first pioneered the use of statistical techniques when studying variations in product quality and consistency at Bell Laboratories in the early 1920's. SPC utilizes statistical tools in the form of control charts (such as Shewhart charts) to observe the performance of the production process in order to predict significant deviations that may

result. Dr. Shewhart created concepts for statistical control and the basis for control charts through a series of carefully designed experiments. While he primarily drew from pure mathematical statistical theories, he understood that data from physical processes seldom produced a normal distribution curve (a Gaussian distribution, also known as a bell curve). Shewhart determined that every process displays variation: some display controlled variation that is natural to the process, while others display uncontrolled variation that is not always present in the process causal system.

SPC, most often used for manufacturing processes, is used in conjunction with experimental designs, process capability analyses, and process improvement plans to monitor product quality and maintain process targets. Six Sigma programs often depend on statistical process controls to provide their data with supportive information. If a process falls outside its preferred operating range, the statistical control can help you determine where and why the process failed.

Benefits of the SPC Method:

- Provides surveillance and feedback for keeping processes in control
- Signals when a problem with the process has occurred
- Detects assignable causes of variation
- Accomplishes process characterization
- Reduces need for inspection
- Monitors process quality
- Provides mechanism to make process changes and track effects of those changes
- Once a process is stable (assignable causes of variation have been eliminated), provides process capability analysis with comparison to the product tolerance

Capabilities of the SPC Method:

- All forms of SPC control charts
- Variable and attribute charts
- Average (X), Range (R), standard deviation (s), Shewhart, CuSum, combined Shewhart-CuSum, exponentially weighted moving average (EWMA)
- Selection of measures for SPC

- Process and machine capability analysis (Cp and Cpk)
- Process characterization
- Variation reduction
- Experimental design
- Quality problem solving
- Cause and effect diagrams

SPC is used to monitor the consistency of processes used to manufacture a product as designed. It aims to get and keep processes under control. No matter how good or bad the design, SPC can ensure that the product is being manufactured as designed and intended. Thus, SPC will not improve a poorly designed product's reliability, but can be used to maintain the consistency of how the product is made and, therefore, of the manufactured product itself and its as-designed reliability.

3.4.1 Methods and Control Charts

Control charts are the basis of statistical process controls methodologies, and are used to distinguish between random/uncontrollable variations and controlled/correctable variations in a system. Control chart detects and monitors process variation over time. It also plays a role as a tool for ongoing control of a process. There are many types of SPC control charts, though centering charts are used most often. The remainder of this article will focus on the different types of centering and dispersion charts. Figure 1 displays single point centering charts and Figure 2 displays subgroup sampling charts. Each figure has a brief description of the chart type within each of the two chart families (centering and dispersion). In the centering chart, the centerline is given by the average of the data samples, where as in the dispersion chart the centerline is the frequency distribution from that average.

Chart Family	Chart Type	Description
Centering Chart	Individual	Uses individual point values to provide a trend.
	Geometric Mean	Uses the geometric mean to provide exponential smoothing.
	Moving Average	Uses the moving average to remove noise and indicate an overall trend.
Dispersion Chart	Range (R chart)	Commonly called an R chart. Plots the range which is the difference between the highest and lowest sample in the range. The number of samples for calculating the range is configured by the user.

Figure1: Control chart types and descriptions for the single point sampling method(click to enlarge)[1].

Chart Family	Chart Type	Description
Centering Chart	Average (XBar)	Commonly called an XBar chart. Plots the average of data in the specified range. All subgroup samples are saved until the specified size is met. The average is then calculated, and the value is written to disk.
	Median	Plots the median value in the same manner as the average chart plots the average value.
Dispersion Chart	Range (R chart)	Commonly called an R chart. Plots the range which is the difference between the highest and lowest sample in the subgroup. Samples are collected until the subgroup is complete, and then sorted in order of size. The average or median is determined for the centering chart, and then the range is calculated.
	Range with Sigma	Plots the R values in the same manner as in the range chart, but the limits are calculated using a deviation value (sigma) that was entered during configuration.
	Root Mean Squared	Used for subgroups of 12 to 25 points. Uses the root mean square (RMS) to calculate the limits and centerline.
	Root Mean Squared with Sigma	Plots in the same manner as the RMS chart, but the limits and the centerline are calculated using a deviation value (sigma) that was entered during configuration.
	Standard Deviation	Plots the standard deviation of the subgroup points.

Figure2: Control chart types and descriptions for the subgroup sampling method(click to enlarge)[1].

A very useful type of centering chart is the Xbar chart, also known as the Shewhart chart mentioned earlier in the article. Figure 3 gives an example of an Xbar chart (on top), as well as an example of a dispersion chart (on bottom). The charts are used in combination with a system of rule based checks to determine whether the system is in statistical control. These rules can be seen in Figure 4 for both the single point centering and subgroup sampling methods. Using these rules, one can inspect a given chart over a period of time and determine whether the system is in control. If the system is not in control they must then check the controllable aspects of the system to see where the problem is occurring.

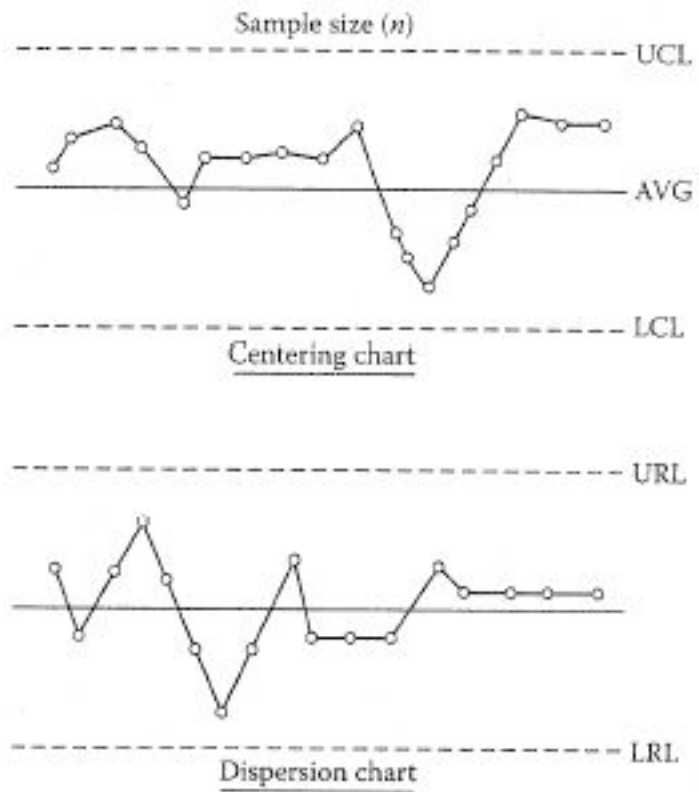


Figure3: The centering Xbar chart (Shewhart Chart) on top is used to determine whether the centering of the process is stable. The dispersion (R) chart on bottom is used to determine whether the spread of the process is stable (click to enlarge)[1].

Centering Chart Type	Criteria which show that the system is not in statistical control
Single Point Values	<ol style="list-style-type: none"> 1. Any of the points fall outside of the control limits. 2. Seven or more consecutive points fall on the same side of the centerline. 3. Ten or eleven consecutive points fall on the same side of the centerline. 4. Three or more consecutive points fall on the same side and all are located closer to the limit than the centerline.
Subgroup Sampling Method	<ol style="list-style-type: none"> 1. Any single subgroup is more than 3 standard deviations away from the centerline (or set point). 2. Two consecutive subgroup values are more than two standard deviations away from the centerline. 3. Three consecutive subgroup values are more than one standard deviation away from the centerline and on the same side of the centerline. 4. Two out of three consecutive subgroup values are more than two standard deviations away from the centerline, with all on the same side of the centerline. 5. Five consecutive subgroup values are on the same side of the centerline.

Figure 4: Table showing the criteria that indicate if a system is not in statistical control for different types of centering charts (click to enlarge)[1].

Note: We only need to see if any one of the criteria objectives are achieved to claim that the system is statistically out of control.

As can be seen from the figures above, the primary tool of SPC is the control chart. Several different descriptive statistics are used in control charts along with several different types of control charts that test for different causes of failure. Control charts are also used with product measurements to analyze process capability and for continuous process improvement efforts.

3.5 Worked out Example 1

KLMM Industries has recent data on their widget making process. The data is shown below. The allowable range of widget width is 19.5-22.5 cm.

Part Number	Width (cm)
1	21.25
2	21.33
3	20.89
4	20.33
5	21.12
6	20.98
7	21.44
8	21.22
9	20.84
10	20.99
11	21.19
12	21.04
13	20.79
14	20.89
15	21.38
16	20.91
17	20.18
18	21.31
19	20.96
20	20.85

- 1) Please from this data calculate the mean and write the mean with its allowable range?
- 2) Next calculate the standard deviation for this data.
- 3) Does this process fall within 4.5 standard deviations?
- 4) 6 standard deviations?

Solution:

$$\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i = \frac{x_1 + x_2 + \cdots + x_N}{N}$$

1)

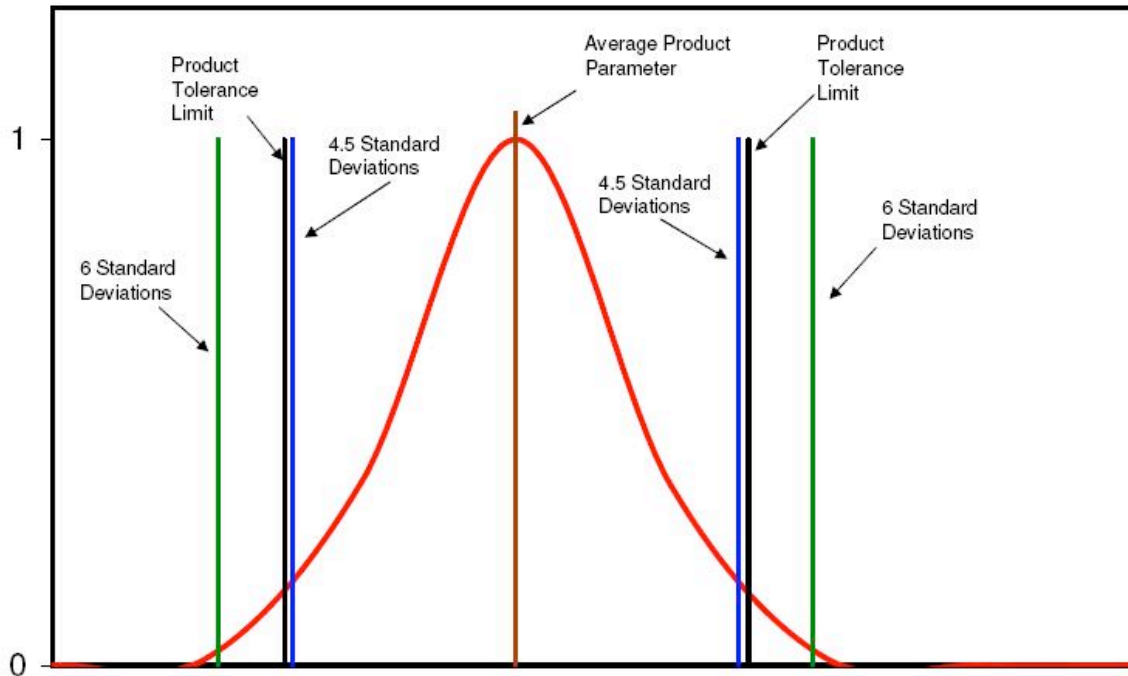
This is also calculated using the average function in excel, from this the average is calculated to be **20.9945**

$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})^2}$$

2)

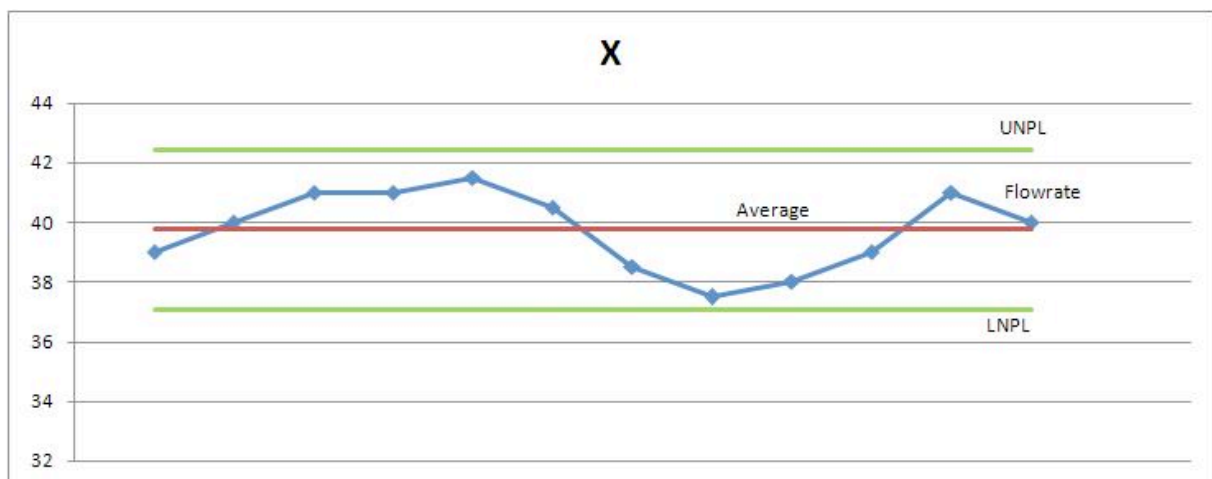
This is also calculated using the STDEV function in excel, from this the standard deviation is calculated to be **0.3206**

- 3) Yes
- 4) No



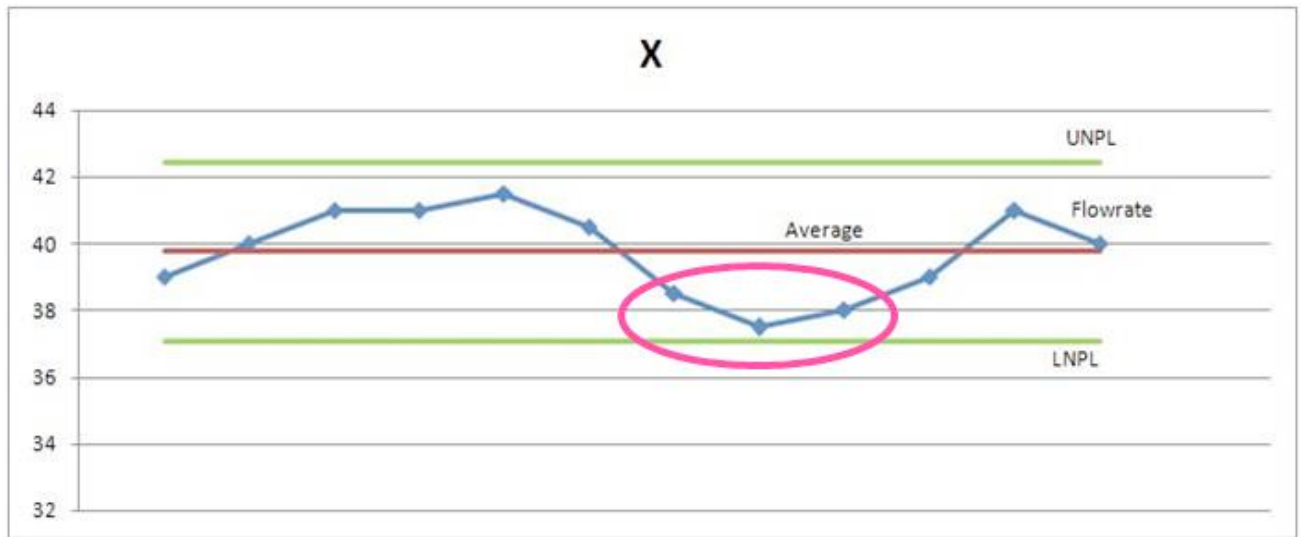
3.6 Worked out Example 2

A chemical engineer at Cool Processes Inc. is in charge of monitoring the flowrate of the cooling water for a reaction. He's new at the company and has asked you for your input. He says that the process is currently in statistical control and does not need to be changed. Below is the centering control chart he has made of the process. Do you agree or disagree with his opinion? Explain.



Solution:

Even though the process appears to be within a reasonable range of oscillation, and none of the data points are exceeding the process limitations, the system is not in statistical control. Centering (X) charts show that a process is not in statistical control if "three or more consecutive points fall on the same side of the centerline and all are located closer to the control limit than to the centerline." (Liptak 2006). The data points circled in the plot below violate that rule.



3.7 Worked Out Example 3

This example will also serve as a small tutorial for using Minitab.

ABC Production is coming out with a new product. One of the chemical engineers has hypothesized that the product thickness is dependent on the process temperature and the concentration of "compound Z." There are currently controls regulating the temperature between 77 and 80°C, and the concentration of Z between 0.0066 and .0073 g/L. Product specifications require that the thickness limits are 1.94 to 2.10 cm. You have been assigned the task of determining if these are good parameters to control. Use the data from random samples and use Minitab with linear regression to make your conclusion.

Sample No.	Thickness (cm)	Temperature (°C)	Concentration (g/L)
1	2.1740228	82	0.066
2	1.8774501	77	0.071
3	1.8774704	77	0.072
4	1.9762727	79	0.069
5	2.0266303	80	0.071
6	2.0994529	81	0.066
7	1.9468132	78	0.067
8	1.8972298	77	0.071
9	1.9169798	77	0.07
10	2.0692626	80	0.066
11	2.1292363	82	0.067
12	2.0479427	80	0.067
13	2.0479598	80	0.069
14	1.8972463	77	0.071
15	1.8774795	77	0.066

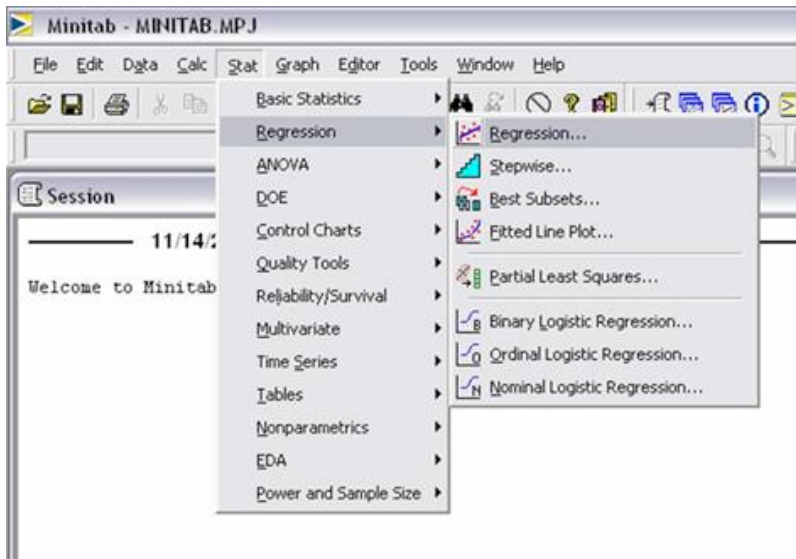
Solution: *Conclusion:* Temperature is much more influential on the thickness than the concentration, so it may be more worthwhile to refine the temperature control than to focus on the concentration controllers. Another option would be to investigate other system parameters (i.e., time in reactor, pressure, etc.) to see if they hold more influence on the thickness.

Using Minitab

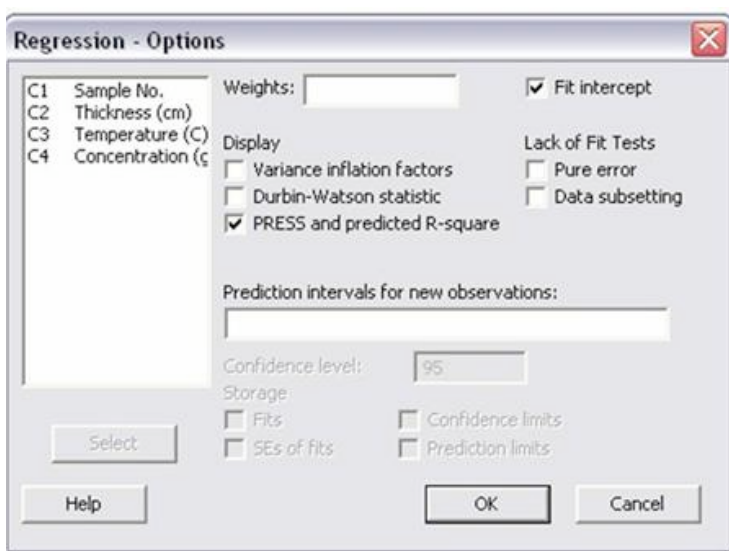
1) Open Minitab and input data

Worksheet 1 ***					
↓	C1	C2	C3	C4	C5
	Sample No.	Thickness (cm)	Temperature (C)	Concentration (g/L)	
1	1	2.17402	82	0.066	
2	2	1.87745	77	0.071	
3	3	1.87747	77	0.072	
4	4	1.97627	79	0.069	
5	5	2.02663	80	0.071	
6	6	2.09945	81	0.066	
7	7	1.94681	78	0.067	
8	8	1.89723	77	0.071	
9	9	1.91698	77	0.070	
10	10	2.06926	80	0.066	
11	11	2.12924	82	0.067	
12	12	2.04794	80	0.067	
13	13	2.04796	80	0.069	
14	14	1.89725	77	0.071	
15	15	1.87748	77	0.066	
16					

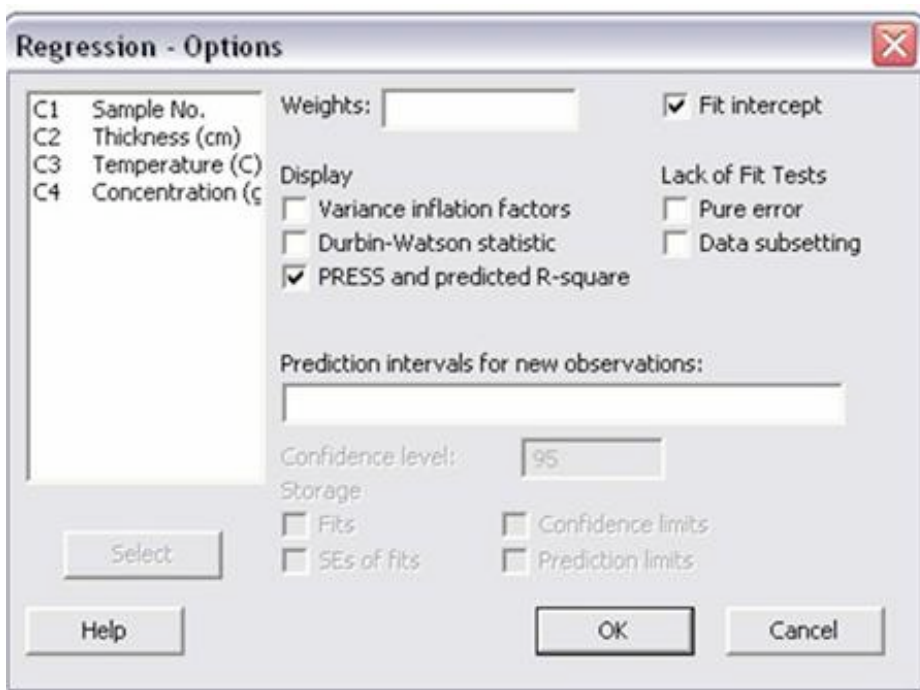
2) Select the “Regression” option from the “Stat” menu and the “Regression” tab



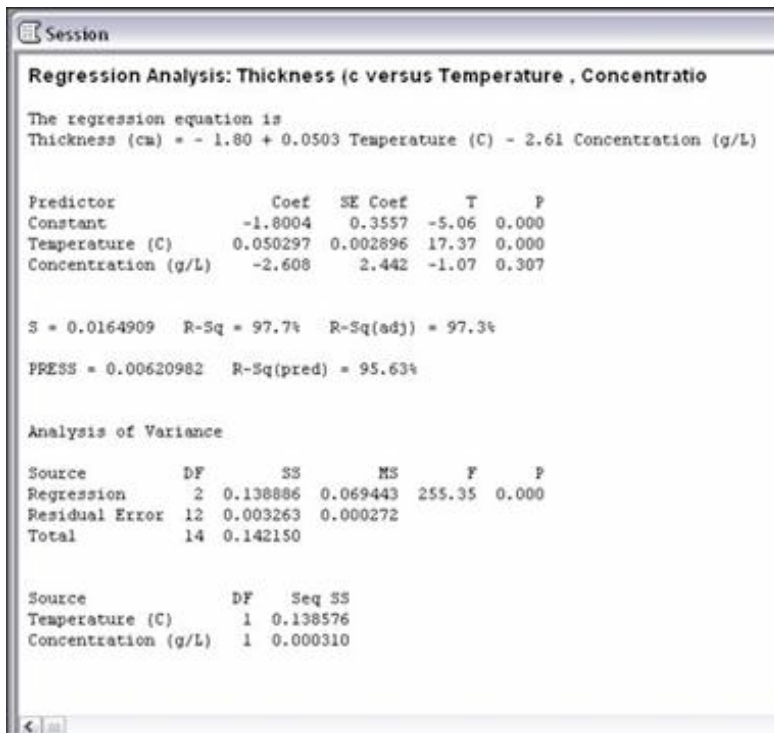
3)The regression window will open; add the “thickness” column for the response, and the Temperature and Concentration columns to the predictors.



4)Click the “Options” button and select “PRESS and predicted R-squared,” then click “OK” on both dialog boxes.



5)The results will appear in the session window:



Regression Analysis: Thickness (c versus Temperature , Concentratio

The regression equation is

Thickness (cm) = - 1.80 + 0.0503 Temperature (C) - 2.61 Concentration (g/L)

Predictor	Coef	SE Coef	T	P
Constant	-1.8004	0.3557	-5.06	0.000
Temperature (C)	0.050297	0.002896	17.37	0.000
Concentration (g/L)	-2.608	2.442	-1.07	0.307

S = 0.0164909 R-Sq = 97.7% R-Sq(adj) = 97.3%

PRESS = 0.00620982 R-Sq(pred) = 95.63%

Analysis of Variance

Source	DF	SS	MS	F	P
Regression	2	0.138886	0.069443	255.35	0.000
Residual Error	12	0.003263	0.000272		
Total	14	0.142150			

Source	DF	Seq SS
Temperature (C)	1	0.138576
Concentration (g/L)	1	0.000310

Interpreting the data

Some of the most important values in the returned data are the p values. These values test the null hypothesis that there is no effect by the inputs (concentration and temperature here) on the output (thickness). The lower the value of p, the more correlation there is between each variable and the result. In this case, the regression has a p value of 0 (under analysis of variance), so the model is significant and at least one of the coefficients is not zero. The p values in the predictor section show a zero value for Temperature (high correlation with thickness) but a 0.3 value for concentration (low correlation with thickness). This indicates that the concentration controller is not significant.

Next we will inspect the R² values. The R-Sq value of 97.7% indicates that the predictors (concentration and temperature) explain that percent of the variance in thickness. The adjusted value (97.3%) accounts for the number of predictors (here, 2) in the model. Since both are high, the model that is given at the beginning of the readout fits the data well.

The predicted R value is also important because it measures the amount of overfit of the model. If this value were not close to the R-Sq value, then the model would only be applicable for this set of data points but would probably not be accurate for any other combination of data points. Since the "R-Sq(pred)" value is close to the R-Sq value, this model is good.

3.8 Sage's Corner


More about Six Sigma...

<http://www.youtube.com/v/j10UMb7UxVc>

3.9 References

- [1]*Instrument Engineer's Handbook: Process Control and Optimization Vol.IV* (2005) edited by Liptak, Bela G. New York: Taylor and Francis Group
- [2]Perlmutter, Barry (2005) *A Six Sigma Approach to Evaluating Vacuum Filtration Technologies* BHS-Filtration INC.
- [3]Chambers & Wheeler *Understanding Statistical Process Control* Tennessee: SPC Press

Section 4. Bayes Rule, conditional probability, independence

Note:  [Video lecture](#) available for this section!

Authors: Brandon Kountz, Ashwini Miryala, Kyle Scarlett, Zachary Zell

Date created: 11/9/06

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

4.1 Introduction

Probability is the likely percentage of times an event is *expected* to occur if the experiment is repeated for a large number of trials. The probability of rare event is close to zero percent and that of common event is close to 100%. Contrary to popular belief, it is not intended to accurately describe a single event, although people may often use it as such. For example, we all know that the probability of seeing the head side of a coin, if you were to randomly flip it, is 50%. However, many people misinterpret this as 1 in 2 times, 2 in 4 times, 5 in 10 times, etc. of seeing the head side of the coin appear. So if you were to flip a coin 4 times and it came up heads every single time, is this 50% probability incorrect? No! It's just that your sample size is small. If you were to flip a coin 10,000 times, you would begin to see a more even distribution of heads and tails. (And if you don't, you should probably get a different coin.) Now, as engineers, even if we know the probability of the system, we don't have time to perform 10,000 trials to verify it. However, you'd be surprised at the small number of trials that are required to get an accurate representation of the system. The following sections describe the relationship between events and their probabilities. These relationships will then be used to describe another probability theory known as Bayes' Theorem.

4.2 Types of Probability

4.2.1 Combination

Combinatorics is the study of all the possible orderings of a finite number of objects into distinct groups. If we use combinatorics to study the possible combinations made from ordering the letters A, B, and C we can begin by counting out all the orderings

$\{(A B C), (A C B), (B C A), (B A C), (C B A), (C A B)\}$

giving us a total of 6 possible combinations of 3 distinct objects. As you can imagine the counting method is simple when the number of objects is small yet, when the number of objects being analyzed increases the method of counting by hand becomes increasingly tedious. The way to do this mathematically is using factorials. If you have n distinct objects then you can order them into $n!$ groups. Breaking the factorial down for our first

example we can say, first there are 3 objects to choose from, then 2, then 1 no matter which object we choose first. Multiplying the numbers together we get $3*2*1=3!$. Now consider finding all the possible orderings using all the letters of the alphabet. Knowing there are 26 letters in the English alphabet, the number of possible outcomes is simply $26!$, a number so large that counting would be difficult.

Now what if there are **n** objects and **m** that are equivalent and you wish to know the number of possible outcomes. By example imagine finding the number of distinct combinations from rearranging the letters of **PEPPER**. There are **6** letters, **2 Es** and **3 Ps** but only **1 R**. Starting with **6!** we need to divide by the repeat possible outcomes

$$(6!)/(3! * 2!) = (6 * 5 * 4 * 3!)/(3! * 2!) = (6 * 5 * 4)/(2) = 6 * 5 * 2 = 60$$

possible arrangements

where on the bottom, the **3!** is for the repeated **Ps** and the **2!** is for the repeated **Es**. **Note: You can cancel same integer factorials just like integers.**

The next topic of importance is choosing objects from a finite set. For example, if 4 hockey teams are made from 60 different players, how many teams are possible? This is found using the following relation:

$$(60 * 59 * 58 * 57)/(4 * 3 * 2 * 1) = 487,635$$

possible teams

Generally, this type of problem can be solved using this relation:

$$\binom{n}{r} = \frac{(n!)}{[(n - r)!r!]} \text{ called } n \text{ choose } r$$

n = number of objects r = number of groups

Using this equation, for the example above the math would be:

$$\binom{60}{4} = \frac{(60!)}{(56! * 4!)}$$

$$\frac{(60 * 59 * 58 * 57 * 56!)}{(56! * 4!)}$$

$$\frac{(60 * 59 * 58 * 57)}{(4!)} =$$

$$487,635$$

possible teams

4.2.2 Joint Probability

Joint probability is the statistical measure where the likelihood of two events occurring together and at the same point in time are calculated. Because joint probability is the probability of two events occurring at the same time, it can only be applied to situations where more than one observation can be made at the same time. When looking at only two random variables, A and B, this is called bivariate distribution, however this can be applied to numerous events or random variables being measured at one time (multivariate distribution). The probability of two events, A and B, both occurring is expressed as:

$$P(A, B)$$

Joint probability can also be expressed as:

$$P(A \cap B)$$

This is read as the probability of the intersection of A and B.

If A, B, and C are independent random variables, then

$$P(A, B, C) = P(A)P(B)P(C)$$

Example Problem

Two cards are selected randomly from a standard deck of cards (no jokers). Between each draw the card chosen is replaced back in the deck. What is the probability of choosing a four then a five? Let P(A) denote the probability that the first card is a four and P(B) denote the probability that the second card is a five.

Solution

If there are 52 cards in a standard card deck with 4 suits, then:

$$P(A) = 4/52 \text{ and } P(B) = 4/52$$

Knowing that the events are independent, each probability is multiplied together to find the overall probability for the set of events. Therefore:

$$P(A, B) = P(A) * P(B)$$

$$P(A, B) = (4/52) * (4/52)$$

$$P(A, B) = 1/169$$

The probability of choosing a four then a five from the deck with replacement is 1/169.

4.2.3 Conditional Probability

Conditional probability is the probability of one event occurring, given that another event occurs. The following expression describes the conditional probability of event A given that event B has occurred:

$$P(A|B)$$

If the events A and B are dependent events, then the following expression can be used to describe the conditional probability of the events:

$$P(A | B) = \frac{P(A, B)}{P(B)}$$

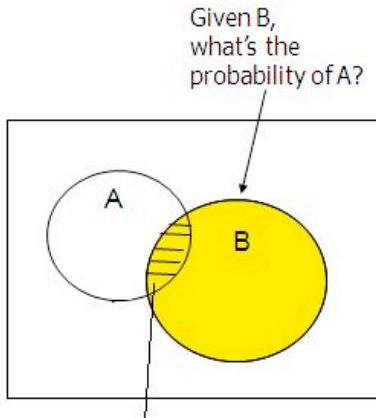
$$P(B | A) = \frac{P(A, B)}{P(A)}$$

This can be rearranged to give their joint probability relationship:

$$P(A, B) = P(B|A) * P(A) = P(A|B) * P(B)$$

This states that the probability of events A and B occurring is equal to the probability of B occurring given that A has occurred multiplied by the probability that A has occurred.

A graphical representation of conditional probability is shown below:



In a conditional probability problem, the sample space is "reduced" to the "space" of the given outcome (e.g. if given B, we now just care about the probability of A occurring "inside" of B)

Conditional probability is often derived from tree diagrams or contingency tables. Suppose you manufacture 100 piston shafts. Event A: feature A is not defective Event B: feature B is not defective

		Feature B: (Roundness)	
		Defective	Not Defective
Feature A (Surface Finish)	Defective	80	9
	Not Defective	6	5

$$P(A \text{ Not Def} \mid B \text{ Def}) = 6 / (80+6) = 0.0698$$

$$P(A \text{ Not Def} \mid B \text{ Not Def}) = 5 / (9+5) = 0.3571$$

Example Problem

Two fair, or unbiased, dice are tossed. Some example outcomes are (1,6) and (3,2). The probability of each possible outcome of the dice is 1/36. When the first die is rolled it results in a value of 2. Once the second die is rolled, what is the probability that the sum of the dice is 7?

Solution

Since it is known that the first value is 2, the possible combination of the two die are as follows:

(2,1) (2,2) (2,3) (2,4) (2,5) (2,6)

This results in six outcomes with equal probabilities since the second die is fair. Therefore, the conditional probability of the outcomes above is 1/6. The conditional probability of the remaining 30 combinations is 0 since the first die is not a 2 in these cases. Finally, since only one of these six outcomes can sum up to 7, (2,5), the probability is 1/6 for rolling a sum of 7 given the value of the first die is a 2.

Example Problem

The probability that a rare species of hamster will give birth to one male and one female is 1/3. The probability that the hamster will give birth to a male is 1/2. What is the probability that the hamster will give birth to a female knowing that the hamster has given birth to a male? Let A denote the probability of giving birth to a male and B denote the probability of giving birth to a female.

Solution

$P(A)$ = Probability of giving birth to a male

$P(B|A)$ = Probability of giving birth to a female given that birth of a male has already occurred

$P(A, B)$ = Probability of giving birth to one male and one female

These events are dependent so the following equation must be used:

$$P(A, B) = P(B|A) * P(A)$$

Rearranging this equation to find $P(B|A)$ would give:

$$P(B|A) = \frac{P(A, B)}{P(A)}$$

Plugging in the known values would give:

$$P(B|A) = (1/3)/(1/2)$$

$$P(B|A) = 2/3$$

Therefore, the probability of giving birth to a female, given that birth of a male already occurred is 2/3.

4.3 Law of Iterative Expectation

An important application of conditional probability is called the "Law of Iterative Expectation". Given simply, it is: $E[X] = E[E[X|Y]]$. If the random variable distribution of X is unknown, but we are given the distribution of the conditional variable of X , then by finding the expectation of the conditional variable twice, we can return to the expectation of the original random variable X . By looking at the expectation of the random variable X , we can deduce the distribution of the random variable X .

The Law of Iterative Expectation is quite useful in mathematics and often used to prove important relationships. Note the example below:

Use the Law of Iterative Expectation to find $\text{Var}[X]$ given only $X|Y$.

Solution

$$E[\text{Var}(X|Y)] = E[X^2] - E[(E[X|Y])^2]$$

$$\text{Var}(E[X|Y]) = E[(E[X|Y])^2] - (E[X])^2$$

$$E[\text{Var}(X|Y)] + \text{Var}(E[X|Y]) = E[X^2] - E[(E[X|Y])^2] + E[(E[X|Y])^2] - (E[X])^2$$

$$\text{Var}[X] = E[(E[X|Y])^2] + E[(E[X|Y])^2] \text{ (by definition)}$$

$$\text{thus } \text{Var}[X] = E[\text{Var}(X|Y)] + \text{Var}(E[X|Y])$$

4.3.1 Marginal Probability

Marginal probability is the unconditional probability of one event; in other words, the probability of an event, regardless of whether another event occurs or not. Finding the marginal probability of an event involves summing all possible configurations of the other event to obtain a weighted average probability. The marginal probability of an event A is expressed as:

$$P(A) = \sum_B P(A, B) = \sum_B P(A|B) * P(B)$$

The marginal probability (of A) is obtained by summing all the joint probabilities. Marginal probability can be used whether the events are dependent or independent. If the events are independent then the marginal probability is simplified to simply the probability. The following example will clarify this computation.

Example Problem 1

The joint probabilities for rain and wind are given in the following table

	No wind	Some wind	Strong wind	Storm
No rain	0.1	0.2	0.05	0.01
Light rain	0.05	0.1	0.15	0.04
Heavy rain	0.05	0.1	0.1	0.05

Marginal probability of no rain = sum of Joint probabilities = .1 + .2 + .05+.01 = .36

Similarly, marginal probability of light rain = .05+.1+.15+.04 = .34

Similarly, marginal probability of heavy rain = .3.

4.3.2 Marginalizing Out a Factor

In a system with two or more factors affecting the probability of the output of another factor, one of these initial factors can be marginalized out to simplify calculations if that factor is unknown.

For instance, consider a system where A and B both affect the output of C. If the condition of B is unknown but its probability is known, it can be marginalized out to put the system in terms of how only A affects C, using the equation below:

$$P(C|A) = \sum_i P(C|A, B_i)P(B_i)$$

Example Problem 2

The table below shows the probability of having a large, small or no sand storm, if there is high, medium or no wind, and depending on if there is rain. The next table shows the probability of rain.

		Sand Storm		
Wind Speed	Rain	P(Large)	P(small)	P(no)
High	yes	0.4	0.4	0.2
High	no	0.6	0.3	0.1
Medium	yes	0.1	0.3	0.6
Medium	no	0.15	0.35	0.5
Low	yes	0	0.1	0.9
Low	no	0	0.25	0.75

Rain	P
Yes	0.25
no	0.75

From this it is possible to calculate the probability of a large, small or no sand storm dependant just on the wind speed:

Similarly as to above:

$P(\text{Sandstorm Size}|\text{Wind Speed}) = P(\text{Sandstorm Size}|\text{Wind Speed, Rain}) * P(\text{Rain}) + P(\text{Sandstorm Size}|\text{Wind Speed, No Rain}) * P(\text{No Rain})$

		Sand Storm	
Wind Speed	P(Large)	P(small)	P(no)
High	$0.4 * 0.25 + 0.6 * 0.75 = 0.55$	$0.4 * 0.25 + 0.3 * 0.75 = 0.325$	$0.2 * 0.25 + 0.1 * 0.75 = 0.125$
Meduim	$0.1 * 0.25 + 0.15 * 0.75 = 0.1375$	$0.3 * 0.25 + 0.35 * 0.75 = 0.3375$	$0.6 * 0.25 + 0.5 * 0.75 = 0.525$
Low	$0 * 0.25 + 0 * 0.75 = 0$	$0.1 * 0.25 + 0.25 * 0.75 = 0.2125$	$0.9 * 0.25 + 0.75 * 0.75 = 0.7575$

4.4 Relationships Between Events

Knowing whether two events are independent or dependent can help to determine which type of probability (joint, conditional, or marginal) can be calculated. In some cases, the probability of an event must be calculated without knowing whether or not related events have occurred. In these cases, marginal probability must be used to evaluate the probability of an event.

4.4.1 Independence

If the two events are considered independent, each can occur individually and the outcome of one event does not affect the outcome of the other event in any way.

Let's say that A and B are independent events. We'll examine what this means for each type of probability.

Independence in Conditional Probability

Independent events technically do not have a conditional probability, because in this case, A is not dependent on B and vice versa. Therefore, the probability of A given that B has already occurred is equal to the probability of A (and the probability of B given A is equal to the probability of B). This can be expressed as:

$$\begin{aligned} P(A|B) &= P(A) \\ P(B|A) &= P(B) \end{aligned}$$

Independence in Joint Probability

Independent events can have a joint probability, even though one event does not rely on the other. For example, joint probability is used to describe an event such as tossing a coin. The outcome when the coin is tossed the first time is not related to the outcome when the same coin tossed a second time. To calculate the joint probability of a set of events we take the product of the individual probabilities of each event in the set. This can be expressed as:

$$P(A, B) = P(A)P(B)$$

Independent events can also occur in a case where there are three events. For example, if two dice are being rolled with a sum of 6 (Event A). Let event B represent that the first die is a 1 and let event C represent that the second rolled die is a 5. To prove if these events are independent, the following relation is considered:

$$P(A, B, C) = P(A)P(B)P(C)$$

$$P(A, B) = P(A)P(B)$$

$$P(A, C) = P(A)P(C)$$

$$P(B, C) = P(B)P(C)$$

If any of these relations are false than the event is not independent. When considering events of more than three, the same relation would follow but with an additional relation to event D.

4.4.2 Dependence

If the two events are considered dependent, then the outcome of the second event depends on the probability of the first event. The probabilities of the individual events must be analyzed with conditional probability.

Let's now say that A and B are dependent events. We'll examine what this means for each type of probability.

Dependence in Conditional Probability

Conditional probability only applies to dependent events. In other words, A must depend on B in order to determine the probability of A occurring given that B has already occurred. Therefore, for dependent events A and B, one can just apply the equations as seen in the conditional probability section.

$$P(A|B) = \frac{P(A, B)}{P(B)}$$

$$P(B|A) = \frac{P(A, B)}{P(A)}$$

Dependence in Joint Probability

Joint probability can also be calculated for dependent events. For example, dependent joint probability can be used to describe cards being drawn from a deck without replacing the cards after each consecutive drawing. In this case, the probability of A and B happening is more complex, since the probability of the B happening depends on the probability of A happening. It can be expressed as:

$$P(A, B) = P(A)P(B|A)$$

Note that this equation is found by rearranging the conditional probability equation.

4.5 Bayes' Theorem

Most probability problems are not presented with the probability of an event "A," it is most often helpful to condition on an event A." At other times, if we are given a desired outcome of an event, and we have several paths to reach that desired outcome, Baye's Theorem will demonstrate the different probabilities of the pathes reaching the desired outcome. Knowing each probability to reach the desired outcome allows us to pick the best path to follow. Thus, Baye's Theorem is most useful in a scenario of which when given a desired outcome, we can condition on the outcome to give us the separate probabilities of each condition that lead to the desired outcome.

The following is Bayes' Theorem:

$$P(B_j|A) = \frac{P(A|B_j)P(B_j)}{\sum_j P(A|B_j) P(B_j)}$$

Where

$$P(A|B_j) = \text{probability of A conditioned on } B_j$$

$$\sum_j P(A|B_j) P(B_j) = \text{the law of total probability}$$

4.5.1 Derivation of Bayes' Theorem

The derivation of Bayes' theorem is done using the third law of probability theory and the law of total probability.

Suppose there exists a series of events: B_1, B_2, \dots, B_n and they are mutually exclusive; that is, $B_1 \cap B_2 \cap \dots \cap B_n = 0$

This means that only one event, B_j , can occur. Taking an event "A" from the same sample space as the series of B_i , we have:

$$A = \cup_j AB_j$$

Using the fact that the events AB_i are mutually exclusive and using the third law of probability theory:

$$P(A) = \sum_j P(AB_j)$$

Conditioning on the above probability, the result below is also called "the law of total probability"

$$P(A) = \sum_j P(A | B_j)P(B_j)$$

Using the definition of conditional probabilities:

$$P(B_j|A) = \frac{P(A|B_j)P(B_j)}{P(A)}$$

Putting the above two equations together, we have the Baye's Theorem:

$$P(B_j|A) = \frac{P(A|B_j)P(B_j)}{\sum_j P(A|B_j) P(B_j)}$$

4.5.2 Real world/Chemical Applications

Bayes' rule can be used to predict the probability of a cause given the observed effects. For example, in the equation assume B represents an underlying model or hypothesis and A represents observable consequences or data. So,

$$P(data|model) = \frac{P(model|data) * P(data)}{P(model)}$$

Where

$P(\text{data}|\text{model})$: probability of obtaining observed data given certain model

$P(\text{model}|\text{data})$: probability that certain model gave rise to observed data

$P(\text{model})$: probability of occurrence of the model prior to taking the data into account

Another application: Bayes' rule estimation is used to identify species in single molecule Fluorescence microscopy. More information can be found on [\[1\]](#)

4.5.3 Underlying Principles and Significance of Bayes' Rule

As stated previously Bayes' Rule allows for changing the probability of an event based on new information about existing knowledge or expertise. For example, in the previous subsection the probability of the occurrence of the model, $P(\text{model})$, would be obtained through many trials conducted previously and thus be considered existing knowledge. The probability of the data, $P(\text{data})$, would then be considered new information. Bayes' Rule essentially uses this new information to upgrade the existing knowledge and then determine the probability of the new information based on the upgraded existing knowledge. Traditional, or Frequentist, statistics would differ from Bayesian statistics by comparing $P(\text{data})$ to $P(\text{model})$ and determine, with 95% confidence, if $P(\text{data})$ is statistically significant to $P(\text{model})$.

Bayesian theory is being used by many companies and institutions to better classify errors and calculate uncertainty. It has proven to perform better than averaging techniques and is used in safety systems as well as computing end states. A few web sites below provide a breadth of information regarding the use of Bayesian statistics.

<http://drambuie.lanl.gov/~bayes/tutorial.htm> - Virtually no probability background is required to understand this article

<http://aiche.com/aiche/2006/techprogram/P69620.HTM>

http://www.sciencedirect.com/science?_obArticleURL

<http://www.dct.tudelft.nl/~verheijen/research/Uerheijen2003a.pdf>

4.6 Worked out Example 1

A true-false question is posed to a team of two ChE students on a quiz show. Both the students will, independently, choose their answer. Team member A knows the correct

answer, while team member B has the wrong answer. Use Marginal Probability to find the best strategy for the team?

4.6.1 Strategy 1

Choose one of them and let that person answer the question without knowing what the other student thought was the correct answer.

4.6.2 Strategy 2

Have both students consider the question and then give the common answer they agree on, or if they disagree, flip a coin to determine which answer to give.

4.6.3 Solution

Strategy 1

We will break down the different possibilities for this situation using the following variables:

C is the event that they submit the correct answer

A is the event that student A is chosen to answer

B is the event that student B is chosen to answer

$$P(C) = P(C, A) + P(C, B) = P(C|A) * P(A) + P(C|B) * P(B)$$

$$P(A) = P(B) = 1/2$$
 because there is an equal chance for either student to be chosen

$$P(C|A) = 1$$
 because student A is correct

$$P(C|B) = 0$$
 because student B is incorrect

$$P(C) = 1 * (1/2) + 0 * (1/2) = 1/2$$

$$P(C) = 1/2$$

Strategy 2

Since we know the students will disagree on their answer, they must flip a coin in order to decide. Therefore the probability is simply 1/2.

Both strategies provide a 1/2 chance in getting the answer correct, therefore they are equally accurate.

4.7 Worked out Example 2

A biologist is studying human cells that are virally infected by a deadly disease, which is present among .01% of the population. When preparing a sample, he mishandles a vial with infected cells and it ends up breaking, cutting through the protective gloves and cutting his hand. Even though he immediately washed his hands, he is worried that he has contracted the disease. Luckily for him, his laboratory has been developing a test for the disease and has performed trials with infected and non-infected patients alike. So, the test is administered and to the biologist's surprise, the test turns up negative. He becomes relieved, but then remembers that the test does not always work, so he decides to use Bayes' Rule to determine the probability that he has the disease. He goes into the laboratory database to get all of the data he needs to determine this.

He wants to determine the probability that he tested negative but is actually positive for the disease, or $P(DIS_{pos}|TEST_{neg})$

From Bayes' Rule,

$$P(DIS_{pos}|TEST_{neg}) = \frac{P(TEST_{neg}|DIS_{pos}) * P(DIS_{pos})}{P(TEST_{neg})}$$

To find the overall probability of a negative test, you need to use marginal probability and sum over all events, that is both having the disease and not having the disease:

$$P(TEST_{neg}) = P(TEST_{neg}|DIS_{pos}) * P(DIS_{pos}) + P(TEST_{neg}|DIS_{neg}) * P(DIS_{neg})$$

Assuming that all people without the virus do not test positive, and that 99% of infected patients test positive, what is the probability that the biologist is actually positive with the disease?

$$P(TEST_{neg}) = .01 * .0001 + 1 * .9999 = 0.999901$$

$$P(DIS_{pos}|TEST_{neg}) = \frac{(0.01 * 0.0001)}{.999901} = 1.0001E - 06$$

The chance that the biologist has the disease is roughly one in a million.

4.8 Worked out Example 3

If there are 52 cards in a standard card deck with 4 suits, then the probability of picking a card of a particular numerical (5 of spades, 5 of clubs, 5 of diamonds, 5 of hearts) value is $P(A) = 1/13$. The probability associated with any subsequent draw of a card is only dependent upon the remaining cards in the deck. If the same card is taken from the deck four times in a row and not returned (resulting in no fives in the deck), what is the probability of picking a four, returning it to the deck and then picking a 6.

This is an example of independence in joint probability.

The probability of each independent event is given below.

$$P(4) = 4/48$$

$$P(6) = 4/48$$

To find the probability of both events happening, one must multiply the probability of each independent event.

$$P = P(4) * P(6) = 1/144.$$

4.9 Worked out Example 4

A Gambler has two coins in his pocket, a fair coin and a two-headed coin. He picks one at random from his pocket, flips it and gets heads. (a) What is the probability that he flipped the fair coin? (b) If he flips the same coin a second time and again gets heads, what is the probability that he flipped the fair coin?

Call F the event he picked the fair coin and B the event he picked the biased coin. There are two coins in his pocket so the probability of picking the either coin is 0.50. Let H₁ be the event "the first flip is heads" and H₂ be the event "the second flip is heads".

For (a)

$$P(F|H_1) = P(H_1|F) * \frac{P(F)}{P(H_1)} = \frac{P(H_1|F)P(F)}{P(H_1|F)P(F) + P(H_1|B)P(B)}$$

Where $P(H_1|F) = 1/2$ and $P(H_1|B) = 1$, so

$$P(F|H_1) = \frac{1/2 * 1/2}{1/2 * 1/2 + 1 * 1/2} = \frac{1}{3}$$

For (b)

This question is solved in the same way as (a)

$$P(F|H_1 \cap H_2) = \frac{P(H_1 \cap H_2|F)P(F)}{P(H_1 \cap H_2|F)P(F) + P(H_1 \cap H_2|B)P(B)} = \frac{1/8}{1/8 + 1/2} = \frac{1}{5}$$

4.10 Worked out Example 5

Consider the situation where you're going on a bus tour of the local refinery and the person you like has asked you to find them because they're going to save a seat for you. There are three buses that are taking the ChemE students on the tour and you need to immediately decide which is the best one to get on. The first bus has room for 25 students, the second has space for 45 and the third has space for 55. To decide which is the best bus, find the **expected value** (or expected number) of passengers for the bus your friend is on, given the following expression:

$$E(X) = \sum_i x_i p(x_i)$$

The expected value of X is the sum of the products of x_i multiplied by $p(x_i)$

$$E(\text{passengers}) = (25*(1/3) + 45*(1/3) + 55*(1/3)) = (25 + 45 + 55)/3 = 135/3 = 45$$

Therefore, the expected number of passengers for the bus your friend is on equals the sum of the passengers on each bus divided by the total number of buses, assuming equal probability of your friend being on any of the 3 buses. This shows that you should get on the second bus in order to find your friend.

Alternative method Now consider that you don't want to give each bus an equal chance that your friend is on it. The objective in this alternative method is to find the probability that your friend is on each bus.

$$P(\text{Bus1}) = 25/135 = 0.185185$$

$$P(\text{Bus2}) = 45/135 = 0.333333$$

$$P(\text{Bus3}) = 55/135 = 0.407407$$

Now using the new probability we can find a more accurate expected number of passengers on the bus your friend is on.

$$E(\text{passengers}) = 25 * (0.18518) + 45 * (0.333333) + 55 * (0.407407) = 42.037$$

This shows a similar result, you should get on the second bus, but the probabilities associated to each bus are adjusted to account for the number of passengers on each one.

4.11 Multiple Choice Question 1

What is conditional probability?

- a. A way of calculating probability under varying conditions
- b. The probability of an event, given that another event has occurred
- c. Probability that can not be determined
- d. Probability that is always very small

4.12 Multiple Choice Question 2

In Bayes' rule, what is P(A)?

- a. The probability of A
- b. The probability of A, given B
- c. The probability of B, given A
- d. The marginal probability of A

Answer: A

4.13 Multiple Choice Question 3

Which type of probability does this statement infer to: What is the probability that a temperature sensor fails given that a flow sensor has failed?

- a. Joint Probability
- b. Conditional Probability
- c. Marginal Probability

Answer: B

4.14 Sage's Corner

An example of Bayes' Rule, illustrated by the Monty Hall problem:

<http://video.google.com/googleplayer.swf?docId=6163049683683917121>

A copy of the slides can be found here: [Unnarrated Slides](#)

A brief description of Bayes' Rule, with two examples:

<http://video.google.com/googleplayer.swf?docId=1332101152106816762>

An unnarrated copy of the slides can be found here: [Bayes Rule](#)

4.15 References

- Ross, Sheldon, A First Course in Probability: Seventh Edition, 2006, Pearson Education, Inc.
- Woolf, Keating, Burge, Yaffe, Statistics and probability primer for computational biologists, spring 2004, MIT.
- [\[2\]](#) University of Oslo
- [\[3\]](#), Wikipedia

Section 5. Bayesian network theory

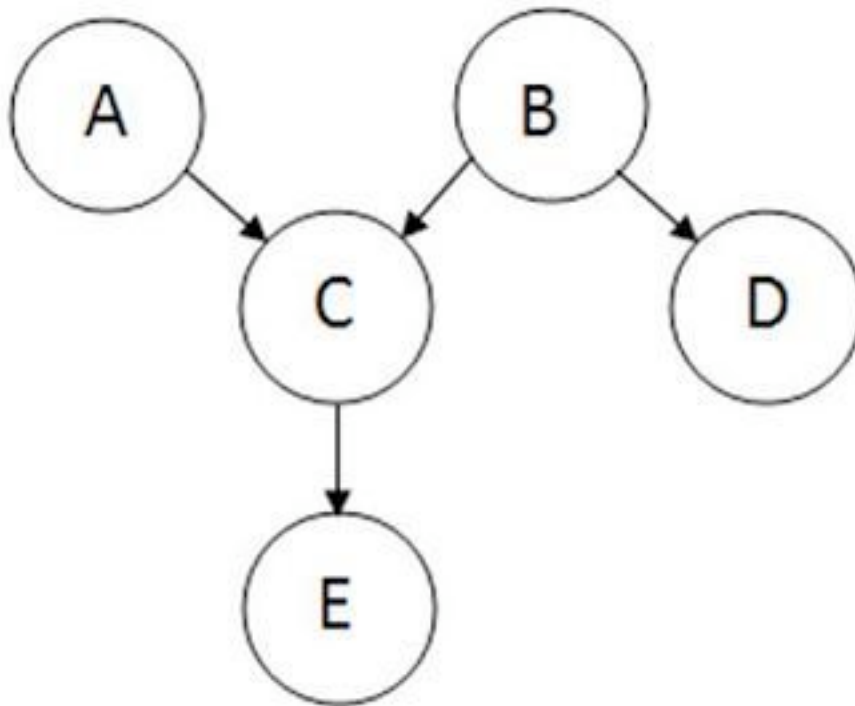
Note: [Video lecture](#) available for this section!

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5.1 Introduction

Bayesian network theory can be thought of as a fusion of [incidence diagrams](#) and [Bayes' theorem](#). A Bayesian network, or belief network, shows conditional probability and causality relationships between variables. The probability of an event occurring given that another event has already occurred is called a conditional probability. The probabilistic model is described qualitatively by a directed acyclic graph, or DAG. The vertices of the graph, which represent variables, are called nodes. The nodes are represented as circles containing the variable name. The connections between the nodes are called arcs, or edges. The edges are drawn as arrows between the nodes, and represent dependence between the variables. Therefore, for any pairs of nodes indicate that one node is the parent of the other so there are no independence assumptions. Independence assumptions are implied in Bayesian networks by the absence of a link. Here is a sample DAG:



The node where the arc originates is called the parent, while the node where the arc ends is called the child. In this case, A is a parent of C, and C is a child of A. Nodes that can be reached from other nodes are called descendants. Nodes that lead a path to a specific node are called ancestors. For example, C and E are descendants of A, and A and C are ancestors of E. There are no loops in Bayesian networks, since no child can be its own ancestor or descendent. Bayesian networks will generally also include a set of probability tables, stating the probabilities for the true/false values of the variables. The main point of Bayesian Networks is to allow for probabilistic inference to be performed. This means that the probability of each value of a node in the Bayesian network can be computed when the values of the other variables are known. Also, because independence among the variables is easy to recognize since conditional relationships are clearly defined by a graph edge, not all joint probabilities in the Bayesian system need to be calculated in order to make a decision.

5.2 Joint Probability Distributions

Joint probability is defined as the probability that a series of events will happen concurrently. The joint probability of several variables can be calculated from the product of individual probabilities of the nodes:

$$P(X_1, \dots, X_n) = \prod_{i=1}^n P(X_i \mid \text{parents}(X_i))$$

Using the sample graph from the introduction, the joint probability distribution is:

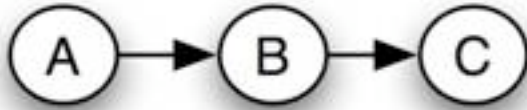
$$P(A, B, C, D, E) = P(A)P(B)P(C|A, B)P(D|B)P(E|C)$$

If a node does not have a parent, like node A, its probability distribution is described as unconditional. Otherwise, the local probability distribution of the node is conditional on other nodes.

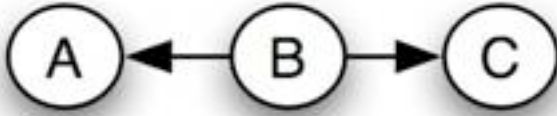
5.3 Equivalence Classes

Each Bayesian network belongs to a group of Bayesian networks known as an equivalence class. In a given equivalence class, all of the Bayesian networks can be described by the same joint probability statement.

As an example, the following set of Bayesian networks comprises an equivalence class:



Network 1



Network 2



Network 3

The causality implied by each of these networks is different, but the same joint probability statement describes them all. The following equations demonstrate how each network can be created from the same original joint probability statement:

Network 1

$$P(A,B,C) = P(A) * P(B | A) * P(C | B)$$

Network 2

$$P(A,B,C) = P(A) * P(B | A) * P(C | B)$$

$$P(A, B, C) = P(A) * \frac{P(A|B) * P(B)}{P(A)} * P(C|B)$$

$$P(A,B,C) = P(A | B) * P(B) * P(C | B)$$

Network 3

Starting now from the statement for Network 2

$$P(A,B,C) = P(A|B) * P(B) * P(C|B)$$

$$P(A, B, C) = P(A|B) * P(B) * \frac{P(B|C) * P(C)}{P(B)}$$

$$P(A,B,C) = P(A|B) * P(B|C) * P(C)$$

All substitutions are based on Bayes rule.

The existence of equivalence classes demonstrates that causality cannot be determined from random observations. A controlled study – which holds some variables constant while varying others to determine each one’s effect – is necessary to determine the exact causal relationship, or Bayesian network, of a set of variables.

5.4 Bayes' Theorem

Bayes' Theorem, developed by the Rev. Thomas Bayes, an 18th century mathematician and theologian, it is expressed as:

$$P(H|E, c) = \frac{P(H|c) \cdot P(E|H, c)}{P(E|c)}$$

where we can update our belief in hypothesis H given the additional evidence E and the background information c. The left-hand term, P(H|E,c) is known as the "posterior probability," or the probability of H after considering the effect of E given c. The term P(H|c) is called the "prior probability" of H given c alone. The term P(E|H,c) is called the "likelihood" and gives the probability of the evidence assuming the hypothesis H and the background information c is true. Finally, the last term P(E|c) is called the "expectedness", or how expected the evidence is given only c. It is independent of H and can be regarded as a marginalizing or scaling factor.

It can be rewritten as

$$P(E|c) = \sum_i P(E|H_i, c) \cdot P(H_i|c)$$

where *i* denotes a specific hypothesis H_i , and the summation is taken over a set of hypotheses which are mutually exclusive and exhaustive (their prior probabilities sum to 1).

It is important to note that all of these probabilities are conditional. They specify the degree of belief in some proposition or propositions based on the assumption that some other propositions are true. As such, the theory has no meaning without prior determination of the probability of these previous propositions.

5.5 Bayes' Factor

In cases when you are unsure about the causal relationships between the variables and the outcome when building a model, you can use Bayes Factor to verify which model describes your data better and hence determine the extent to which a parameter affects the outcome of the probability. After using Bayes' Theorem to build two models with different variable dependence relationships and evaluating the probability of the models based on the data, one can calculate Bayes' Factor using the general equation below:

$$BF = \frac{p(model1|data)}{p(model2|data)} = \frac{\frac{p(data|model1)p(model1)}{p(data)}}{\frac{p(data|model2)p(model2)}{p(data)}} = \frac{p(data|model1)}{p(data|model2)}$$

The basic intuition is that prior and posterior information are combined in a ratio that provides evidence in favor of one model versus the other. The two models in the Bayes' Factor equation represent two different states of the variables which influence the data. For example, if the data being studied are temperature measurements taken from multiple sensors, Model 1 could be the probability that all sensors are functioning normally, and Model 2 the probability that all sensors have failed. Bayes' Factors are very flexible, allowing multiple hypotheses to be compared simultaneously.

BF values near 1, indicate that the two models are nearly identical and BF values far from 1 indicate that the probability of one model occurring is greater than the other. Specifically, if BF is > 1, model 1 describes your data better than model 2. IF BF is < 1, model 2 describes the data better than model 1. In our example, if a Bayes' factor of 5 would indicate that given the temperature data, the probability of the sensors functioning normally is five times greater than the probability that the sensors failed. A table showing the scale of evidence using Bayes Factor can be found below:

scale of evidence for Bayes factors	
Bayes factor	Interpretation
B.F. < 1/10	Strong evidence for Model 2
1/10 < B.F. < 1/3	Moderate evidence for Model 2
1/3 < B.F. < 1	Weak evidence for Model 2
1 < B.F. < 3	Weak evidence for Model 1
3 < B.F. < 10	Moderate evidence for Model 1
B.F. > 10	Strong evidence for Model 1

Although Bayes' Factors are rather intuitive and easy to understand, as a practical matter they are often quite difficult to calculate. There are alternatives to Bayes Factor for model assessment such as the Bayesian Information Criterion (BIC).

The formula for the BIC is:

$$-2 \cdot \ln p(x|k) \approx \text{BIC} = -2 \cdot \ln L + k \ln(n).$$

x = the observed data; n = the number of data points in x , the number of observations, or equivalently, the sample size; k = the number of free parameters to be estimated. If the estimated model is a linear regression, k is the number of regressors, including the constant; $p(x|k)$ = the likelihood of the observed data given the number of parameters; L = the maximized value of the likelihood function for the estimated model.

This statistic can also be used for non-nested models. For further information on Bayesian Information Criterion, please refer to:[\[1\]](#)

5.6 Advantages and Limitations of Bayesian Networks

The advantages of Bayesian Networks are as follows:

- Bayesian Networks visually represent all the relationships between the variables in the system with connecting arcs.
- It is easy to recognize the dependence and independence between various nodes.
- Bayesian networks can handle situations where the data set is incomplete since the model accounts for dependencies between all variables.
- Bayesian networks can map scenarios where it is not feasible/practical to measure all variables due to system constraints (costs, not enough sensors, etc.)
- Help to model noisy systems.
- Can be used for any system model - from all known parameters to no known parameters.

The limitations of Bayesian Networks are as follows:

- All branches must be calculated in order to calculate the probability of any one branch.
- The quality of the results of the network depends on the quality of the prior beliefs or model. A variable is only a part of a Bayesian network if you believe that the system depends on it.
- Calculation of the network is NP-hard (nondeterministic polynomial-time hard), so it is very difficult and possibly costly.
- Calculations and probabilities using Baye's rule and marginalization can become complex and are often characterized by subtle wording, and care must be taken to calculate them properly.

5.7 Inference

Inference is defined as the process of deriving logical conclusions based on premises known or assumed to be true. One strength of Bayesian networks is the ability for inference, which in this case involves the probabilities of unobserved variables in the

system. When observed variables are known to be in one state, probabilities of other variables will have different values than the generic case. Let us take a simple example system, a television. The probability of a television being on while people are home is much higher than the probability of that television being on when no one is home. If the current state of the television is known, the probability of people being home can be calculated based on this information. This is difficult to do by hand, but software programs that use Bayesian networks incorporate inference. One such software program, Genie, is introduced in [Learning and analyzing Bayesian networks with Genie](#).

5.8 Marginalization

Marginalization of a parameter in a system may be necessary in a few instances:

- If the data for one parameter (P1) depends on another, and data for the independent parameter is not provided.
- If a probability table is given in which P1 is dependent upon two other system parameters, but you are only interested in the effect of one of the parameters on P1.

Imagine a system in which a certain reactant (R) is mixed in a CSTR with a catalyst (C) and results in a certain product yield (Y). Three reactant concentrations are being tested (A, B, and C) with two different catalysts (1 and 2) to determine which combination will give the best product yield. The conditional probability statement looks as such:

$$P(R, C, Y) = P(R)P(C)P(Y|R, C)$$

The probability table is set up such that the probability of certain product yield is dependent upon the reactant concentration *and* the catalyst type. You want to predict the probability of a certain product yield given only data you have for catalyst type. The concentration of reactant must be marginalized out of $P(Y|R, C)$ to determine the probability of the product yield without knowing the reactant concentration. Thus, you need to determine $P(Y|C)$. The marginalization equation is shown below:

$$P(Y|C) = \sum_i P(Y|R_i, C)P(R_i)$$

where the summation is taken over reactant concentrations A, B, and C.

The following table describes the probability that a sample is tested with reactant concentration A, B, or C:

Reactant	P(Reactant)
A	0.2
B	0.5
C	0.3

This next table describes the probability of observing a yield - High (H), Medium (M), or Low (L) - given the reactant concentration and catalyst type:

Reactant	Catalyst	P(Y=H)	P(Y=M)	P(Y=L)
A	1	0.51	0.08	0.41
A	2	0.3	0.2	0.5
B	1	0.71	0.09	0.2
B	2	0.92	0.05	0.03
C	1	0.21	0.4	0.39
C	2	0.12	0.57	0.31

The final two tables show the calculation for the marginalized probabilities of yield given a catalyst type using the marginalization equation:

Catalyst	P(Y=H)	P(Y=M)	P(Y=L)
1	$0.2 \cdot 0.51 + 0.5 \cdot 0.71 + 0.3 \cdot 0.21$	$0.2 \cdot 0.08 + 0.5 \cdot 0.09 + 0.3 \cdot 0.4$	$0.2 \cdot 0.41 + 0.5 \cdot 0.2 + 0.3 \cdot 0.39$
2	$0.2 \cdot 0.3 + 0.5 \cdot 0.92 + 0.3 \cdot 0.12$	$0.2 \cdot 0.2 + 0.5 \cdot 0.05 + 0.3 \cdot 0.57$	$0.2 \cdot 0.5 + 0.5 \cdot 0.03 + 0.3 \cdot 0.31$

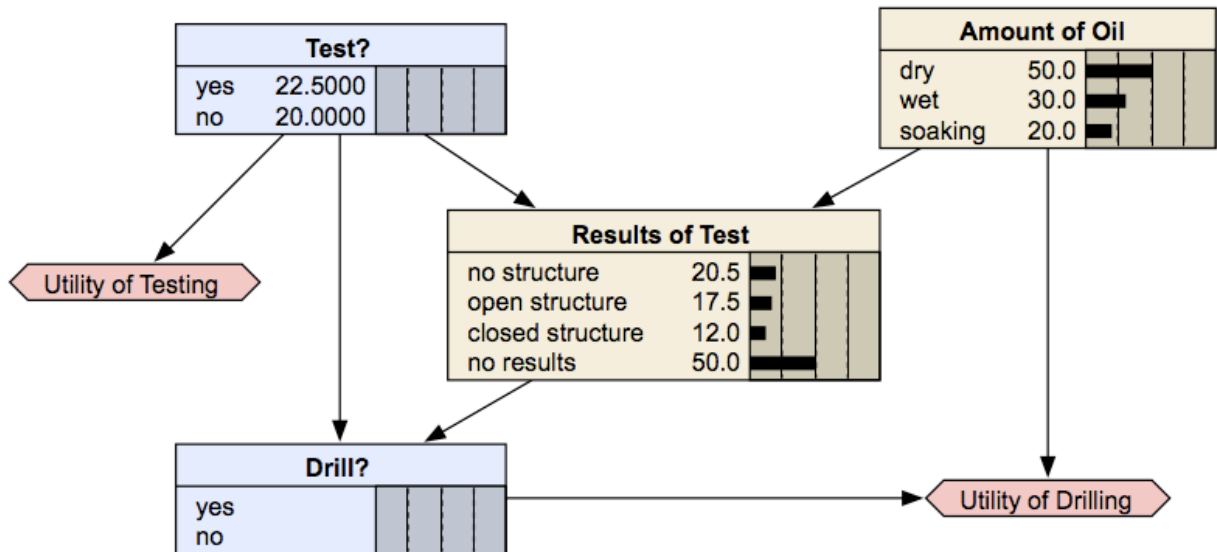
Catalyst	P(Y=H)	P(Y=M)	P(Y=L)
1	0.520	0.181	0.299
2	0.556	0.236	0.208

5.9 Dynamic Bayesian Networks

The static Bayesian network only works with variable results from a single slice of time. As a result, a static Bayesian network does not work for analyzing an evolving system that changes over time.

Below is an example of a static Bayesian network for an oil wildcatter:

Oil Wildcatter

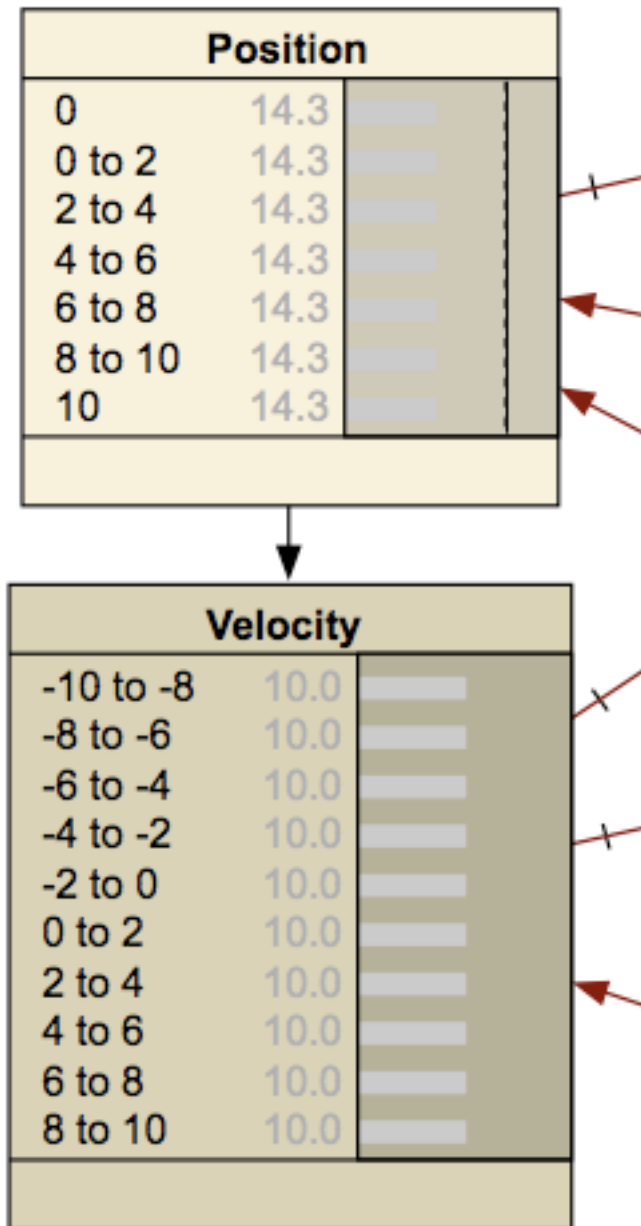


<http://www.norsys.com/netlibrary/index.htm>

An oil wildcatter must decide either to drill or not. However, he needs to determine if the hole is dry, wet or soaking. The wildcatter could take seismic soundings, which help determine the geological structure at the site. The soundings will disclose whether the terrain below has no structure, which is bad, or open structure that's okay, or closed structure, which is really good. As you can see this example does not depend on time.

Dynamic Bayesian network (DBN) is an extension of Bayesian Network. It is used to describe how variables influence each other over time based on the model derived from past data. A DBN can be thought as a [Markov chain model](#) with many states or a discrete time approximation of a differential equation with time steps.

An example of a DBN, which is shown below, is a frictionless ball bouncing between two barriers. At each time step the position and velocity changes.



<http://www.norsys.com/netlibrary/index.htm>

An important distinction must be made between DBNs and Markov chains. A DBN shows how variables affect each other over time, whereas a Markov chain shows how the state of the entire system evolves over time. Thus, a DBN will illustrate the probabilities of one variable changing another, and how each of the individual variables will change over time. A Markov chain looks at the state of a system, which incorporates the state of each individual variable making up the system, and shows the probabilities of the system changing states over time. A Markov chain therefore incorporates all of the variables present in the system when looking at how said system evolves over time. Markov chains can be derived from DBNs, but each network represents different values and probabilities.

There are several advantages to creating a DBN. Once the network has been established between the time steps, a model can be developed based on this data. This model can then be used to predict future responses by the system. The ability to predict future responses can also be used to explore different alternatives for the system and determine which alternative gives the desired results. DBN's also provide a suitable environment for model predictive controllers and can be useful in creating the controller. Another advantage of DBN's is that they can be used to create a general network that does not depend on time. Once the DBN has been established for the different time steps, the network can be collapsed to remove the time component and show the general relationships between the variables.

A DBN is made up with interconnected time slices of static Bayesian networks. The nodes at certain time can affect the nodes at a future time slice, but the nodes in the future can not affect the nodes in the previous time slice. The causal links across the time slices are referred to as temporal links, the benefit of this is that it gives DBN an unambiguous direction of causality.

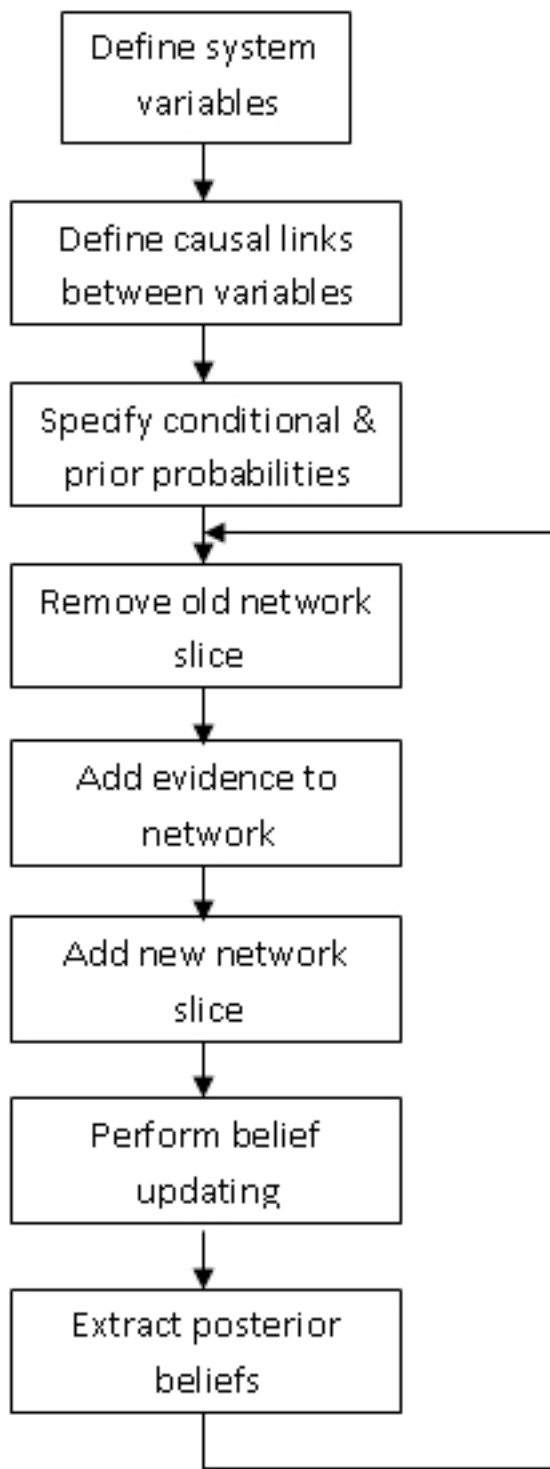
For the convenience of computation, the variables in DBN are assumed to have a finite number of states that the variable can have. Based on this, conditional probability tables can be constructed to express the probabilities of each child node derived from conditions of its parent nodes.

Node C from the sample DAG above would have a conditional probability table specifying the conditional distribution $P(C|A,B)$. Since A and B have no parents, so it only require probability distributions $P(A)$ and $P(B)$. Assuming all the variables are binary, means variable A can only take on A1 and A2, variable B can only take on B1 and B2, and variable C can only take on C1 and C2. Below is an example of a conditional probability table of node C.

A	B	C	
		C1	C2
A1	B1	$P(C=C1 A=A1, B=B1)$	$P(C=C2 A=A1, B=B1)$
A1	B2	$P(C=C1 A=A1, B=B2)$	$P(C=C2 A=A1, B=B2)$
A2	B1	$P(C=C1 A=A2, B=B1)$	$P(C=C2 A=A2, B=B1)$
A2	B2	$P(C=C1 A=A2, B=B2)$	$P(C=C2 A=A2, B=B2)$

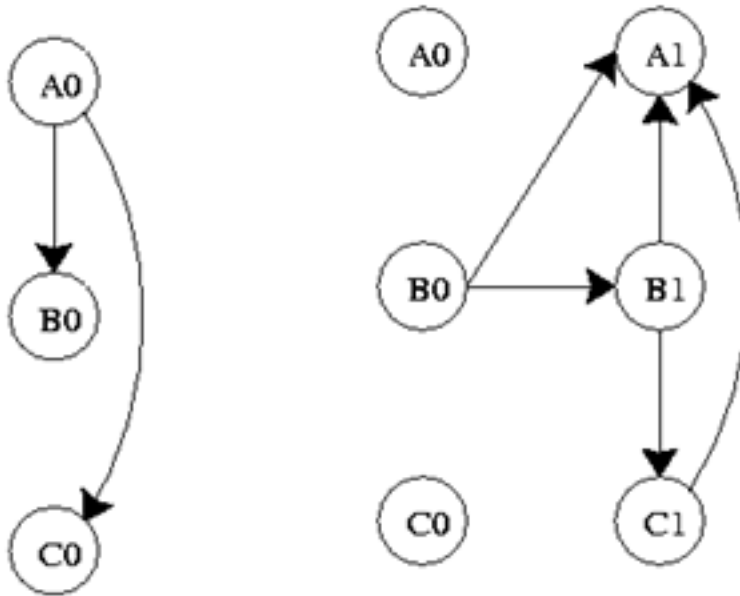
The conditional probabilities between observation nodes are defined using a sensor node. This sensor node gives conditional probability distribution of the sensor reading given the actual state of system. It embodies the accuracy of the system.

The nature of DBN usually results in a large and complex network. Thus to calculate a DBN, the outcome old time slice is summarized into probabilities that is used for the later slice. This provides a moving time frame and forms a DBN. When creating a DBN, temporal relationships between slices must be taken into account. Below is an implementation chart for DBN.



The graph below is a representation of a DBN. It represents the variables at two different time steps, $t-1$ and t . $t-1$, shown on the left, is the initial distribution of the variables. The

next time step, t , is dependent on time step $t-1$. It is important to note that some of these variables could be hidden.

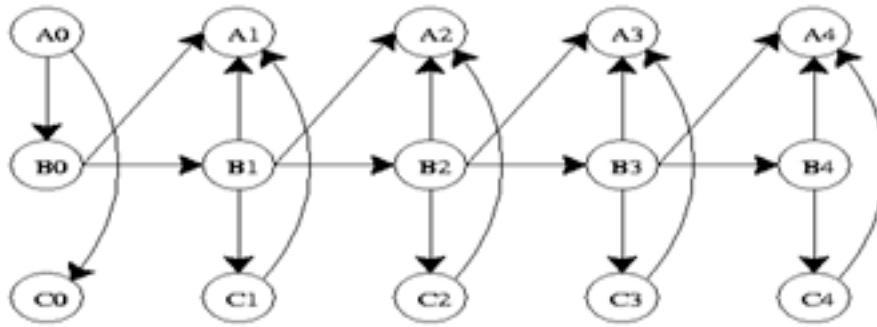


Where A_0, B_0, C_0 are initial states and A_i, B_i, C_i are future states where $i=1,2,3,\dots,n$.

The probability distribution for this DBN at time t is...

$$P(Z_t | Z_{t-1}) = \prod_{i=1}^N P(Z_t^i | \pi(Z_t^i))$$

If the process continues for a larger number of time steps, the graph will take the shape below.

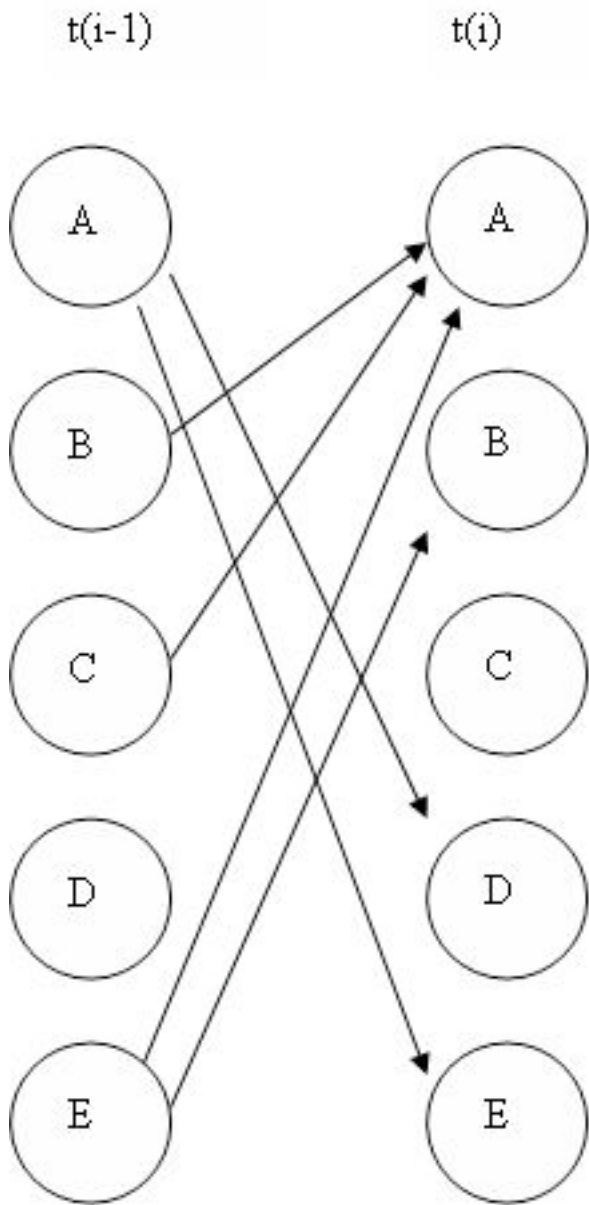


Its joint probability distribution will be...

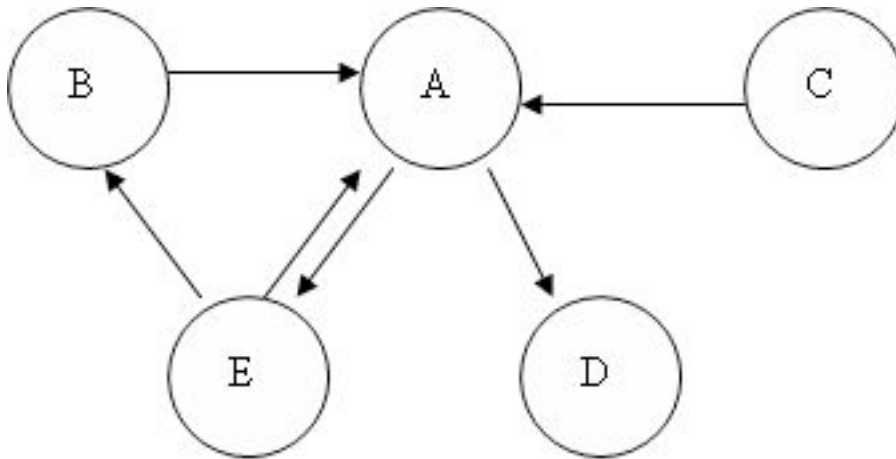
$$P(\mathbf{Z}_{1:T}) = \prod_{t=1}^T \prod_{i=1}^N P(Z_t^i \mid \boldsymbol{\pi}(Z_t^i))$$

DBN's are useful in industry because they can model processes where information is incomplete, or there is uncertainty. Limitations of DBN's are that they do not always accurately predict outcomes and they can have long computational times.

The above illustrations are all examples of "unrolled" networks. An unrolled dynamic Bayesian network shows how each variable at one time step affects the variables at the next time step. A helpful way to think of unrolled networks is as visual representations of numerical solutions to differential equations. If you know the states of the variables at one point in time, and you know how the variables change with time, then you can predict what the state of the variables will be at any point in time, similar to using Euler's method to solve a differential equation. A dynamic Bayesian network can also be represented as a "rolled" network. A rolled network, unlike an unrolled network, shows each variable's effect on each other variable in one chart. For example, if you had an unrolled network of the form:



then you could represent that same network in a rolled form as:



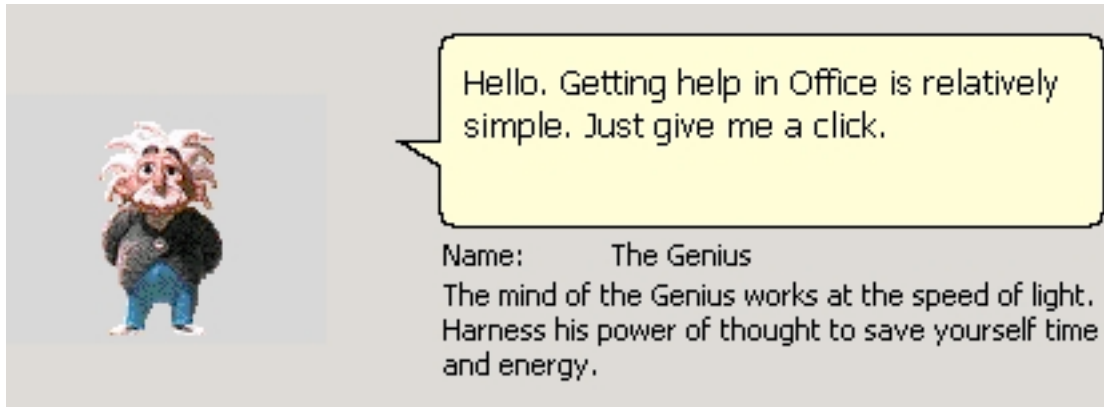
If you examine each network, you will see that each one provides the exact same information as to how the variables all affect each other.

5.10 Applications

Bayesian networks are used when the probability that one event will occur depends on the probability that a previous event occurred. This is very important in industry because in many processes, variables have conditional relationships, meaning they are not independent of each other. Bayesian networks are used to model processes in a wide variety of applications. Some of these include...

1. Gene regulatory networks
2. Protein structure
3. Diagnosis of illness
4. Document classification
5. Image processing
6. Data fusion
7. Decision support systems
8. Gathering data for deep space exploration
9. Artificial Intelligence
10. Prediction of weather

11. On a more familiar basis, Bayesian networks are used by the friendly Microsoft office assistant to elicit better search results.



12. Another use of Bayesian networks arises in the credit industry where an individual may be assigned a credit score based on age, salary, credit history, etc. This is fed to a Bayesian network which allows credit card companies to decide whether the person's credit score merits a favorable application.

5.11 Summary: A General Solution Algorithm for the Perplexed

Given a Bayesian network problem and no idea where to start, just relax and try following the steps outlined below.

Step 1: What does my network look like? Which nodes are parents (and are they conditional or unconditional) and which are children? How would I model this as an incidence diagram and what conditional probability statement defines it?

Step 2: Given my network connectivity, how do I tabulate the probabilities for each state of my node(s) of interest? For a single column of probabilities (parent node), does the column sum to 1? For an array of probabilities (child node) with multiple possible states defined by the given combination of parent node states, do the rows sum to 1?

Step 3: Given a set of observed data (usually states of a child node of interest), and probability tables (aka truth tables), what problem am I solving?

- Probability of observing the particular configuration of data, order unimportant

Solution: Apply multinomial distribution

- Probability of observing the particular configuration of data in that particular order

Solution: Compute the probability of each individual observation, then take the product of these

- Probability of observing the data in a child node defined by 2 (or n) parents given only 1 (or n-1) of the parent nodes

Solution: Apply marginalization to eliminate other parent node

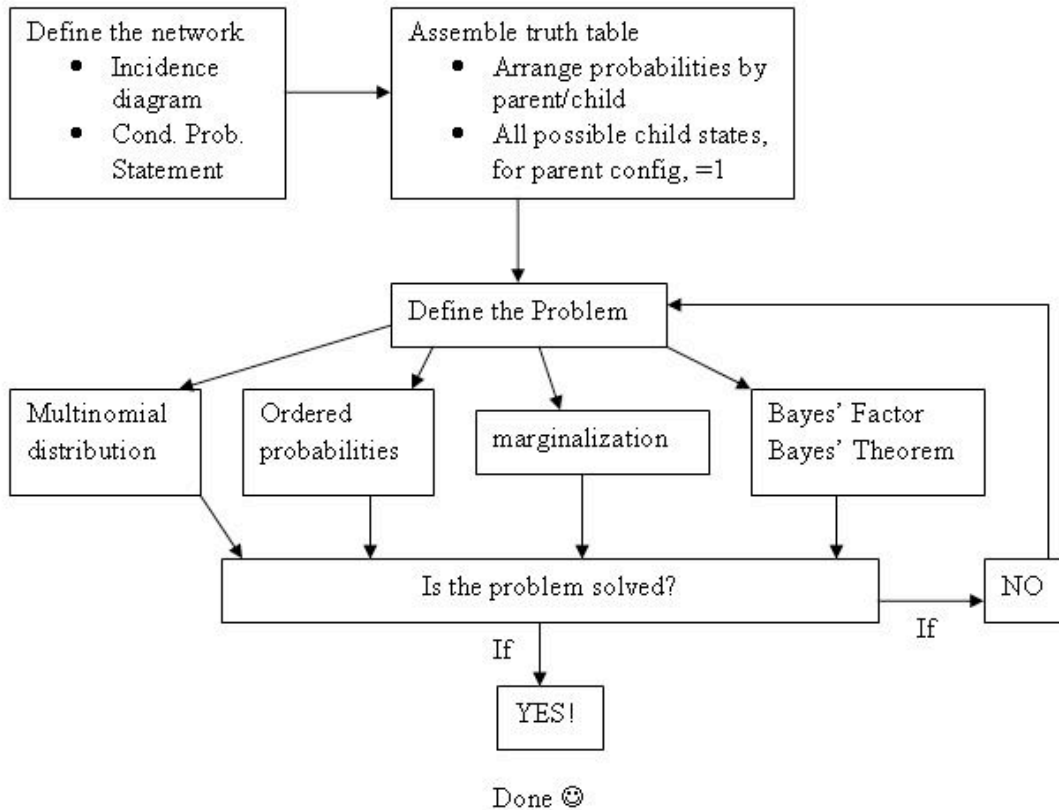
- Probability of a parent node being a particular state given data in the form of observed states of the child node

Solution: Apply Bayes' Theorem
Solve for Bayes' Factor to remove
incalculable denominator terms generated by applying Bayes'
Theorem, and to compare the parent node state
of interest to a base case, yielding a more meaningful data
point

Step 4: Have I solved the problem? Or is there another level of complexity? Is the problem a combination of the problem variations listed in step 3?

- If problem is solved, call it a day and go take a baklava break
- If problem is not solved, return to step 3

Graphically:

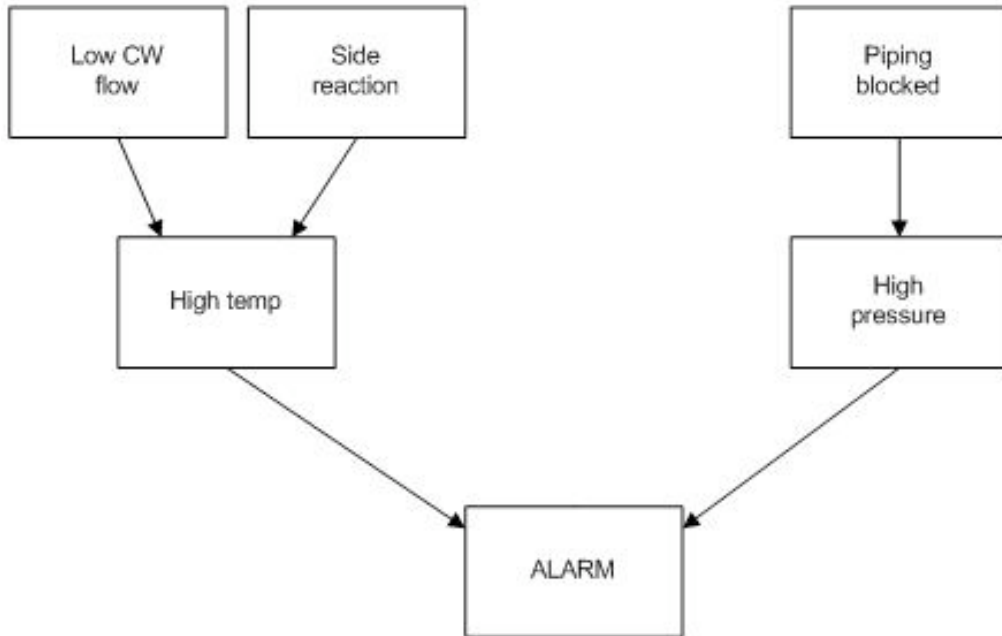


5.12 Worked out Example 1

A multipurpose alarm in a plant can be tripped in 2 ways. The alarm goes off if the reactor temperature is too high or the pressure in a storage tank is too high. The reactor temperature may be too high because of a low cooling water flow (1% probability), or because of an unknown side reaction (5% probability). The storage tank pressure might be too high because of a blockage in the outlet piping (2% probability). If the cooling water flow is low and there is a side reaction, then there is a 99% probability that a high temperature will occur. If the cooling water flow is normal and there is no side reaction, there is only a 3% probability a high temperature will occur. If there is a pipe blockage, a high pressure will always occur. If there is no pipe blockage, a high pressure will occur only 2% of the time.

Create a DAG for the situation above, and set up the probability tables needed to model this system. All the values required to fill in these tables are not given, so fill in what is possible and then indicate what further values need to be found.

Answer:



The following probability tables describe the system, where CFL = Cold water flow is low, SR = Side reaction present, PB = Pipe is blocked, HT = High temperature, HP = High pressure, A = Alarm. T stands for true, or the event did occur. F stands for false, or the event did not occur. A blank space in a table indicates an area where further information is needed.

P(CFL=T)	0.01
P(CFL=F)	0.99
P(SR=T)	0.05
P(SR=F)	0.95
P(PB=T)	0.02
P(PB=F)	0.98

CFL	SR	P(HT=T)	P(HT=F)
T	T	0.99	0.01
T	F		
F	F	0.03	0.97
F	T		

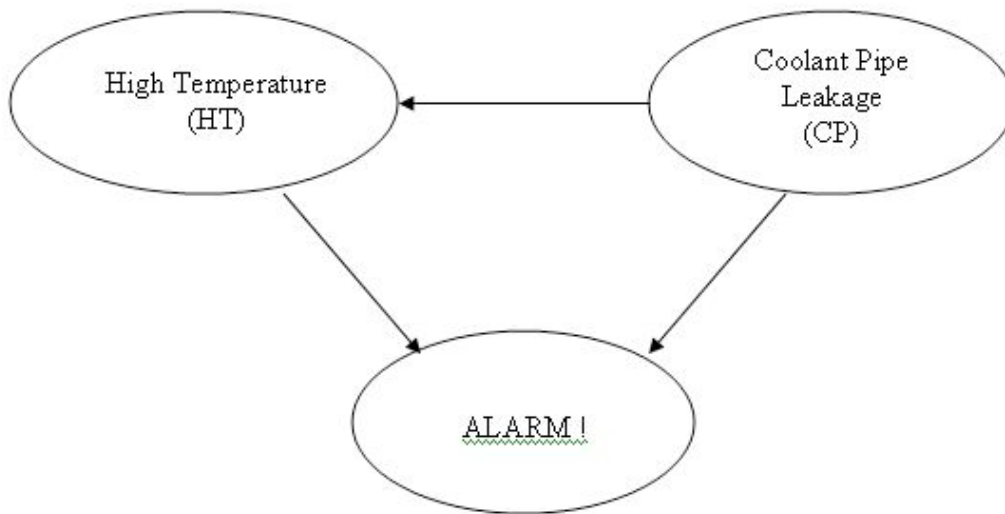
PB	P(HP=T)	P(HP=F)
F	0.02	0.98
T	1.00	0.00

HT	HP	P(A=T)	P(A=F)
T	T		
T	F		
F	F		
F	T		

An advantage of using DAGs becomes apparent. For example, you can see that there is only a 3% chance that there is a high temperature situation given that both cold water flow is not low and that there is no side reaction. However, as soon as the cold water becomes low, you have at least a 94% chance of a high temperature alarm, regardless of whether or not a side reaction occurs. Conversely, the presence of a side reaction here only creates a 90% chance of alarm trigger. From the above probability calculations, one can estimate relative dominance of cause-and-effect triggers. For example you could now reasonably conjecture that the cold water being low is a more serious event than a side reaction.

5.13 Worked out Example 2

The DAG given below depicts a different model in which the alarm will ring when activated by high temperature and/or coolant water pipe leakage in the reactor.



The table below shows the truth table and probabilities with regards to the different situations that might occur in this model.

CP		HT	
T	F	T	F
0.3	0.7	0.9	0.1
		F	1

HT	CP	A	
F	F	T	F
F	T	0	1
T	F	0.7	0.3
T	T	0.9	0.1
T	T	0.99	0.01

The joint probability function is:

$$P(A, HT, CP) = P(A | HT, CP)P(HT | CP)P(CP)$$

A great feature of using the Bayesian network is that the probability of any situation can be calculated. In this example, write the statement that will describe the probability that the temperature is high in the reactor given that the alarm sounded.

Answer:

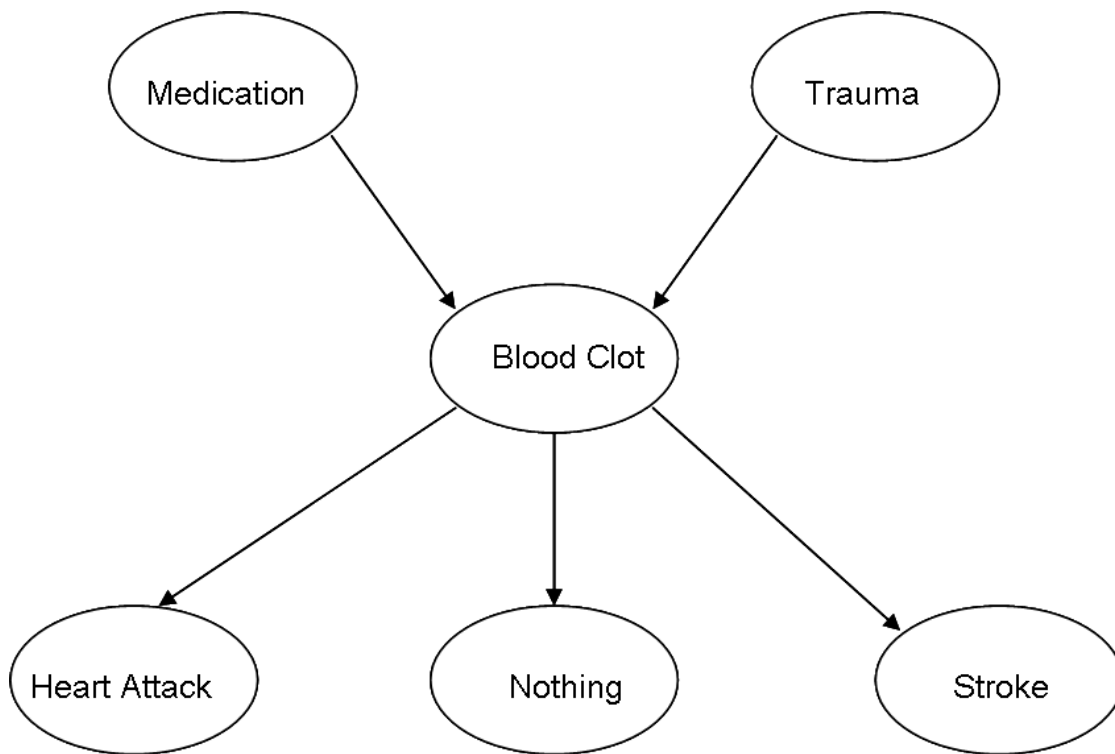
$$P(CP = T \mid A = T) = \frac{P(A = T, CP = T)}{P(A = T)} = \frac{\sum_{HT \in \{T, F\}} P(A = T, HT, CP = T)}{\sum_{HT, CP \in \{T, F\}} P(A = T, HT, CP)}$$

5.14 Worked out Example 3

Certain medications and traumas can both cause blood clots. A blood clot can lead to a stroke, heart attack, or it could simply dissolve on its own and have no health implications.

a. Please create a DAG that represents this situation.

Answer:



b. The following probability information is given where M = medication, T = trauma, BC = blood clot, HA = heart attack, N = nothing, and S = stroke. T stands for true, or this event did occur. F stands for false, or this event did not occur.

P(M=T)	0.2
P(M=F)	0.8
P(T=T)	0.05
P(T=F)	0.95

M	T	P(BC=T)	P(BC=F)
T	T	0.95	0.05
T	F	0.3	0.7
F	T	0.6	0.4
F	F	0.9	0.1

BC	P(HA=T)	P(HA=F)	P(S=T)	P(S=F)	P(N=T)	P(N=F)
T	0.4	0.6	0.35	0.65	0.25	0.75
F	0.15	0.85	0.1	0.9	0.75	0.25

What is the probability that a person will develop a blood clot as a result of both medication and trauma, and then have no medical implications?

Answer: $P(N, BC, M, T) = P(N | BC) P(BC | M, T) P(M) P(T) = (0.25) (0.95) (0.2) (0.05) = 0.2375\%$

5.15 Worked out Example 4

Suppose you were given the following data.

Catalyst	p(Catalyst)
A	0.40
B	0.60

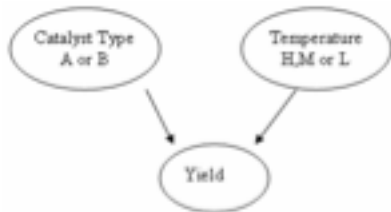
Temperature	Catalyst	P(Yield = H)	P(Yield = M)	P(Yield = L)
H	A	0.51	0.08	0.41
H	B	0.30	0.20	0.50
M	A	0.71	0.09	0.20
M	B	0.92	0.05	0.03
L	A	0.21	0.40	0.39

L	B	0.12	0.57	0.31
---	---	------	------	------

How would you use this data to find $p(\text{yield}|\text{temp})$ for 9 observations with the following descriptions?

# Times Observed	Temperature	Yield
4x	H	H
2x	M	L
3x	L	H

An DAG of this system is below:



Answer: Marginalization! The state of the catalyst can be marginalized out using the following equation:

$$p(\text{yield} | \text{temp}) = \sum_{i=A,B} p(\text{yield} | \text{temp}, \text{cat}_i) p(\text{cat}_i)$$

The two tables above can be merged to form a new table with marginalization:

Temperature	P(Yield = H)	P(Yield = M)	P(Yield = L)
H	$0.51*0.4 + 0.3*0.6 = 0.384$	$0.08*0.4 + 0.2*0.6 = 0.152$	$0.41*0.4 + 0.5*0.6 = 0.464$
M	$0.71*0.4 + 0.92*0.6 = 0.836$	$0.09*0.4 + 0.05*0.6 = 0.066$	$0.20*0.4 + 0.03*0.6 = 0.098$
L	$0.21*0.4 + 0.12*0.6 = 0.156$	$0.40*0.4 + 0.57*0.6 = 0.502$	$0.39*0.4 + 0.31*0.6 = 0.342$

$$p(\text{yield}|\text{temp}) = \frac{9!}{4!2!3!} * (0.384^4 * 0.098^2 * 0.156^3) = 0.0009989$$

5.16 Worked Out Example 5

A very useful use of Bayesian networks is determining if a sensor is more likely to be working or broken based on current readings using the Bayesian Factor discussed earlier. Suppose there is a large vat in your process with large turbulent flow that makes it difficult to accurately measure the level within the vat. To help you use two different level sensors positioned around the tank that read whether the level is high, normal, or low. When you first set up the sensor system you obtained the following probabilities describing the noise of a sensor operating normally.

Tank Level (L)	p(S=High)	p(S=Normal)	p(S=Low)
Above Operating Level Range	0.80	0.15	0.05
Within Operating Level Range	0.15	0.75	0.10
Below Operating Level Range	0.10	0.20	0.70

When the sensor fails there is an equal chance of the sensor reporting high, normal, or low regardless of the actual state of the tank. The conditional probability table for a fail sensor then looks like:

Tank Level (L)	p(S=High)	p(S=Normal)	p(S=Low)
Above Operating Level Range	0.33	0.33	0.33
Within Operating Level Range	0.33	0.33	0.33
Below Operating Level Range	0.33	0.33	0.33

From previous data you have determined that when the process is acting normally, as you believe it is now, the tank will be operating above the level range 10% of the time, within the level range 85% of the time, and below the level range 5% of the time. Looking at the last 10 observations (shown below) you suspect that sensor 1 may be broken. Use Bayesian factors to determine the probability of sensor 1 being broken compared to both sensors working.

Sensor 1	Sensor 2
High	Normal
Normal	Normal
Normal	Normal
High	High
Low	Normal

Low	Normal
Low	Low
High	Normal
High	High
Normal	Normal

From the definition of the Bayesian Factor we get.

$$BF = \frac{p(model1|data)}{p(model2|data)} = \frac{\frac{p(data|model1)p(model1)}{p(data)}}{\frac{p(data|model2)p(model2)}{p(data)}} = \frac{p(data|model1)}{p(data|model2)}$$

For this set we will use the probability that we get the data given based on the model.

$$\frac{p(data|model1)}{p(data|model2)}$$

If we consider model 1 both sensors working and model 2 sensor 2 being broken we can find the BF for this rather easily.

$$p(data | model 1) = p(s1 data | model 1) * p(s2 data | model 1)$$

For both sensors working properly:

The probability of the sensor giving each reading has to be calculated first, which can be found by summing the probability the tank will be at each level and multiplying by probability of getting a specific reading at that level for each level.

$$p(s1 = high | model 1) = [(.10)*(.80) + (.85)*(.15) + (.05)*(.10)] = 0.2125$$

$$p(s1 = normal | model 1) = [(.10)*(.15) + (.85)*(.75) + (.05)*(.20)] = 0.6625$$

$$p(s1 = low | model 1) = [(.10)*(.05) + (.85)*(.10) + (.05)*(.70)] = 0.125$$

Probability of getting sensor 1's readings (assuming working normally)

$$p(s1 data | model1) = (.2125)^4 * (.6625)^3 * (.125)^3 = 5.450 * 10^{-6}$$

The probability of getting each reading for sensor 2 will be the same since it is also working normally

$$p(s2data \mid model1) = (.2125)^2 * (.6625)^7 * (.125)^1 = 3.162 * 10^{-4}$$

$$p(data \mid model1) = (5.450 * 10^{-6}) * (3.162 * 10^{-4}) = 1.723 * 10^{-9}$$

For sensor 1 being broken:

The probability of getting each reading now for sensor one will be 0.33.

$$p(s1data \mid model2) = (0.33)^4 * (0.33)^3 * (0.33)^3 = 1.532 * 10^{-5}$$

The probability of getting the readings for sensor 2 will be the same as model 1, since both models assume sensor 2 is acting normally.

$$p(data \mid model2) = (1.532 * 10^{-5}) * (3.162 * 10^{-4}) = 4.844 * 10^{-9}$$

$$BF = \frac{1.723 * 10^{-9}}{4.844 * 10^{-9}} = 0.356$$

A BF factor between 1/3 and 1 means there is weak evidence that model 2 is correct.

5.17 True or False?

1. Is the other name for Bayesian Network the "Believer" Network?
2. The nodes in a Bayesian network can represent any kind of variable (latent variable, measured parameter, hypothesis..) and are not restricted to random variables.
3. Bayesian network theory is used in part of the modeling process for artificial intelligence.

Answers:

1. F
2. T
3. T

5.18 Sage's Corner

http://www.youtube.com/v/x_3E0sE6ugs

Unnarrated Slides:

http://controls.engin.umich.edu/wiki/index.php/Image:Bayesian_Network_Theory.ppt

<http://video.google.com/googleplayer.swf?docId=-8662996094538220092>
Example Adapted from <<http://www.dcs.qmw.ac.uk/~norman/BBNs/BBNs.htm>>
Unnarrated Slides:
<http://controls.engin.umich.edu/wiki/index.php/Image:Bayesian.ppt>

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Section 6. Learning and analyzing Bayesian networks with Genie

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Date Revised: November 29, 2007

6.1 Introduction

Genie (Graphical network interface) is a software tool developed at the University of Pittsburgh for Microsoft Windows and available free of charge at [Genie](#). It is useful for decision analysis and for graphically representing the union of probability and networked occurrences. Particularly, Genie can be used for the analysis of [Bayesian networks](#), or directed acyclic graphs (i.e. occurrences in a web of happenings are conditionally independent of each other). Bayesian networks or Dynamic Bayesian Networks (DBNs) are relevant to engineering controls because modelling a process using a DBN allows for the inclusion of noisy data and uncertainty measures; they can be effectively used to predict the probabilities of related outcomes in a system. In Bayesian networks, the addition of more nodes and inferences greatly increases the complexity of the calculations involved and Genie allows for the analysis of these complicated systems. Additionally, the graphical interface facilitates visual understanding of the network (Charniak, 1991).

This [link](#) gives an example of a complex Bayesian network depicted in the graphical interface of Genie. As can be seen, Genie arranges the network of nodes and inferences in a topology that is easily visualized and is useful for both simple and extremely complex systems.

6.2 Using Genie to Construct and Analyze Dynamic Bayesian Networks

This section will include instructions for downloading and installing the Genie software as well as describe the procedure for using Genie to analyze simple Bayesian networks.

6.2.1 Downloading and Installing Genie

The Genie software download is available the Genie [website](#), depicted below:



To download Genie, click on the “Downloads” link on the left menu of the page and highlighted in red in the figure above.

A registration page will appear which requires some basic user information. After this has been entered, click on the Register link.

A Downloads page with several download options will appear. Click on the GeNie 2.0 link highlighted in red on the figure below. This will initiate the download.

NOTE: The Genie Software download is only available for Windows.

Downloads

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GeNIe top

Windows EXE GeNIe 2.0 [8.35 MB] (September 12, 2007)

Comments:
This is build 2.0.2811.0. [Changelog](#)

Install the software by following the steps indicated in the Genie installation program.

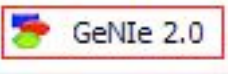
NOTE: You will not be able to install the software onto University of Michigan computers without administrative rights. You must install this software on your home PC.

The installation of the Genie software is now complete. Please note the help section of the software features many tutorials describing how to use a wide array of functions. However, this article will be focused on the analysis of Dynamic Bayesian Networks.

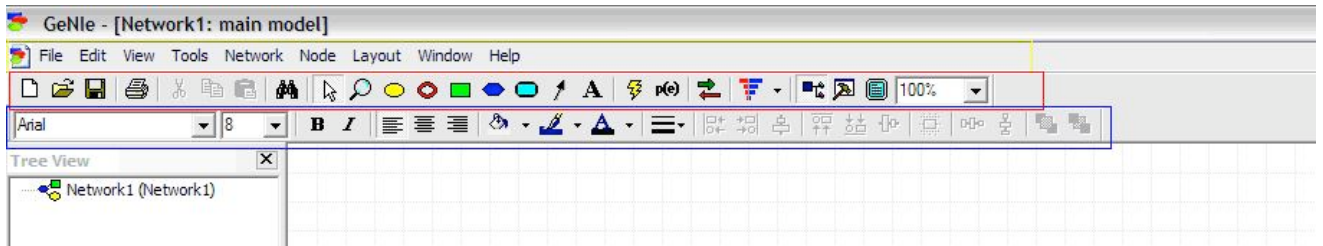
- All informational materials used to create this tutorial come from [GeNIe](#)

6.2.2 Using GeNIe to Analyze Dynamic Bayesian Networks

If the program was installed in the default location given in the installation wizard a shortcut to GeNIe can be found in the start menu listed under All Programs. Click on the

GeNIe 2.0 Icon as seen below: 

The main interface will appear as shown in the figure below:



Note the important tool bars highlighted on the figure above: the menu bar (yellow), the standard toolbar (red), and the format toolbar (blue).

Consider this simple illustration of how to build a Dynamic Bayesian Network using GeNie:

Polly popular is the most popular girl on the UM campus who only dates other UM students. It is common knowledge that Polly only accepts 30% of the invitations she receives to go on a date. Of the invitations that she accepts, 40% of them come from guys with high GPAs, 40% of them come from guys with medium GPAs and 20% of them come from guys with low GPAs. Of the invitations that she rejects, 10% of them come from guys with high GPAs, 30% of them come from guys with medium GPAs, and 60% of them come from guys with low GPAs.

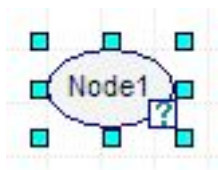
NOTE: In this example, the variable of GPA is discretized into categories of high, medium, and low. This is necessary for analysis using GeNie because otherwise there would exist infinite states for each node in the DBN (Charniak, 1991).

Creating a Bayesian network allows for determinations to be made about probabilities of Polly accepting or rejecting certain date invitations. Shown below is how to use GeNie to find the probability of Polly accepting a date invitation from a guy if she knows the guy inviting her has a high GPA.

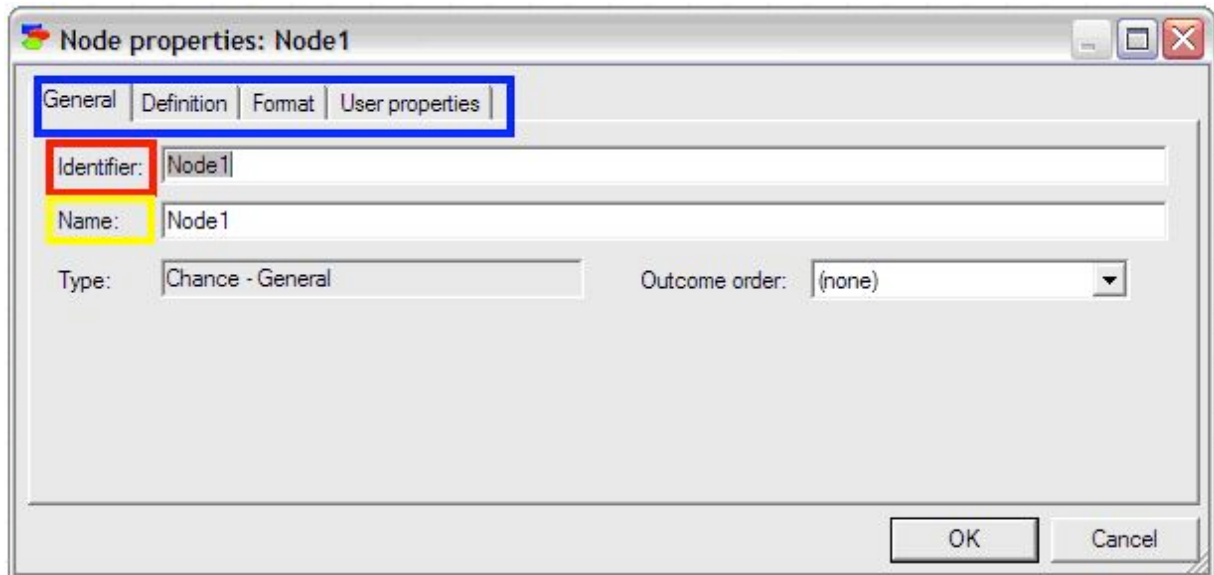
First, a node is created for the variable called acceptance of invitation. Select the “chance” node from the standard toolbar as is shown in the figure below highlighted in red.



Left-click on a clear part of the graph area of the screen. An oval will appear with “Node1” inside as seen in the figure below.

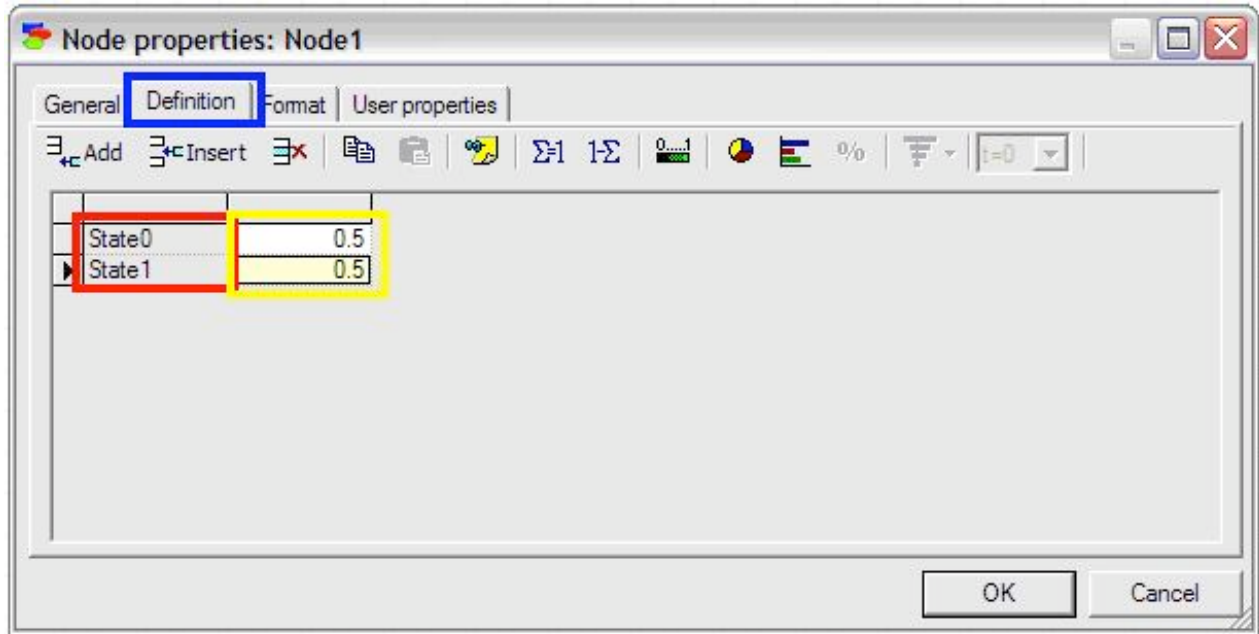


The edit mode for the node should come up automatically; if not, simply double-click on the node to pull up the edit screen as depicted in the figure below.




Enter an identifier for the node (must be a valid variable name in a programming language) and enter a name for the node (can be a string of any length). For this example, the identifier is entered as “Acceptance” and the name is entered as “Acceptance of Invitation”.

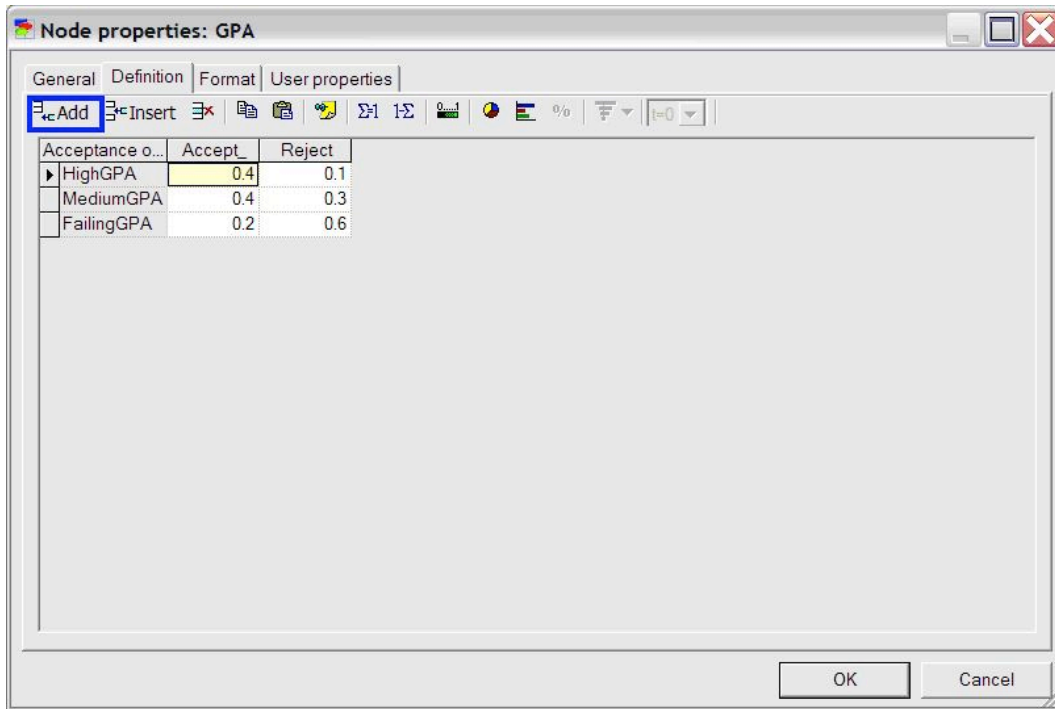
To define the probabilities of the node, click on the definition tab highlighted in blue as shown below. The names of the states can be edited by double clicking on the name fields (highlighted in red in the figure below) and the probabilities can be edited by clicking on the probability field (highlighted in yellow in the figure below).



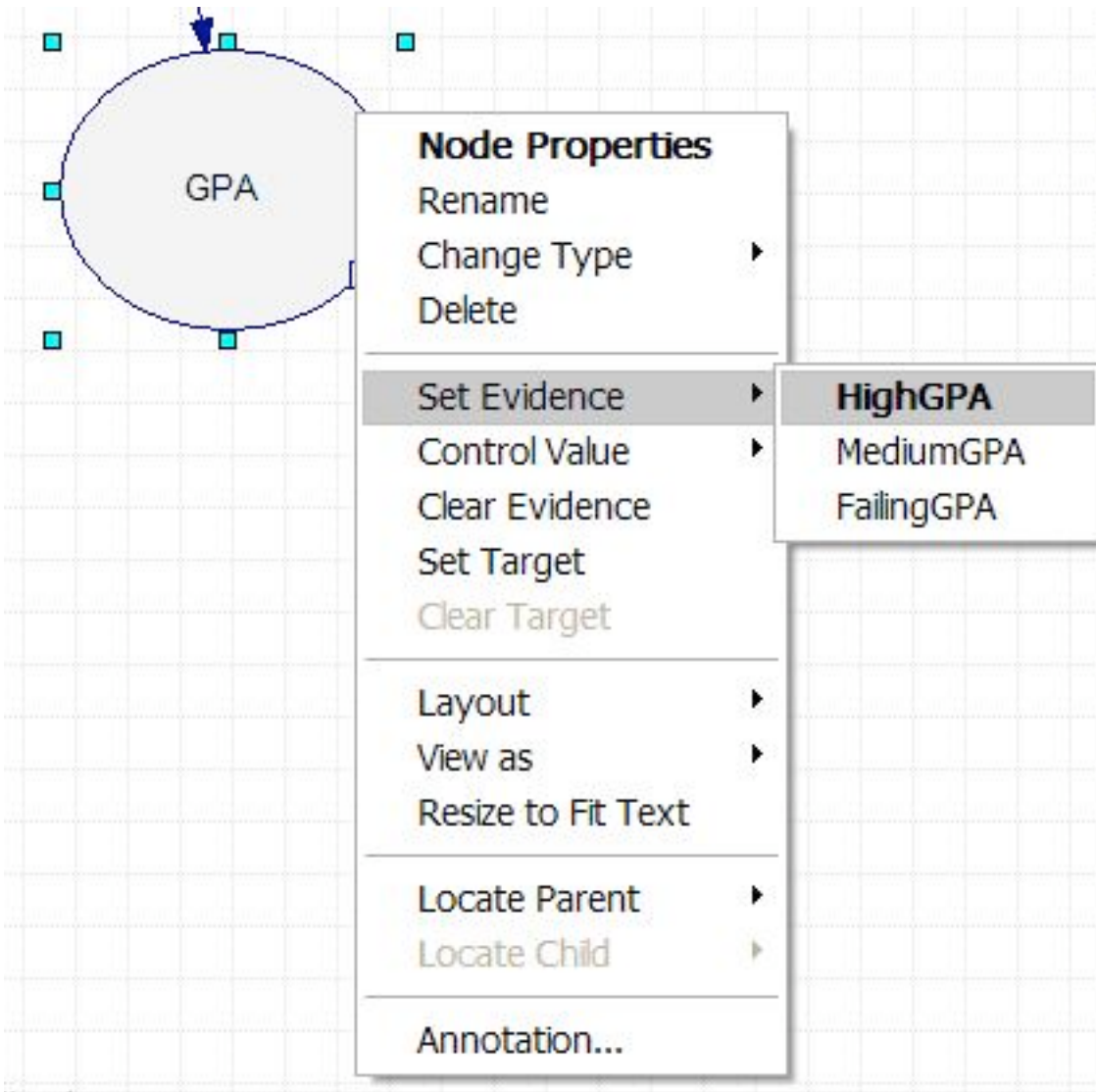
In this example, “State0” is changed to “Accept” and “State1” is changed to “Reject”. The default probabilities are entered as 0.3 for Accept and 0.7 for Reject.


To create a second node for the variable GPA, simply click the change node again and place a second node under the “Acceptance” node. Define the name and identifier of this node as done with the “Acceptance” node. Then define the probabilities for the “GPA” node by first adding another outcome by clicking the “add outcome” button highlighted in blue in the figure below. Change state0, state1, and state2 to HighGPA, MediumGPA, and LowGPA respectively. To finish defining this node, fill in the probabilities listed in the problem statement (shown in the figure below) and press ok.

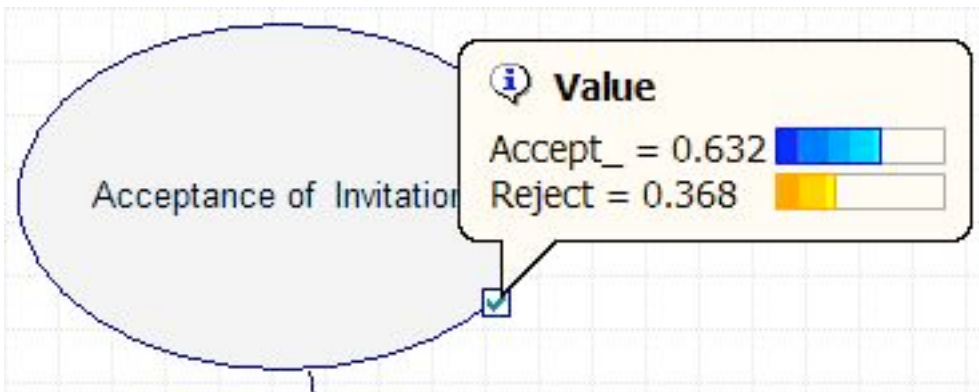
After the creation and definition of both nodes, connect these two nodes with an influence arc to represent that GPA affects how Polly accepts or rejects the invitations she receives. To do this, click on the Arc tool (found on the standard toolbar), , and click on the “Acceptance” node and drag the arrow to the new “GPA” node.



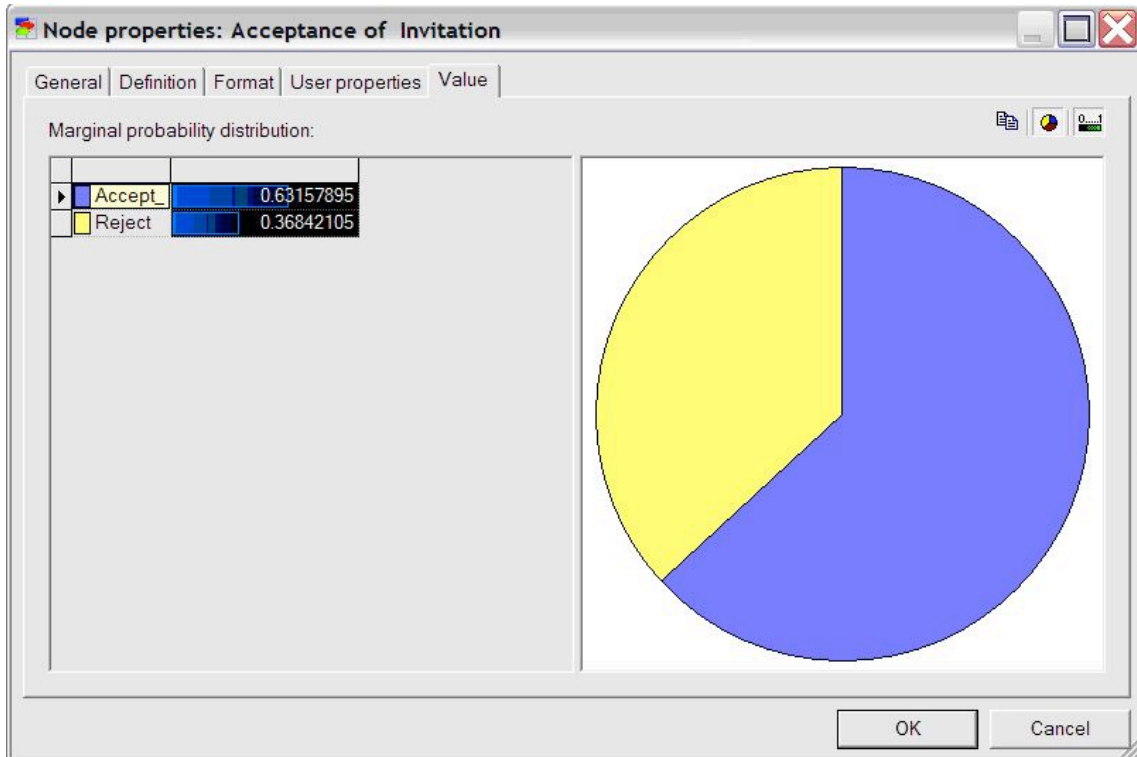
The Bayesian network describing this problem is now fully defined within the Genie program. To determine the probability of Polly accepting a date invitation from a guy if she knows the guy has a high GPA, first right click on the GPA node, scroll down to "Set Evidence", and select "HighGPA". This is shown in the figure below.



Then, update the network by clicking the update icon in the standard toolbar, . After the update, view the results by holding the mouse pointer over the check mark on the corner of the Acceptance node, as shown in the Figure below.



The results can also be accessed by double clicking the Acceptance node and selecting the value tab, shown in the figure below.



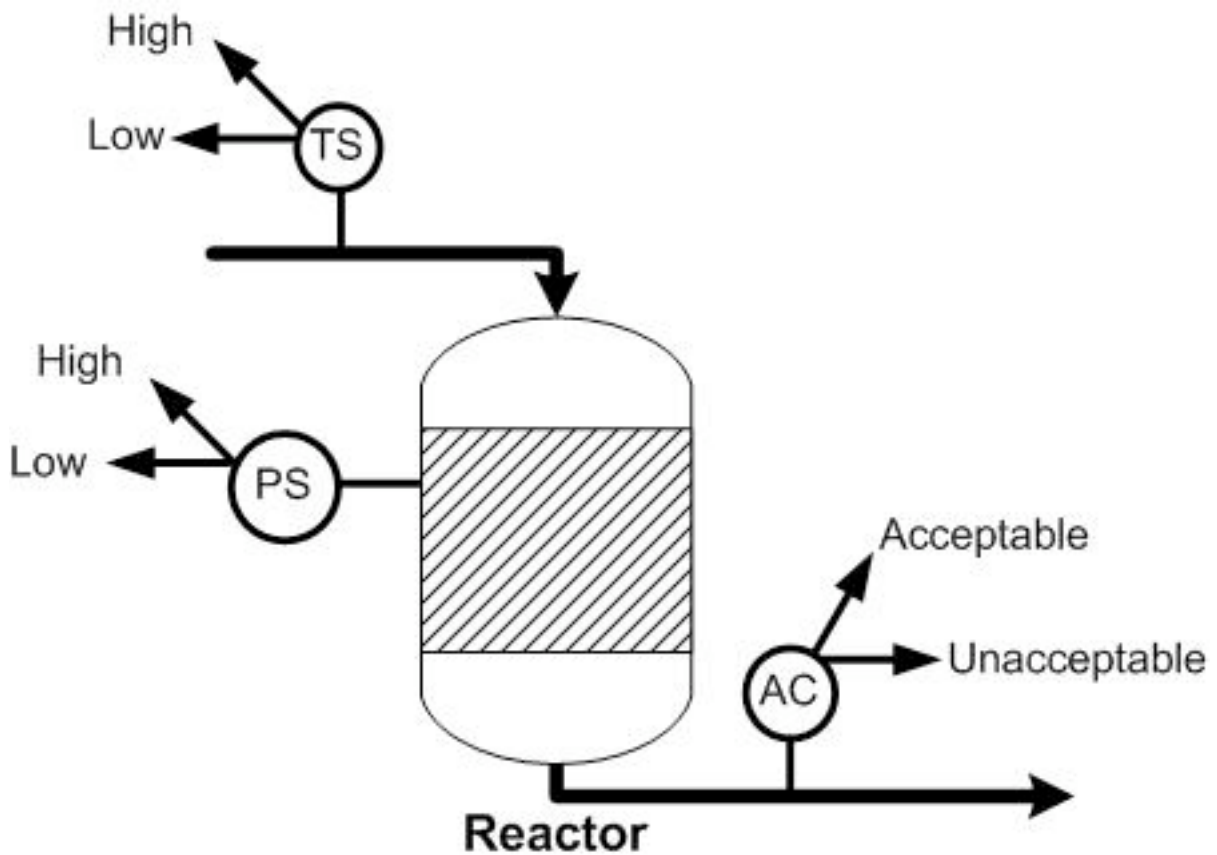
As can be seen in the figure above, Polly will accept the date invitation 63.16% of the time when she knows the guy inviting her has a high GPA. Other probabilities related to this example can be determined similarly.

The logic and procedure involved in this simple problem can be applied to complex systems with many interconnected nodes. Please see the Worked Out Examples sections for more examples of how to use GeNIe to analyze Bayesian networks.

- All informational materials used to create this tutorial come from [GeNIe](#)

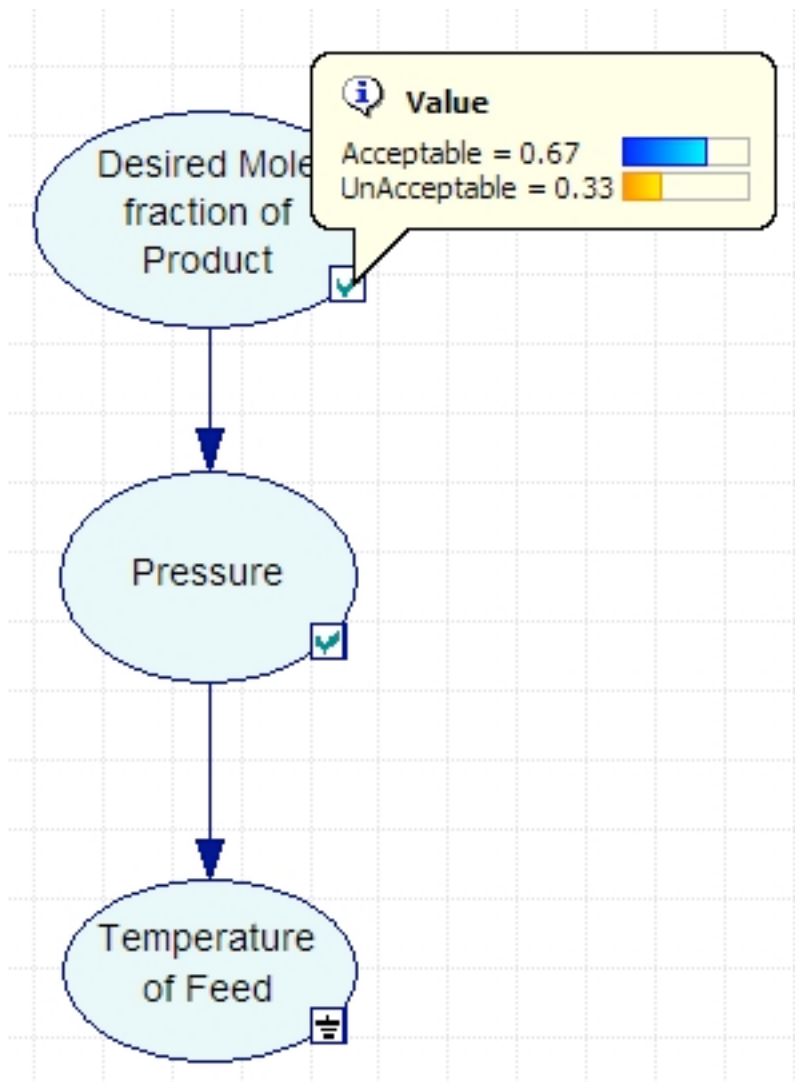
6.3 Worked out Example 1

For the reactor shown below, the probability that the effluent stream will contain the acceptable mole fraction of product is 0.5. For the same reactor, if the effluent stream contains the acceptable mole fraction, the probability that the pressure of the reactor is high is 0.7. If the effluent stream does not contain the acceptable fraction, the probability that the pressure is low is 0.85. If the pressure of the reactor is high, the probability that the temperature of the feed is high is 0.9 and if the pressure of the reactor is low, the probability that temperature of the feed is low is 0.75. Given that the temperature of the feed is low, what is the probability that the effluent stream contains the acceptable mole fraction of product?



Solution:

The variables to be included in the Bayesian network are the acceptable mole fraction of product in the effluent stream, the pressure of the reactor, and the temperature of the reactor. The variables are connected in an acyclic network as shown in the image below. After the nodes were created and the incidence arcs were defined, the probability was calculated by updating the network and moving the pointer over the checkmark on the node. As can be seen in the figure, the probability of the effluent stream containing the acceptable mole fraction of product given that the feed temperature is low is 67%.



A GeNIe file containing the full solution of the problem is located [here](#). In this file, the values entered into Genie for the probabilities and stages can be accessed by double-clicking on the nodes.

6.4 Worked out Example 2

The following example is complicated and contains many layers of information. It is intended to illustrate how many elements can be put together in a Bayesian Network and analyzed using Genie such that the problem is not impossibly complicated. Assume that detailed statistical experiments were conducted to find all the stated probabilities.

Consider a CSTR with a cooling jacket and an exothermic reaction with $A \rightarrow B$. The feed stream is pure A and the cooling stream in the jacket has a sufficient flow rate high such that the ambient temperature is constant.

The pumps transporting the reactor feed stream are old, and sometimes do not pump at their full capacity. 98% of the time the pumps work normally, but at other times the feed flow rate is slightly lower than normal. The preheating process for the feed stream is inefficient, and sometimes does not heat the reactants to 80°C. There is a 95% chance the feed stream is slightly cooler than desired. Finally, the pumps for the cooling water sometimes lose power, causing the ambient temperature for the reactor to climb higher than usual. There is a 1% chance of this power loss occurring.

The concentration of A in the reactor depends on the feed flow rate. If this flow rate is normal, then there is a 98% chance CA is normal, and a 1% chance each that it is slightly higher or lower than normal. If the flow rate is low, then there is a 40% chance that CA will be higher than normal and a 60% chance that CA will be normal.

The reactor temperature depends on the feed temperature and the ambient temperature. If both T0 and Ta are normal, there is a 98% chance T is normal, and a 1% chance each that it is slightly higher or lower than normal. If T0 is normal and Ta is high, there is a 90% chance T is normal and a 10% chance it is high. If Ta is normal and T0 is low, there is a 80% chance T is normal and a 20% T is low. Finally, if T0 is low and Ta is high, there is a 90% chance T is normal, a 8% chance T is low, and a 2% chance T is high.

The conversion depends on CA and T. If one of these variables is high and the other low, there is an equal chance that X will be low, normal, or high. If both CA and T are normal, there is a 98% chance X is normal, and a 1% chance each that it is slightly higher or lower than normal. If both CA and T are low, there is equal chance that X will be low or normal. If both CA and T are high, there is equal chance that X will be normal or high. If CA is normal and T is low, there is a 75% chance X is normal and a 25% chance X is low. If CA is normal and T is high, there is a 75% chance X is normal and a 25% chance X is high. Finally, if T is normal and CA is low or high, there is a 85% chance X is normal and a 15% chance that X is low or high, respectively.

Create a model in Genie for this system that can be used to determine probabilities of related events occurring.

Solution:

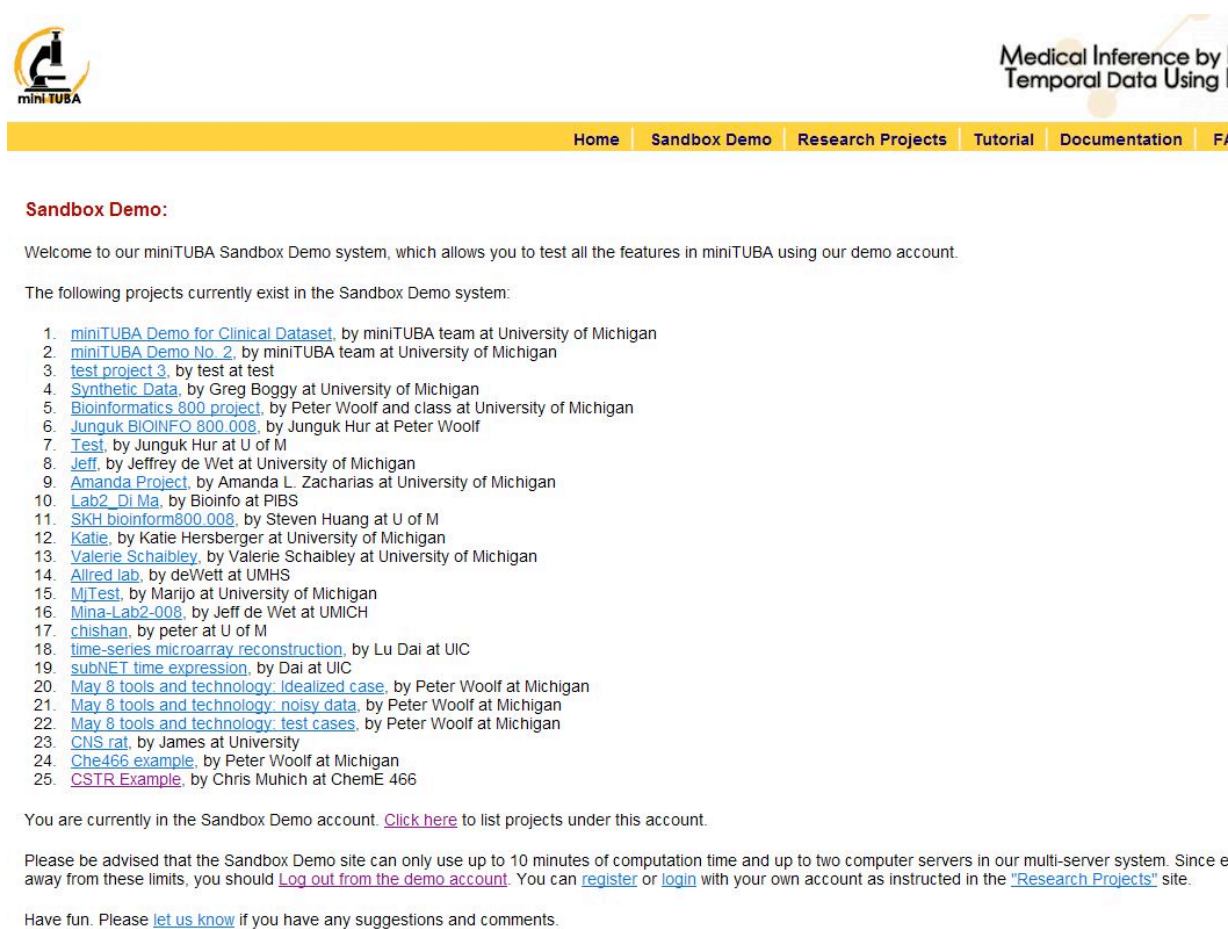
A GeNIe file containing the Bayesian Network of this problem is located [here](#).

This model can be used to answer questions such as (1) if a composition sensor for B in the exit stream tells us that the conversion is slightly low, what is the probability that the feed temperature is normal and (2) if a temperature sensor in the reactor tells us that the reactor temperature is high what is the probability that the ambient temperature is normal?

6.5 miniTuba

MiniTuba is a program that allows the creation of Bayesian Networks thought time, with only the final data sets. This was created by Zuoshuang Xiang, Rebecca M. Minter, Xiaoming Bi, Peter Woolf, and Yongqun He, to analysis medical data, but can be used to create Bayesian Networks for any propose. In oder to use this program go to <http://www.minituba.org/> and go to the Sandbox demo Tab. From here one can either start a new project or merly modify an old project. This wiki will talk though how to create a new project.

First Log in: to do this click the Log In link at the bottom of the page and enter demo@e.d.u as the user name and demo as the password this should bring up this screen:



Sandbox Demo:

Welcome to our miniTUBA Sandbox Demo system, which allows you to test all the features in miniTUBA using our demo account.

The following projects currently exist in the Sandbox Demo system:

1. [miniTUBA Demo for Clinical Dataset](#), by miniTUBA team at University of Michigan
2. [miniTUBA Demo No. 2](#), by miniTUBA team at University of Michigan
3. [test project 3](#), by test at test
4. [Synthetic Data](#), by Greg Boggy at University of Michigan
5. [Bioinformatics 800 project](#), by Peter Woolf and class at University of Michigan
6. [Junguk BIOINFO 800 008](#), by Junguk Hur at Peter Woolf
7. [Test](#), by Junguk Hur at U of M
8. [Jeff](#), by Jeffrey de Wet at University of Michigan
9. [Amanda Project](#), by Amanda L. Zacharias at University of Michigan
10. [Lab2_DiMa](#), by Bioinfo at PIBS
11. [SKH bioinform800 008](#), by Steven Huang at U of M
12. [Katie](#), by Katie Hersberger at University of Michigan
13. [Valerie Schaibley](#), by Valerie Schaibley at University of Michigan
14. [Allred lab](#), by deWett at UMHS
15. [MiTest](#), by Marijo at University of Michigan
16. [Mina-Lab2-008](#), by Jeff de Wet at UMICH
17. [chishan](#), by peter at U of M
18. [time-series microarray reconstruction](#), by Lu Dai at UIC
19. [subNET time expression](#), by Dai at UIC
20. [May 8 tools and technology: idealized case](#), by Peter Woolf at Michigan
21. [May 8 tools and technology: noisy data](#), by Peter Woolf at Michigan
22. [May 8 tools and technology: test cases](#), by Peter Woolf at Michigan
23. [CHS rat](#), by James at University
24. [Che466 example](#), by Peter Woolf at Michigan
25. [CSTR Example](#), by Chris Muhich at ChemE 466

You are currently in the Sandbox Demo account. [Click here](#) to list projects under this account.

Please be advised that the Sandbox Demo site can only use up to 10 minutes of computation time and up to two computer servers in our multi-server system. Since e away from these limits, you should [Log out from the demo account](#). You can [register](#) or [login](#) with your own account as instructed in the "[Research Projects](#)" site.

Have fun. Please [let us know](#) if you have any suggestions and comments.

and click My Projects and then Creat New Project.

The user needs to know how many variables (EX: Temperature, Pump speed, Yield, flowrate in ChemE), data sets (EX: Reactors, Tanks ect) and the average number of time steps that will be analyzed.

In this example we will have a CSTR whose yeild may be affected by the reactor Volume, the motor speed, the temperature or the concentraion. This means that there are 5 variable. Lets say that we have 5 reactors runing this experiment with differeing either high or low Moter speed, temperature, and yeild and either high medium or low volume and concentrion. In this example Yeild is only affected by the moter speed and Temperature with the folloing probability

Motor/Temp (high or low)	yeild	
	H	L
M+T+	0.96	0.04
M+T-	0.3	0.7
M-T+	0.6	0.4
M-T-	0	100

Enter the requested data in miniTuba and then click open project from the list. Then click "load/updata data"

this example will use the following data:

[Media:CSTRExample.xls](#)

To insert the data, simply copy and paste in the data to open box, then click LOAD DATA. In Order to run the analysis click "Start DBN botton"

Here you can slect which data series and vaiables you would like to analyze. Now miniTuba gives several different options for the data. The data can be analysies and a

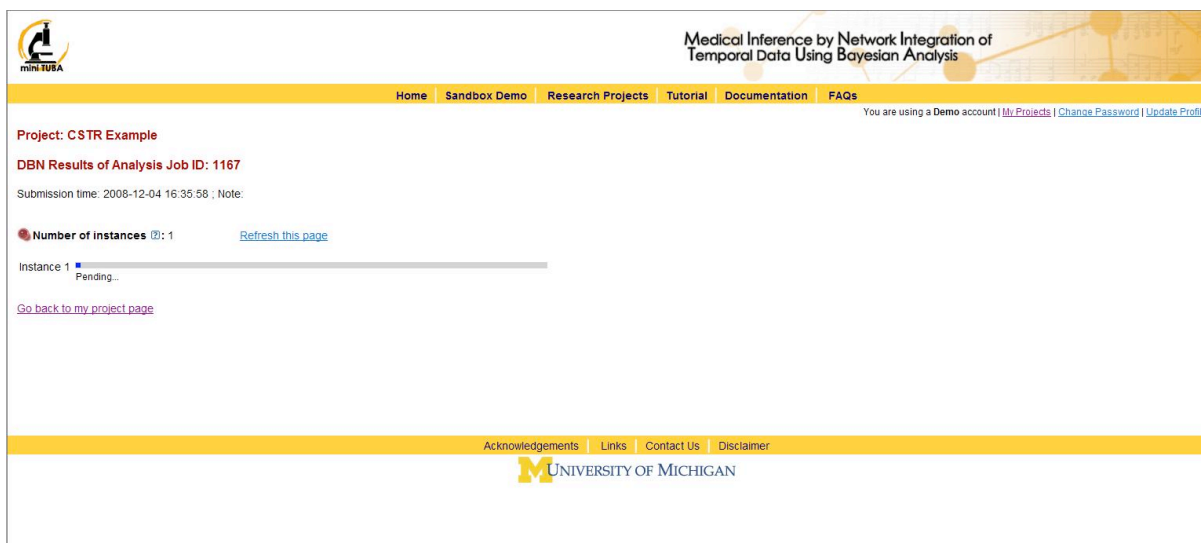
child a parent or both. A Child means that the data isn't affected by the other data that, Parent means the data doesn't affect the other data, and both means that the data can be affected and affect other variables. In our example, the motor speed is the only thing that we know is not affected by the other variables, so we will select it as a parent.

Discretization Policy tells MiniTuba how to bin the. In our case, as things are exactly high, med or low represented by 0,1,2 it is easy to decide how to discretize the data, but it is ok if the data isn't already bin (ie in 0s 1s and 2s). Quantile splits the data into even chunks (ie if you select quantile 2, it will find the mean and then everything above that is in one bin and everything below that mean is in a different bin). Interval bins things that are in equal sized intervals around each other.

Select Natural fit for spline fitting (this will allow you to have some data points missing ex: no volume reading in 1 data set) Lets select 2 intervals for motor speed, temperature and yield and then 3 intervals for volume and concentration.

MiniTuba also give you the option to force it to come up with some relationships whether MiniTuba thinks they should or not. MiniTuba also allows you to choose the method used to solve this, we will select simulated annealing Number of Instances allows you to choose the number of computers used to solve the problem, we will just leave it at 1 In the Demo version, the max calculation time is 1 min.

When everything is done, click Run Bayesian Analysis. By clicking Check Progress the following screen will show up. Click Update every so often to check whether the solution has been computed.

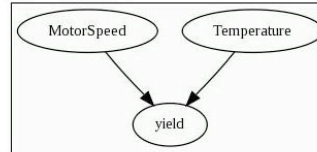


The screenshot shows the MiniTuba web interface. At the top left is the MiniTuba logo. The main header reads "Medical Inference by Network Integration of Temporal Data Using Bayesian Analysis". A navigation bar includes links for Home, Sandbox Demo, Research Projects, Tutorial, Documentation, and FAQs. A user notice states "You are using a Demo account | [My Projects](#) | [Change Password](#) | [Update Profile](#)". The main content area displays "Project: CSTR Example" and "DBN Results of Analysis Job ID: 1167". It shows a submission time of "2008-12-04 16:35:58" and a "Note". A "Number of instances" field is set to 1, with a "Refresh this page" link. Below this, a progress bar for "Instance 1" is shown as "Pending...". A "Go back to my project page" link is at the bottom. The footer contains "Acknowledgements | Links | Contact Us | Disclaimer" and the University of Michigan logo.

This will output the following screen when it is done

Networks Generated:

Top 10 Networks: [No 1.](#) [No 2.](#) [No 3.](#) [No 4.](#) [No 5.](#) [No 6.](#) [No 7.](#) [No 8.](#) [No 9.](#) [No 10.](#)
[Score Distribution of Top 10 Networks ?](#) [Conserved Subnetworks among Top 10 Networks ?](#)



Probability Table and Possible Scatter Plot:

Please click a variable in above network to check its probability table and possible scatter plot.

Run Prediction:

[Click here](#) to run prediction based on current analysis.

Generate Subnetwork: please select a subset from available variables:

Vol
MotorSpeed
Temperature
yield

in No 1 scoring network

Show sub network of selected variables

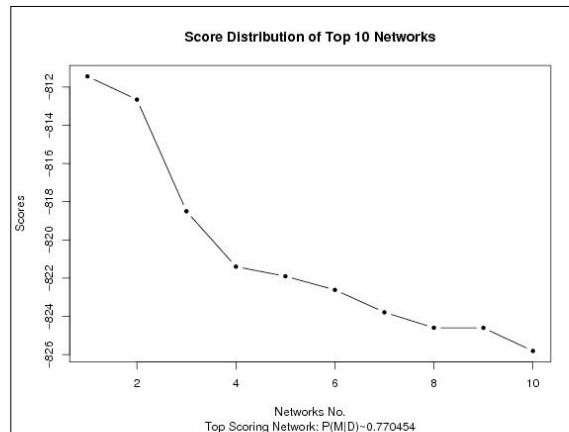
Note: To select more than one nodes, press "Ctrl" or "Shift" button in the keyboard, hold it and click on specific nodes.

[Go back to my project page](#)

As you can see, the yield depends on the motor speed and the temperature alone, just like we crated the modle to show. Top Ten networks, shows the 10 most likely networks. Click Score Distribution of Top Ten Networks shows the relative probability of each network, and the probability that the number 1 network is the correct network out of the top 10. In our example the best network has a probability of 0.77 as seen below.

Networks Generated:

Top 10 Networks: [No 1.](#) [No 2.](#) [No 3.](#) [No 4.](#) [No 5.](#) [No 6.](#) [No 7.](#) [No 8.](#) [No 9.](#) [No 10.](#)
[Score Distribution of Top 10 Networks ?](#) [Conserved Subnetworks among Top 10 Networks ?](#)



6.6 Sage's Corner

An example of using Genie to analyze a Bayesian network

<http://video.google.com/googleplayer.swf?docId=9222502903336100020>

For the powerpoint slides without narration, please [click here](#)

A brief narration for better understanding GENIE

http://www.youtube.com/v/FCy_p1BeDrM


Un-narrated slides can be found at: [Unnarrated Slides](#)

6.7 References

- Charniak, Eugene (1991). "Bayesian Networks without Tears", *AI Magazine*, 50-62.
- GeNIe Helpfile at [GeNIe & SMILE](#)
- Murphy, Kevin. (2002). "Dynamic Bayesian Networks."
- Xiang Z., Minter R., Bi X., Woolf P., and He Y.(2007). "miniTUBA: medical inference by network integration of temporal data using Bayesian analysis," *Bioinformatics*, v. 23, 2423-2432, 2007.

Section 7. Occasionally dishonest casino?: Markov chains and hidden Markov models

Subtitle: Occasionally dishonest casino?: Markov chains and hidden Markov models

Note:  [Video lecture](#) available for this section!

Authors: Nicole Blan, Jessica Nunn, Pamela Roxas, Cynthia Sequerah

Stewards: Kyle Goszyk, So Hyun Ahn, Sam Seo, Mike Peters

Date Presented: 11/21/06; Revised: 11/19/07

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

7.1 Introduction

Basic probability can be used to predict simple events, such as the likelihood a tossed coin will land on heads rather than tails. Instinctively, we could say that there is a 50% chance that the coin will land on heads.

But let's say that we've just watched the same coin land on heads five times in a row, would we still say that there is a 50% chance of the sixth coin toss will results in heads? No – intuitively, we sense that there is a very low probability (much less than 50%) that the coin will land on heads six times in a row.

What causes us to rethink the probability of the coin landing on heads? The same coin is being tossed, but now we are taking into account the results of previous tosses. Basic probability can be used to predict an isolated event. But more advanced probability concepts must be used to assess the likelihood of a certain sequence of events occurring. This wiki article provides an introduction to concepts such as Bayes rule, Markov chains, and hidden Markov models, which are more useful for predicting real world scenarios (which are rarely singular, isolated events).

7.2 Bayes' Rule

Recall the wiki article that discusses [Bayes Rule](#):

$$P(A | B) = \frac{P(B | A)P(A)}{P(B)}$$

Bayes' rule is a foundational concept for finding the probability of related series of events. It relates the probability of event A conditional to event B and the probability of event B conditional to event A, which are often not the same probabilities.

Another interpretation of Bayes' rule: it's a method for updating or revising beliefs (i.e. probability of landing on heads) in light of new evidence (knowing that the coin landed on heads the last five tosses).

Please refer to the [Bayes Rule](#) wiki for a more detailed explanation behind this rule.

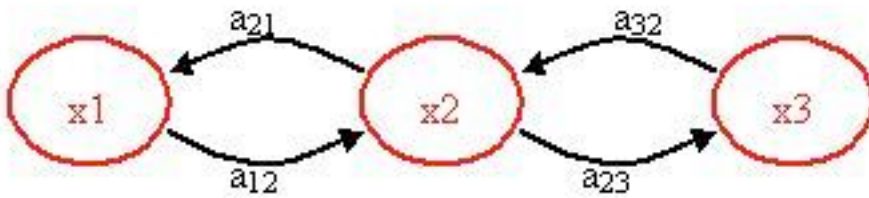
7.3 Markov Chains

A Markov chain is a particular way of modeling the probability of a series of events. A Markov chain is a sequence of random values whose probabilities at a time interval depend only upon the value of the number at the previous time. A Markov chain, named after Andrey Markov, is a stochastic process with the Markov property. This means that, given the present state, future states are independent of the past states. In other words, the description of the present state fully captures all the information that could influence the future evolution of the process, so that future states of the system will be reached through a probabilistic (determined from current data) process instead of a deterministic one (from past data).

At each point in time, the system could either change its state from the current state to a different state, or remain in the same state. This happens in accordance with the specified probability distribution. These changes of state are called transitions, and the probabilities associated with various state changes are called transition probabilities.

For example, let's say we want to know the probability of an elevator moving more than five floors up in a 30-floor building (including the lobby). This is an example of a Markov chain because the probability does not depend on whether the elevator was on the 6th floor at 7:00 am or on the 27th floor at 10:30 pm. Instead the probability is dependent on what floor the elevator is on right before it starts to move. More specifically, the fact that the elevator is on the top floor at t_1 results in a zero probability that the elevator will be five floors higher at t_2 .

The figure below helps to visualize the concept of a Markov Model.



$x_1, x_2, x_3 =$ states

$a_{12}, a_{21}, a_{23}, a_{32} =$ transition probabilities

A transition probability is simply the probability of going from one state to another state. Please note that there may be other paths or transition probabilities for state x_1 , say to state x_3 or back to itself. The sum of the transition probabilities must always equal to 1.

$$\sum_{i=1} a_{1,i} = a_{11} + a_{12} + a_{13} + \dots a_{1n}$$

7.4 Transition Probability

The transition probabilities of each state for one system can be compiled into a transition matrix. The transition matrix for a system can represent a one-step transition or a multiple-step transition. A n-step transition matrix is simply a one-step transition matrix rised to the n-th power.

For state i to make a transition into state j , the transition probability P_{ij} must be greater than 0. so:

$$P_{i,j} \geq 0, i, j \geq 0$$

$$\sum_{j=0} P_{ij} = 1, i = 0, 1, \dots$$

Let \mathbf{P} be the matrix of a one-step transition matrix,

$$\mathbf{P} = \begin{pmatrix} P_{0,0} & P_{0,1} & P_{0,2} & \cdots \\ P_{1,0} & P_{1,1} & P_{1,2} & \cdots \\ \vdots & \ddots & \vdots & \\ P_{i,0} & P_{i,1} & P_{i,2} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix}$$

$P_{i,1}$ would denote the probability of going from state i to 1

Example: Will It Rain Tomorrow? [ref: Ross]

Suppose that whether or not it rains today depends on previous weather conditions through the last two days. Specifically, suppose that if it has rained for the past two days, then it will rain tomorrow with probability 0.7; if it rained today but not yesterday, then it will rain tomorrow with probability 0.5; if it rained yesterday but not today, then it will rain tomorrow with probability 0.4; if it has not rained in the past two days, then it will rain tomorrow with probability 0.2.

The transition matrix for the above system would be:

state 0: if it rained both today and yesterday

state 1: if it rained today but not yesterday

state 2: if it rained yesterday but not today

state 3: if it did not rain either yesterday or today

$$\mathbf{P} = \begin{pmatrix} 0.7 & 0 & 0.3 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0.4 & 0 & 0.6 \\ 0 & 0.2 & 0 & 0.8 \end{pmatrix}$$

7.5 Applications of Markov Chains

Since this concept is quite theoretical, examples of applications of this theory are necessary to explain the power this theory has. Although these following applications are not chemical control related, they have merit in explaining the diversity of operations in which Markov chains can be used. Hopefully, by seeing these examples, the reader will

be able to use Markov chains in new, creative approaches to solve chemical controls problems.

Queuing Theory

Markov chains can be applied to model various elements in something called queuing theory. Queuing theory is simply the mathematical study of waiting lines (or queues).

This theory allows for the analysis of elements arriving at the back of the line, waiting in the line, and being processed (or served) at the front of the line. This method uses the variables including the average waiting time in the queue or the system, the expected number waiting or receiving service and the probability of encountering the system in certain states, such as empty, full, having an available server or having to wait a certain time to be served. These variables are all unique to the system at hand. A link that explains this theory in more detail can be found below:

[Queuing Theory](#)

Although Queuing Theory is generally used in customer service, logistics and operations applications, it can be tailored to chemical processing. For instance, it is essential to model how long a particular product will be in an assembly line before it makes it to the desired end process. Thus, this theory is robust for all kinds of uses.

7.6 Queuing Problem Example

On a sunny Tuesday morning in the Computer Engineering Building, a group of Chemical Engineering students are finishing their engineering laboratory reports and have stayed up all night writing ambivalent fluid mechanics questions, they need some prestigious coffee for refreshment instead of Red Bull. Coffee shop called "Dreamcaster's Cafè" was opened by a University of Michigan Chemical Engineering graduate. Business is going very well for "Dreamcaster's Cafè" and there are many people, m people, waiting in line in front of the Chemical Engineering students. The service time for the first person in line (not necessarily a Chemical Engineering student) is an exponential distribution

$$\frac{1}{\mu}$$

with an average waiting time of $\frac{1}{\mu}$. Since the Chemical Engineering students have to return to the Computer Engineering Building to finish their report, they have a finite patience waiting in line and their patience is an exponential distribution with an average

$$\frac{1}{\theta}$$

of $\frac{1}{\theta}$. The group of Chemical Engineering students does not care how long the service

time is. Find the probability that the *i*th Chemical Engineering student to wait long enough to get coffee.

Solution

X_j = the patience of person # j in line

$X_j \sim \text{Exp}(\mu)$

Let Y = time it takes to serve the first customer

$Y \sim \text{Exp}(\mu)$

P_j = probability that the j^{th} person waited long enough to get coffee

For the first person, $n=1$:

$$P_1 = P\{X_1 > Y\} = \frac{\mu}{\mu + \mu}$$

For the n -th person in line, we can use the memoryless property of exponential functions:

$A_n = \{\text{Person } n \text{ served}\}$

$B_n = \{\text{person } n \text{ leaves before buying coffee, he/she is out of patience}\} = \{X_n < \min\{X_1, X_2, \dots, X_{n-1}, Y\}\}$

Note that $P_n = P(A_n)$

$$P_n = P(A_n | B_n) + P(A_n | B_n^c)$$

$$P_n = P(A_n | B_n) P(B_n)$$

$$P_n = P(A_n | B_n) \frac{(n-1)\mu + \mu}{n\mu + \mu}$$

$$P_n = P(A_n | B_n) \frac{(n-1)\mu + \mu}{n\mu + \mu}$$

$$P_n = \frac{\mu}{n\mu + \mu}$$

Since there were already m people on the line, the i -th student is really the n -th person minus the m people on the line, so:

$$P_i = \frac{\mu}{(m+1)\mu + \mu}$$

Google's Page Ranking System

The PageRank of a webpage as used by Google is defined by a Markov chain.

PageRank is the probability to be at page i in the following Markov chain on all (known) webpages. If N is the number of known webpages, and a page i has k_i links then it has transition probability

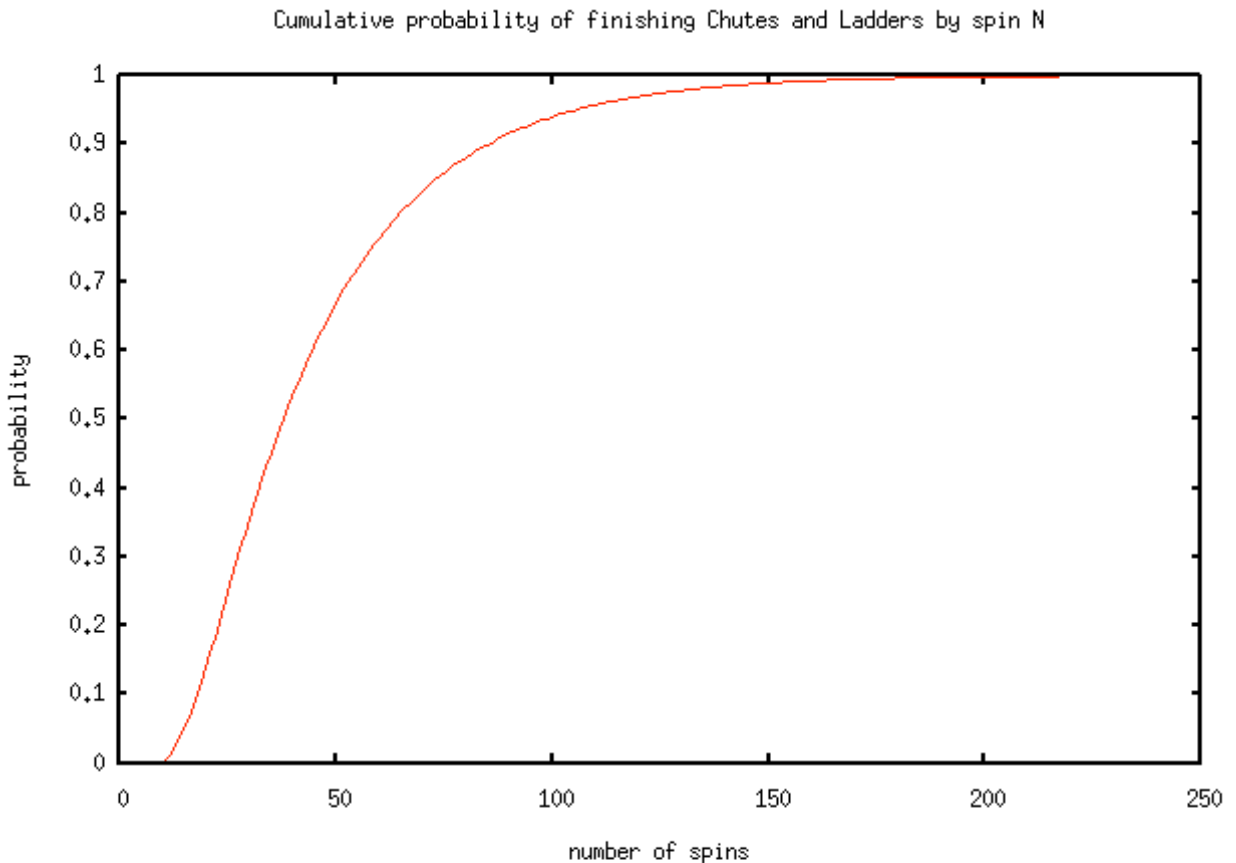
$$(1 - q) / k_i + q / N$$

for all pages that are linked to and q/N for all pages that are not linked. The constant q is around 0.15.

Children's Games

Markov chains are used in the children's games "Chutes and Ladders," "Candy Land" and "Hi Ho! Cherry-O!" These games utilize the Markov concept that each player starts in a given position on the game board at the beginning of each turn. From there, the player has fixed odds of moving to other positions.

To go into further detail, any version of Snakes and Ladders can be represented exactly as a Markov chain, since from any square the odds of moving to any other square are fixed and independent of any previous game history. The Milton Bradley version of Chutes and Ladders has 100 squares, with 19 chutes and ladders. A player will need an average of 45.6 spins to move from the starting point, which is off the board, to square 100.



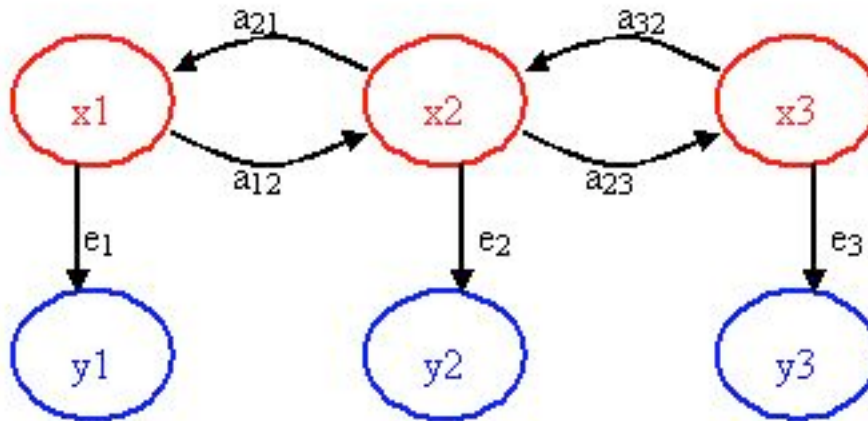
One last game of interest is Monopoly. This can be modeled using Markov chains. Check out the following link to see a simulation of the probability of landing on a particular property in the Monopoly game:

Monopoly Simulation

7.7 Hidden Markov Models

Building further on the concept of a Markov chain is the hidden Markov model (HMM). A hidden Markov model is a statistical model where the system being modeled is assumed to be a Markov process with unknown parameters or casual events. HMMs are primarily helpful in determining the hidden parameters from the observable parameters.

Again, the figure below may help visualize the Hidden Markov Model concept.



x_1, x_2, x_3 = hidden/unknown states

$a_{12}, a_{21}, a_{23}, a_{32}$ = transition probabilities

y_1, y_2, y_3 = observable states

e_1, e_2, e_3 = emission probabilities

The key point of the figure above is that only the blue circles are seen, but you suspect or know that these *observable states* are directly related or dependent on some *hidden state*. These hidden states (the red circles) are what actually dictates the outcome of the observable states. The challenge is to figure out the hidden states, the emission probabilities and transition probabilities.

For example, say you have a data acquisition program that continuously records the outlet temperature of your product stream which you are heating up through a heat exchanger. The heat exchanger provides a constant supply of heat. You observe that the temperature has some step disturbances and is not always constant. The temperature is the observable parameter, but the cause of its deviations/states is actually the stream's flowrate. When the flowrate fluctuates, the outlet temperature also fluctuates since the heat exchanger is providing the same amount of heat to the stream. So, the stream flowrate is the hidden

parameter (since you do not have access to this measured variable) and the probability that the flowrates switches from say 100 to 150 to 300 L/h are the transition probabilities. The emission probability is the probability that the observed outlet temperature is directly caused by the flowrate. This emission probability is not necessarily 1 since temperature variations could also be due to noise, etc.

Another common scenario used to teach the concept of a hidden Markov model is the “Occasionally Dishonest Casino”. If a casino uses a fair die, each number has a $1/6$ probability of being landed on. This type of probability that represents a known parameter is known as emission probability in HMMs. Sometimes a casino can tip the odds by using a loaded die, where one number is favored over the other five numbers and therefore the side that is favored has a probability that is higher than $1/6$.

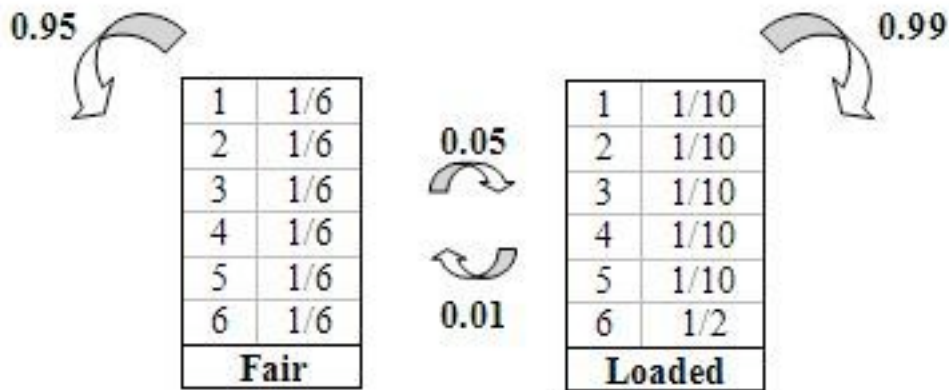
But how does one know that the casino is being dishonest by using a loaded die? Pretend that the die is loaded in such a way that it favors the number 6. It would be difficult to differentiate between a fair die and loaded die after watching only one roll. You may be able to get a better idea after watching a few tosses and see how many times the die landed on 6. Let’s say that you saw the following sequence of die tosses:

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It is still difficult to say with certainty whether the die is loaded or not. The above sequence is a feasible for both a fair die and a loaded die. In this particular case, the above numbers that represent what was rolled are the observable parameters. The hidden parameter is the type of die used just because we do not know which type produced the above sequence of numbers.

Instead of relying on a sneaking suspicion that the casino is being dishonest, one can use a hidden Markov model to prove that a loaded die is being used occasionally. Please note that if a loaded die was used all the time it would be more blatantly obvious. In order to get away with this “slight” unfairness, the casino will switch the fair die with a loaded one every so often. Let’s say that if a fair die is being used there is a 5% chance that it will be switched to a loaded die and a 95% chance that it will remain fair. These are known as transition probabilities because they represent the likelihood of a causal event changing to another causal event.

Below is a picture representing the transition probabilities (probability of staying or changing a type of die) as well as the emission probabilities (probability of landing on a number).



Using the basic diagram above that show the emission and transition properties, conditioned statements in Excel can be used to model the probability that a loaded die is being used. Please refer to example two for the hidden Markov model Excel sheet.

HMMs can be modeled using Matlab. Follow the link to the site which contains information in installing the HMM toolbox in Matlab:

[HMMs in Matlab](#)

7.8 Worked out Example 1: "What should I wear?"

Being a student of the University of Michigan, one of your daily concerns is the weather. The weather affects important issues such as, choice of clothing, shoes, washing your hair, and so many more. Considering the bizarre weather in Ann Arbor, you wish to be able to calculate the probability that it will rain given the data of the last three consecutive days. Applying your chemical engineering skills and empowered by the knowledge from this Wiki article, you sit down and decide to be the next Weather-Person.

You know the following information since you have been an avid fan of the Weather Channel since age 5.

Weather	P(rain weather)	P(blizzard weather)
Sunny	0.15	0.05
Blizzard	0.25	0.15
Rainy	0.6	0.1

You then record the weather for the past 3 days.

Day	Weather
1	Rain
2	Rain
3	Blizzard
4	?

Solution

Since the last day was a blizzard you use a matrix expressing a 100% chance in the past, and multiply this by the probabilities of each weather type.

$$[0 \quad 1 \quad 1] \begin{bmatrix} .8 & .15 & .05 \\ .6 & .25 & .15 \\ .3 & .6 & .1 \end{bmatrix} = [.6 \quad .25 \quad .15]$$

This means that there is a 60% chance of sun, a 25% chance of rain and a 15% chance of a blizzard. This is because a Markov process works based on the probability of the immediately previous event. Thus, you decide that is a low enough risk and happily decide to wear your best new outfit AND wash your hair.

7.9 Worked out Example 2: "What should I wear for the weekend?"

Turns out it does rain the next day and you get your favorite clothes soaked. However, you are leaving for a weekend with your family and must decide what to wear for the next two days. What is the prediction for the next two days?

Solution

Predicting for the first day is like the previous example substituting rain in for a blizzard.

$$[0 \quad 0 \quad 1] \begin{bmatrix} .8 & .15 & .05 \\ .6 & .25 & .15 \\ .3 & .6 & .1 \end{bmatrix} = [.3 \quad .6 \quad .1]$$

In order to predict for the second day we must use our previous data to predict how the weather will act. Since we predict two days ahead we multiply the probabilities twice, effectively squaring them.

$$\begin{bmatrix} 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} .8 & .15 & .05 \\ .6 & .25 & .15 \\ .3 & .6 & .1 \end{bmatrix}^2 = \begin{bmatrix} .63 & .255 \end{bmatrix}$$

Alternatively, we can take the prediction from the previous day and multiply that by the probability of weather.

$$\begin{bmatrix} .3 & .6 & 1 \end{bmatrix} \begin{bmatrix} .8 & .15 & .05 \\ .6 & .25 & .15 \\ .3 & .6 & .1 \end{bmatrix} = \begin{bmatrix} .63 & .255 & .115 \end{bmatrix}$$

Both ways give you the same answer. Therefore, you decide to pack for both sunny and rainy weather.

7.10 Worked out Example 3: OSEH Example

Now, back to REAL chemical engineering applications, the probability theories described above can be used to check if a piece of equipment is working. For example, you are an OSEH inspector and you have to analyze a set of data recording the pollutant levels of a plant. If they use the scrubber they have, the probability of pollutant levels being high is low. However, if the scrubber is not used, the probability of pollutant levels being high increases. You have gotten some inside information that the operators use the scrubbers only 70% off the time. Your task is to create a model based on the data recordings and using probability theories to *predict* WHEN they switch their scrubbers ON and OFF, so that you can catch them red-handed in the act!

There are 6 possible pollutant levels: none, low, med-low, med, med-high, and high. If the level = high, then this is above the allowable limit. Every other level is considered allowable. If the scrubber is ON, there is equal chance that any of the states will occur. If the scrubber is OFF, there is a 50% chance that a *high* pollutant level will be recorded.

Given the following data:

$P(E_{on}) = 0.7$	<i>probability of equipment is operating</i>								
$P(E_{off}) = 0.3$	<i>probability of equipment is NOT operating</i>								
six possible states of pollutant quantity: none, low, med-low, med, med-high, high, Let pollutant quantity of <i>high</i> be over the allowable limit by OSEH									
Readings are taken every hour by a composition analyzer									
Scrubber on									
$P(<limit E_{on})$	<i>probability of pollutant quantity being less than the allowable limit i.e. none, low, med-low, med, med-high</i>								
$P(<limit E_{on})$	(5/6)								
$P(limit E_{on})$	<i>probability of pollutant quantity being equal or more than the allowable limit i.e. high</i>								
$P(limit E_{on})$	(1/6)								
Scrubber off									
$P(<limit E_{off})$	0.5								
$P(=limit E_{off})$	0.5								

Solution

Formulas used are listed below:

(1)

$$P(Data|E_{on}) = P(<limit|E_{on})^{n-1} P(limit|E_{on})^n = \left(\frac{5}{6}\right)^{n-1} \left(\frac{1}{6}\right)^n$$

(2)

$$P(Data|E_{off}) = P(<limit|E_{off})^{n-1} P(limit|E_{off})^n = \left(\frac{1}{2}\right)^{n-1} \left(\frac{1}{2}\right)^n$$

(3)

$$P(Data) = P(Data|E_{on}) * P(E_{on}) + P(Data|E_{off}) * P(E_{off})$$

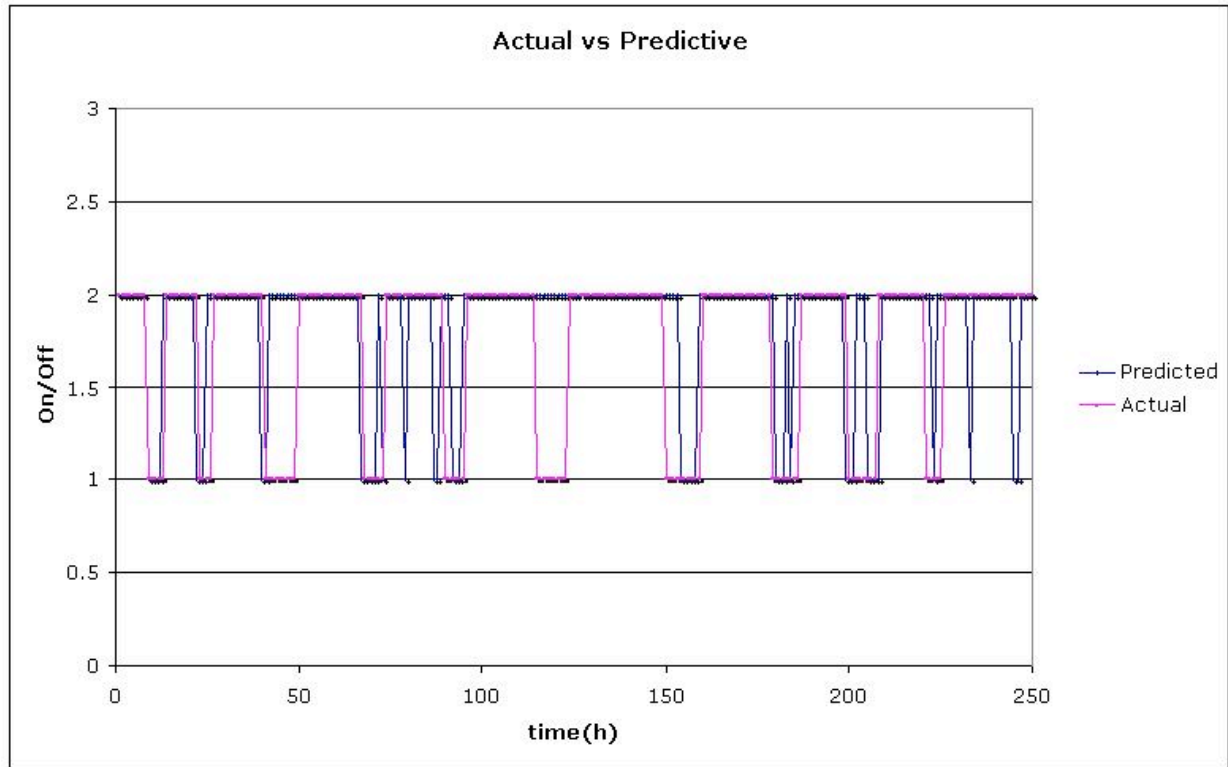
$$P(E_{on}|Data) = \frac{P(Data|E_{on}) * P(E_{on})}{P(Data)}$$

(4)

Please refer to the attached Excel File for the predictive model. [OSEHExample](#)

From our results in the Excel file, we graphed the predicted vs actual times when the scrubber was turned off. The value of "1" was chosen arbitrarily to represent when the

scrubber was OFF and "2" when it was "ON".



7.11 Multiple Choice Question 1

What is the key property of a Markov chain?

- A) Probability of each symbol depends on FUTURE symbols.
- B) Probability of each symbol depends on ALL preceding symbols.
- C) Probability of each symbol depends on NONE of the preceding symbols.
- D) Probability of each symbol depends only on the value of the PREVIOUS symbol.

7.12 Multiple Choice Question 2

What kind of parameters does emission probability represent?

- A) unknown parameters
- B) Markov parameters
- C) known parameters
- D) Bayes' parameters

7.13 Sage's Corner

The Occasionally Dishonest Casino explained and applied to a short example:

<http://video.google.com/googleplayer.swf?docId=-2874032065834002418>

Please click the following link for a copy of the PowerPoint slides: [Occasionally Dishonest Casinos](#)

7.14 References

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- For more information on when to reference see [the following wikipedia entry](#).
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Section 8. Continuous Distributions: normal and exponential

Title: Continuous Distributions: normal and exponential

Authors: Navin Raj Bora, Dallas Burkholder, Nina Mohan, Sarah Tschirhart

Date Presented: November 21, 2006

Date Revised:

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

8.1 Introduction

Random variables whose spaces are not composed of a countable number of points but are intervals or a union of intervals are said to be of the continuous type. Continuous distributions are probability models used to describe variables that do not occur in discrete intervals, or when a sample size is too large to treat each individual event in a discrete manner (please see [Discrete Distributions](#) for more details on discrete distributions). The main difference between continuous and discrete distributions is that continuous distributions deal with a sample size so large that its random variable values are treated on a continuum (from negative infinity to positive infinity), while discrete distributions deal with smaller sample populations and thus cannot be treated as if they are on a continuum. This leads to a difference in the methods used to analyze these two types of distributions: continuous and discrete distributions are analyzed using calculus, while discrete distributions are analyzed using arithmetic. There are many different types of continuous distributions including some such as Beta, Cauchy, Log, Pareto, and Weibull. In this wiki, though, we will only cover the two most relevant types of continuous distributions for chemical engineers: Normal (Gaussian) distributions and Exponential distributions.

In chemical engineering, analysis of continuous distributions is used in a number of applications. For example in error analysis, given a set of data or distribution function, it is possible to estimate the probability that a measurement (temperature, pressure, flow rate) will fall within a desired range, and hence determine how reliable an instrument or piece of equipment is. Also, one can calibrate an instrument (eg. temperature sensor) from the manufacturer on a regular basis and use a distribution function to see if the variance in the instruments' measurements increases or decreases over time.

8.2 Normal Distributions

8.2.1 What is a Gaussian (normal) distribution curve?

A Gaussian distribution can be used to model the error in a system where the error is caused by relatively small and unrelated events.

This distribution is a curve which is symmetric about the mean (i.e. a Bell shaped curve) and has a range measured by standard deviations above and below the mean of the data set (please see [Basic Statistics](#) for a further discussion on these statistical parameters). To better explain, consider that a certain percentage of all data points will fall within one standard deviation of the mean. Likewise, more data points will fall within two standard deviations of the mean, and so on. However, under this model it would require an infinite range to capture ALL the data points thus presenting a minor difficulty in this approach.

The figure below is a possible Gaussian distribution, where the mean (μ) is 10 and standard deviation (σ) is 2. $F(x)$ is the number of times a certain value of x occurs in the population. The mean is simply the numerical average of all the samples in the population, and the standard deviation is the measure of how far from the mean the samples tend to deviate. The following sections explain how and why a normal distribution curve is used in control and what it signifies about sets of data.

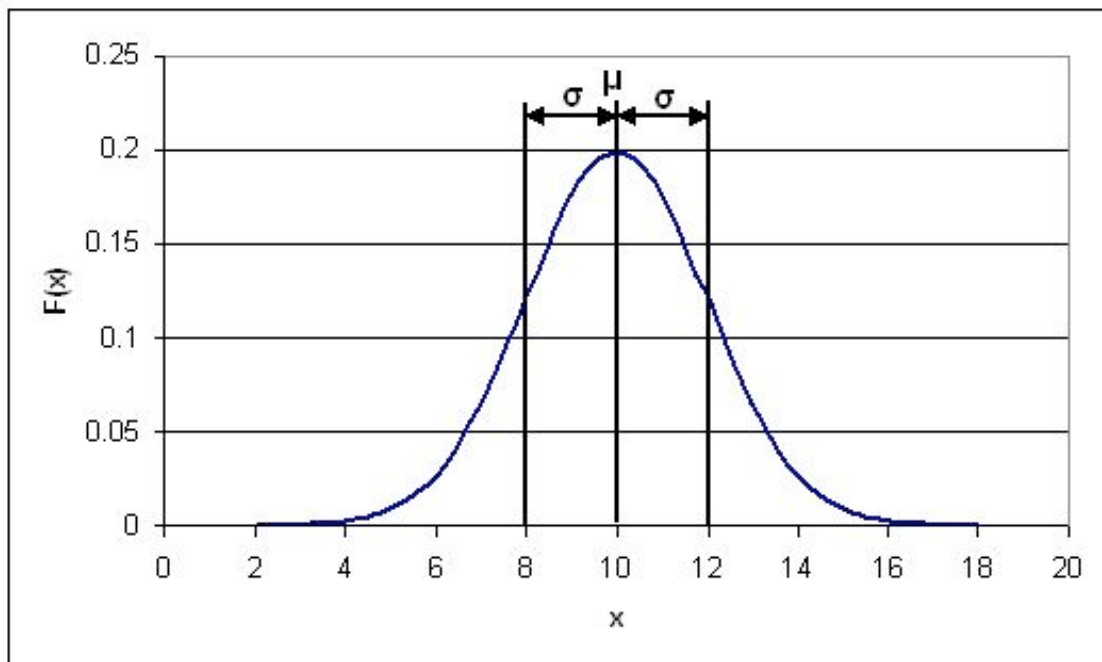


Figure 1: Generic Normal Distribution curve

8.2.2 The Probability Density Function (PDF) for a normal distribution

As was mentioned in the Introduction section, distribution curves can be used to determine the probability, $P(x)$, of a certain event occurring. When this is done, the distribution curve is known as a Probability Density Function (**PDF**). In the figure shown above, the x-axis represents the range of possible events (eg. the range of ages in a sample population or the magnitude of noise generated by a temperature sensor). The y-axis represents the number of times a certain x value occurs in a population. The PDF can be described mathematically as follows:

$$P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} * e^{-(x-\mu)^2/2*\sigma^2}$$

In some cases, it might not be necessary to know the probability of just one event occurring. Rather, you may want to know the probability of a range of events (eg. what is the probability that the noise generated by my temperature sensor will fall in the range of 5-10 Hz?). When this happens, you must integrate the above PDF over the desired range, in the following manner:

$$P(k_1 < x < k_2) = \int_{k_1}^{k_2} \left(\frac{1}{\sqrt{2\pi\sigma^2}} * e^{-(x-\mu)^2/2*\sigma^2} \right) dx$$

where k_1 and k_2 are the limits of your desired range. This integral results in the following expression:

$$P(k_1 < x < k_2) = \frac{1}{2} \left(\text{Erf}f\left[\frac{k_2 - \mu}{\sigma\sqrt{2}}\right] - \text{Erf}f\left[\frac{k_1 - \mu}{\sigma\sqrt{2}}\right] \right)$$

The *Erf* function can be found in most scientific calculators and can also be calculated using tables of *Erf* values. For example, its use here parallels what we learned in ChE 342, Heat and Mass Transfer. Determine the value inside the brackets of the erf function through simple arithmetic, then take this value and find the corresponding Erf number from a table. Finally use this value in the calculation to determine the probability of a certain point, x, falling within a range bound from k1 to k2.

Sample Calculation

Given a data set with an average of 20 and a standard deviation of 2, what is the probability that a randomly selected data point will fall between 20 and 23?

Solution 1

To solve simply substitute the values into the equation above. This yields the following equation:

$$P(20 < x < 23) = \frac{1}{2} \left(\text{Erf} \left[\frac{23 - 20}{2\sqrt{2}} \right] - \text{Erf} \left[\frac{20 - 20}{2\sqrt{2}} \right] \right)$$

$$P(20 < x < 23) = \frac{1}{2} (\text{Erf} [1.061] - \text{Erf} [0])$$

These Erf values must be looked up in a table and substituted into the equation. Doing this yields

$$P(20 < x < 23) = \frac{1}{2} (0.933255 - 0.5) = 0.433255$$

Thus there is a 43.3255% chance of randomly selecting a number from the data set with a value between 20 and 23.

Graphically speaking, the PDF is just the area under the normal distribution curve between k_1 and k_2 . So, for the distribution shown above, the PDF for $8 < x < 12$ would correspond the area of the orange shaded region in the figure below:

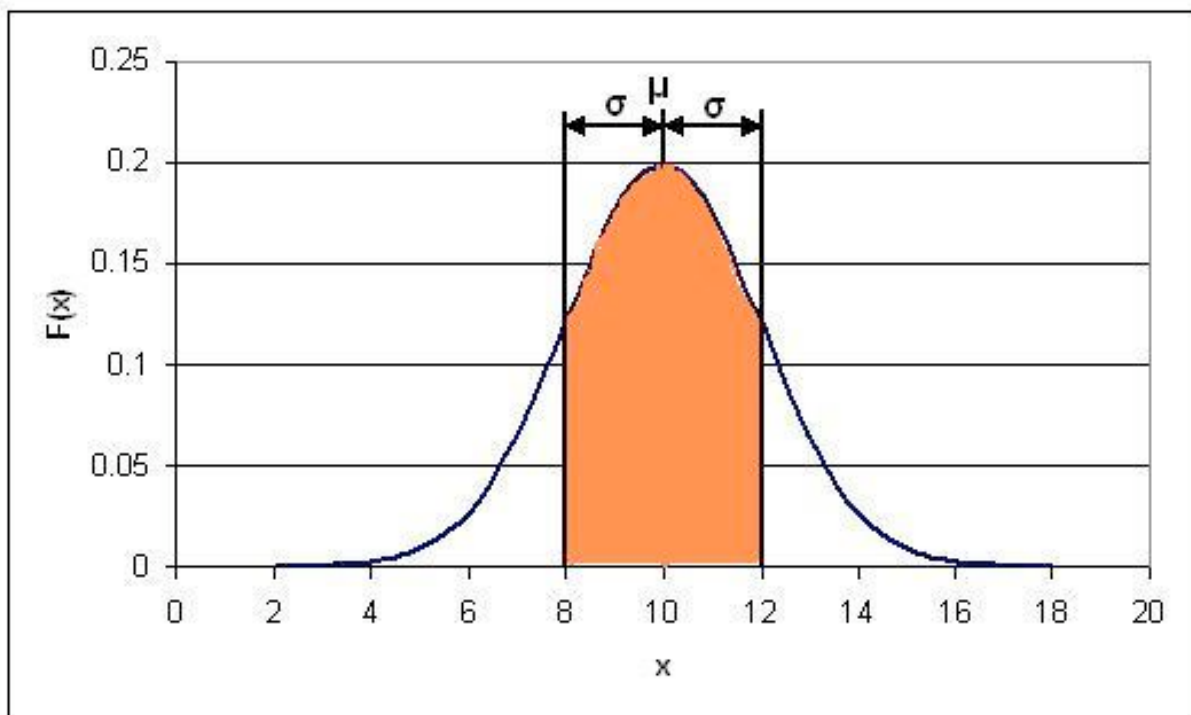


Figure 2: PDF for $8 < x < 12$

Solution 2

Alternatively, rather than using the error function, Mathematica's built-in probability density function can be used to solve this problem. This probability density function can be applied to the normal distribution using the syntax shown below.

```
NIntegrate[PDF[NormalDistribution[ $\mu$ , $\sigma$ ],x],{x,x1,x2}]
```

In this syntax, μ represents the mean of the distribution, σ represents the standard deviation of the distribution, and x_1 and x_2 represent the limits of the range.

This function can be applied to this problem as shown below.

```
In[1]:= NIntegrate[PDF[NormalDistribution[20, 2], x], {x, 20, 23}]  
Out[1]= 0.433193
```

This shows that the probability of a randomly selected data point falling between 20 and 23 is 0.4332, or 43.32%. As expected, this value calculated using the built-in probability density function in Mathematica matches the value calculated from using the error function. Mathematica provides a faster solution to this problem.

An important point to note about the PDF is that when it is integrated from negative infinity to positive infinity, the integral will always be equal to one, regardless of the mean and standard deviation of the data set. This implies that there is a 100% chance that your random variable x will fall between negative infinity and positive infinity. Likewise, the integral between negative infinity and the mean is 0.5, or there is a 50% chance of finding a value in this region due to the symmetric nature of the distribution.

8.2.3 The Cumulative Density Function (CDF) for a normal distribution

To transition our argument to a more holistic perspective regarding the probability density function for a normal distribution, we present the cumulative density function, which represents the integral (area under the curve) of the PDF from negative infinity to some given value on the y -axis of the graph incrementally according to the x axis, which remains the same as before. Because of this type of definition, we may circumvent the rigorous error function analysis presented above by simply subtracting one CDF point from another. For example, if engineers desire to determine the probability of a certain value of x falling within the range defined by k_1 to k_2 and possess a chart featuring data of the relevant CDF, they may simply find $CDF(k_2) - CDF(k_1)$ to find the relevant probability.

The Cumulative Density Function (**CDF**) is simply the probability of the random variable, x , falling at or below a given value. For example, this type of function would be used if you wanted to know the probability of your temperature sensor noise being less than or equal to 5 Hz. The CDF for a normal distribution is described using the following expression:

$$P(-\infty < x < k) = \frac{1}{2} \left(\text{Erf} \left[\frac{k - \mu}{\sigma \sqrt{2}} \right] + 1 \right)$$

where k is the maximum allowable value for x .

The main difference between the PDF and CDF is that the PDF gives the probability of your variable x falling within a definite range, where the CDF gives the probability of your variable x falling at or below a certain limit, k . The following figure is the CDF for a normal distribution. You'll notice that as x approaches infinity, the CDF approaches 1. This implies that the probability of x falling between negative and positive infinity is equal to 1.

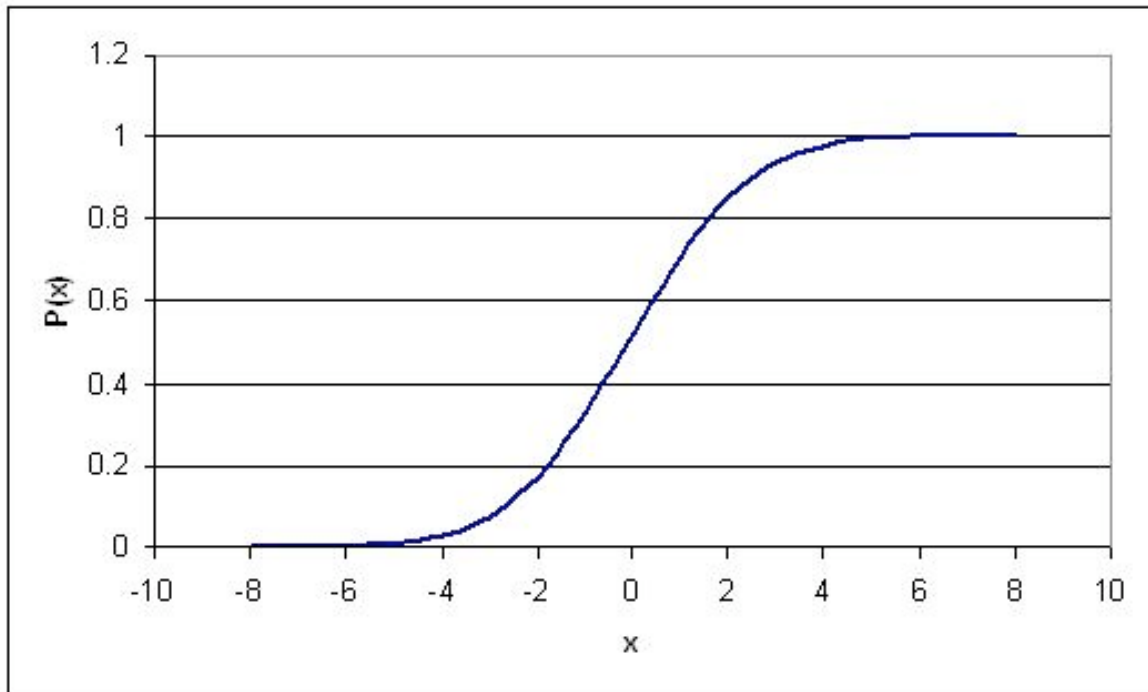


Figure 3: CDF plot for a Normal Distribution

8.2.4 Standard Normal Distribution

A special type of probability distribution curve is called the **Standard Normal Distribution**, which has a mean (μ) equal to 0 and a standard deviation (σ) equal to 1.

This simplified model of distribution typically assists engineers, statisticians, business strategists, economists, and other interested professionals to model process conditions, and to associate the attention and time needed to address particular issues (i.e. higher probability for a failed condition necessitate additional attention, etc.). Also, our grades in many of the courses here at the U of M, both in and outside of the college of engineering, are based either strictly or loosely off of this type of distribution. For example, the B range typically falls within +/- of one standard deviation.

The following figure is a Standard Normal Distribution curve:

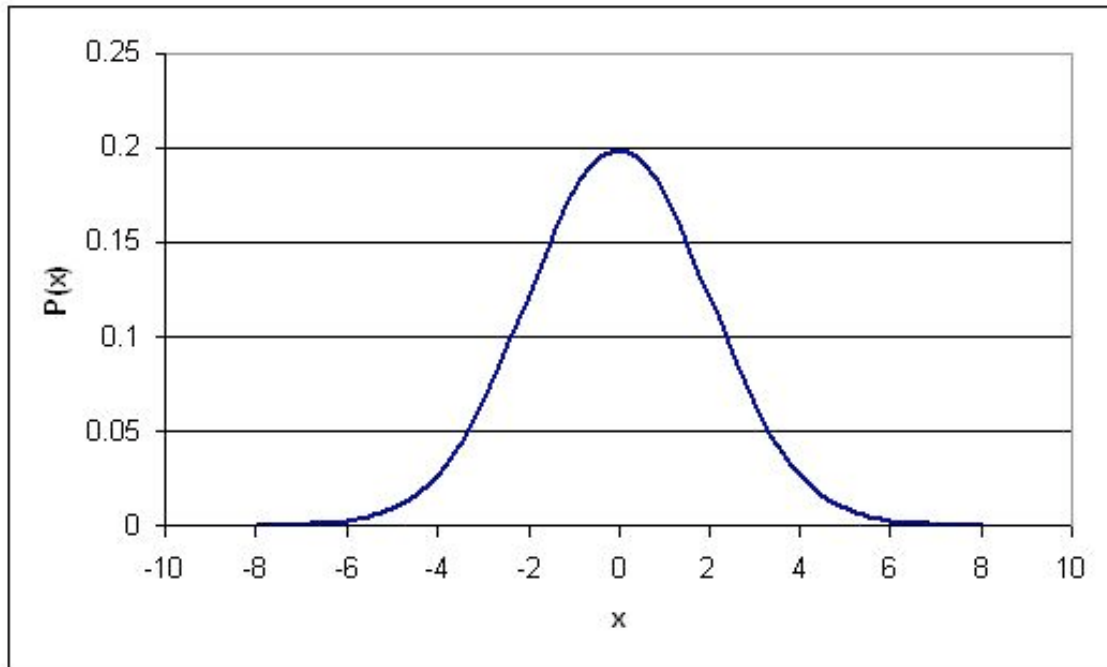


Figure 4: Standard Normal Distribution Curve

The benefit of the standard normal distribution is it can be used in place of the $Erf[]$ function, if you do not have access to a scientific calculator or $Erf[]$ tables. To use the Standard Normal Distribution curve, the following procedure must be followed:

1.Perform a z-transform. This is a transformation which essentially normalizes any normal distribution into a standard normal distribution. It is done using the following relationship:

$$z = \frac{x - \mu}{\sigma}$$

Mathematically speaking, the z transform normalizes the data by changing all the raw data points into data points that dictate how many standard deviations they fall away from the mean. So, regardless of the magnitude of

the raw data points, the standardization allows multiple sets of data to be compared to each other.

2. Use a standard normal table to find the p-value. A standard normal table has values for z and corresponding values for F(x), where F(x) is known as the p-value and is just the cumulative probability of getting a particular x value (like a CDF). A standard normal table may look like the following table (it should be noted that if you are dealing with a Standard Normal Table that contains only positive z values, the following property can be used to convert your negative z values into positive ones: $F(-z) = 1 - F(z)$):

Table 1: Standard Normal Table

z	F(x)	z	F(x)	z	F(x)
-2.5	0.006	-1	0.159	0.5	0.691
-2.4	0.008	-0.9	0.184	0.6	0.726
-2.3	0.011	-0.8	0.212	0.7	0.758
-2.2	0.014	-0.7	0.242	0.8	0.788
-2.1	0.018	-0.6	0.274	0.9	0.816
-2	0.023	-0.5	0.309	1	0.841
-1.9	0.029	-0.4	0.345	1.1	0.864
-1.8	0.036	-0.3	0.382	1.2	0.885
-1.7	0.045	-0.2	0.421	1.3	0.903
-1.6	0.055	-0.1	0.46	1.4	0.919
-1.5	0.067	0	0.5	1.5	0.933
-1.4	0.081	0.1	0.54	1.6	0.945
-1.3	0.097	0.2	0.579	1.7	0.955
-1.2	0.115	0.3	0.618	1.8	0.964
-1.1	0.136	0.4	0.655	1.9	0.971

A more detailed standard normal table can be found [here](#) (Note: This table is the same table used in the 'Basic Statistics' wiki).

3. What if I want the probability of z falling between a range of x=a and x=b? First, find your two z values that correspond to a and b. So these would

be $z_a = \frac{a - \mu}{\sigma}$ and $z_b = \frac{b - \mu}{\sigma}$, respectively. The probability of x falling in between a and b is just: $F(z_b) - F(z_a)$, where $F(z_b)$ and $F(z_a)$ are found from the standard normal tables.

Sample Calculation

Lets take the same scenario as used above, where you have a data set with an average of 20 and standard deviation of 3 and calculate the probability of a randomly selected data point being between 20 and 23.

Solution

To do this simply subtract the two Z scores:

$$z_a = \frac{23 - 20}{2} = 1.5$$
$$z_b = \frac{0 - 20}{2} = -10$$

These Z scores correspond to probabilities of 0.933 and 0.5 respectively. Their difference, 0.433, is the probability of a randomly selected value falling between the two. Notice that this is almost identical to the answer obtained using the Erf method. Note that obtaining this answer also required much less effort. This is the main advantage of using Z scores.

8.3 Properties of a Normal Distribution

There are several properties for normal distributions that become useful in transformations.

1 If X is a normal with mean μ and σ^2 often noted $X \sim N(\mu, \sigma^2)$, then the transform of a data set to the form of $aX + b$ follows a $\sim N(a * \mu + b, a^2 * \sigma^2)$.

2 A normal distribution can be used to approximate a binomial distribution (n trials with probability p of success) with parameters $\mu = np$ and $\sigma^2 = np(1 - p)$. This is derived using the limiting results of the central limit theorem.

3 A normal distribution can be used to approximate a Poisson distribution (parameter λ) with parameters $\mu = \sigma^2 = \lambda$. This is derived using the central limit theorem.

4 The a sum of random variables following the same normal distribution $\sim N(n\mu, n\sigma^2)$. This

$$\sim N\left(\mu, \frac{\sigma^2}{n}\right)$$

result shows how the sample mean

5 The square of a standard normal variable is a chi-squared variable with one degree of freedom.

6 Combining 4 and 5 yields the sum of n squared standard normal variables is a chi-squared variable with n degrees of freedom. This has application for chi-square testing as seen other sections of this text.

8.4 Exponential Distribution

The exponential distribution can be thought of as a continuous version of the geometric distribution without any memory. It is often used to model the time for a process to occur at a constant average rate. Events that occur with a known probability for a given x value build the theory developed previously (i.e. F(x) vs. x, F(x) in this case is different than before), where x may indicate distance between mutations on a DNA strand., for one example application, rate of instrument failure, or time required for a radioactive particle to decay (the decay RATE) for the below applications.

However, do remember that the assumption of a constant rate rarely holds as valid in actuality. The rate of incoming phone calls differs according to the time of day. But if we focus on a time interval during which the rate is roughly constant, such as from 2 to 4 p.m. during work days, the exponential distribution can be used as a good approximate model for the time until the next phone call arrives.

One can implement the exponential distribution function into Mathematica using the command: `ExponentialDistribution[lambda]`.

Or, for a more grass-roots understanding of the function reference the following website, detailing the number of sharks seen in area one square mile in different one hour time periods. Use the "Fish" button to run the applet. To change the parameter lambda, type in the value and hit the "Clear" button.

http://www.math.csusb.edu/faculty/stanton/m262/poisson_distribution/Poisson_old.html

8.4.1 The Probability Density Function (PDF)

A few notes are worth mentioning when differentiating the PDF from the two-parameter Exponential Distribution function. As λ is decreased in value, the distribution is stretched out to the right, and as λ is increased, the distribution is pushed toward the origin. This distribution has no shape parameter as it has only one shape, i.e. the exponential, and the only parameter it has is the failure rate, λ . The distribution starts at $T = 0$ at the level of $f(T = 0) = \lambda$ and decreases thereafter exponentially and monotonically as T increases, and is convex. The PDF for an exponential distribution is given in the form below, where λ is the rate parameter and x is random variable:

$$P(x) = \begin{cases} \lambda e^{-\lambda x} & x \geq 0 \\ 0 & x < 0 \end{cases}$$

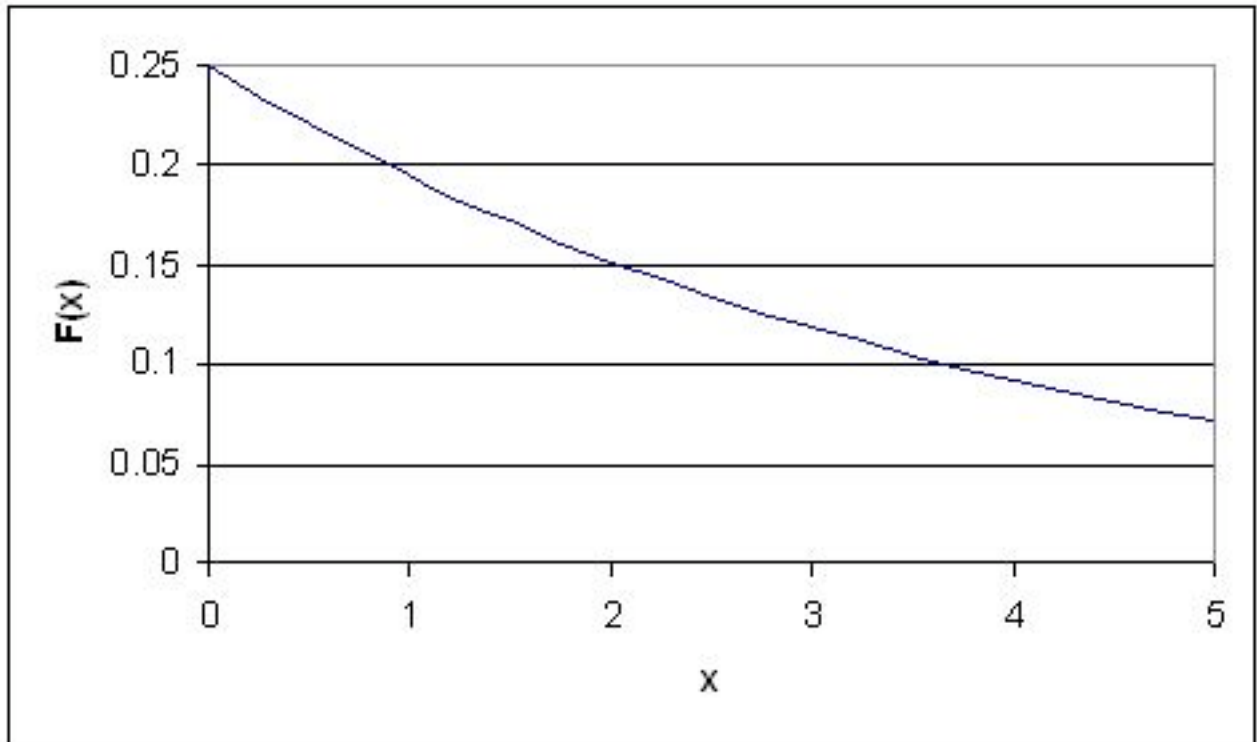


Figure 5: PDF ($\lambda = 0.25$) for Exponential Distribution

Here, x could represent time while the rate parameter could be the rate in which decay occurs. The rate parameter must be constant and greater than 0. The PDF decreases continuously in this diagram because of its definition as a decay example. Exponential decay typically models radioactive particles which lose mass per unit of time. Thus $F(x)$ represents the mass of the particle with x equalling elapsed time since the start of the decay. As time passes, the mass falls due to radioactive decay (particle emits radiation as a form of energy release, any energy that results subtracts from mass, $E = MC^2$).

8.4.2 The Cumulative Distribution Function (CDF)

The CDF for an exponential distribution is expressed using the following:

$$P(x) = \begin{cases} 1 - e^{-\lambda x} & x \geq 0 \\ 0 & x < 0 \end{cases}$$

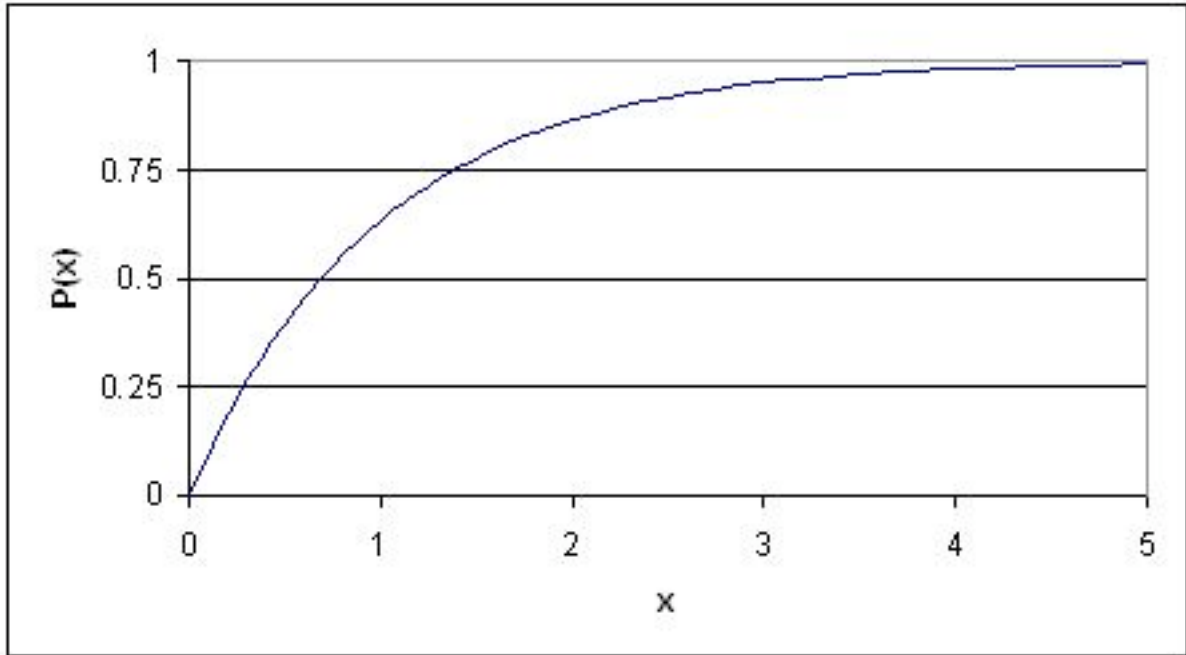


Figure 6: CDF ($\lambda = 1$) for Exponential Distribution

Following the example given above, this graph describes the probability of the particle decaying in a certain amount of time (x).

8.5 Properties of the Exponential Distribution

Among the distribution functions, the exponential distribution function has two unique properties, they are the memoryless property and a constant hazard rate.

--The Memoryless Property--

If a random variable, X , survived for " t " units of time, then the probability of X surviving an additional " s " units of time is the same as the probability of X surviving " s " units of time. The random variable has "forgotten" that it has survived for " t " units of time, thus this property is called the "memoryless" property.

A random variable, X , is *memoryless* if

$$P\{X > s+t \mid X > t\} = P\{X > s\} \text{ for all } s, t \geq 0 \quad (1)$$

From using (1) above and the definition of conditional probability:

$$\frac{P(X > s, X > t)}{P(X > t)} = P(x > s) \quad (2)$$

and so:

$$P\{X > s+t\} = P\{X > s\}P\{X > t\} \quad (3)$$

to prove the above property, we suppose that there is a function such that $F(x) = P\{X > x\}$.

by equation 3 above, we have

$$F(x+t) = F(s)F(t) \quad (4)$$

By elementary calculus, the only continuous solution for this kind of functiona equation is

$$F(x) = e^{-\lambda x} \quad (5)$$

It is thus proven the only distribution that can solve equation (4), or the memoryless property, is an exponential function.

--The Constant Hazard Rate Property--

Suppose the random variable, X , survived for "t" units of time, and $r(t)$ represents the conditional probability that the t-year-old variable will fail. Mathematically the hazard rate, or the failure rate, is defined as:

$$r(t) = \frac{f(t)}{1 - F(t)} \quad (6)$$

For the exponential distribution, the hazard rate is constant since

$$f(t) = e^{-\lambda t},$$

and

$$r(t) = \frac{\lambda e^{-\lambda t}}{e^{-\lambda t}}$$

$$r(t) = \lambda$$

the above proved that $r(t)$ is constant for exponential distribution.

8.5.1 Standard Exponential Distribution

When an exponential distribution has $\lambda = 1$, this is called the standard exponential distribution. The equation and figure for this function is described below:

$$P(x \geq 0) = e^{-x}$$

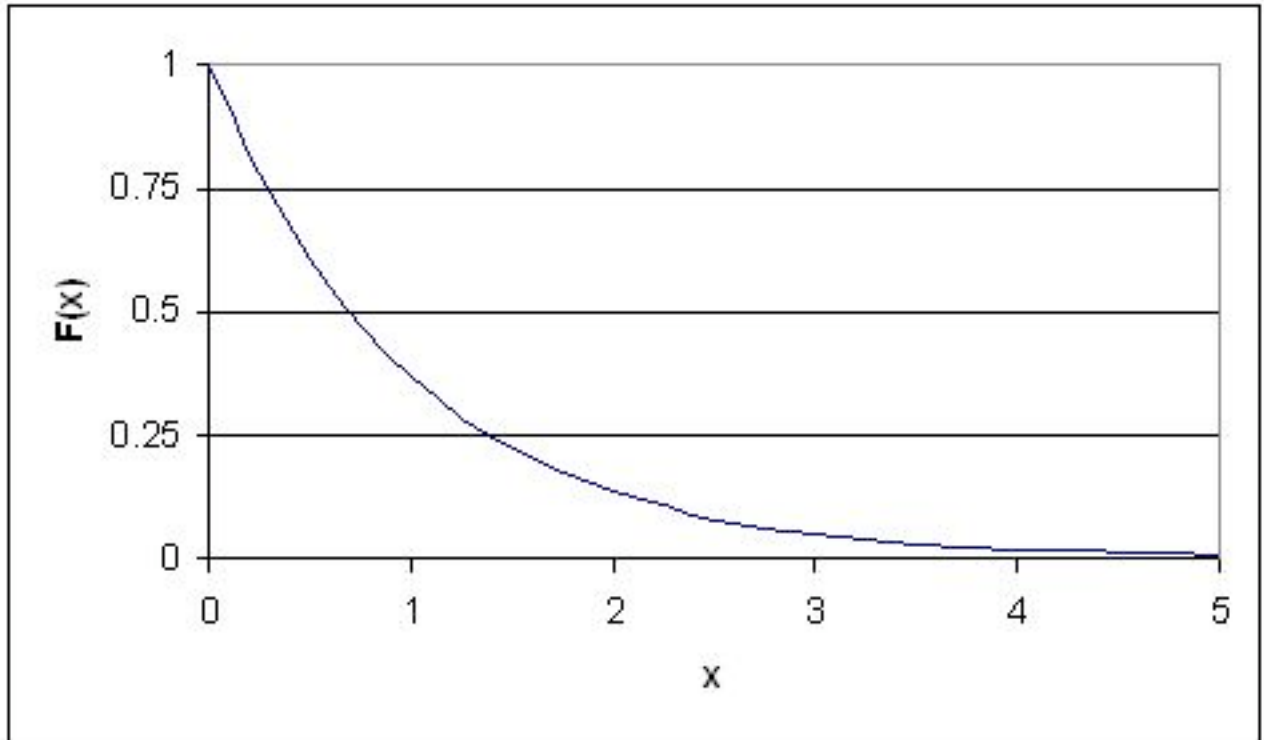


Figure 7: Standard Exponential Distribution Curve

This type of distribution is a way of standardizing your graph. This parallels our previous example of standard normal distribution, however, since time is now the x variable, it may not be negative (as an assumption of our hypothetical scenario). Thus, decay occurs only for positive time (as the radioactive particle emits mass).

8.6 Worked out Example 1

You are the lead process engineer for a leading pharmaceutical company, and your newest responsibility is to characterize one of your bioreactors. Part of this characterization is to determine the temperature variance within the reactor during the last step in an isothermal reaction. After taking data during this reaction for two weeks straight, you determine that the average temperature of the reaction is 30 C, with a standard deviation of your set of data being 3 C. Also, the data fits a normal distribution (ie. it is not skewed either side of the average) The higher-ups, ie. the ones who give you

the raises, decide that this reactor needs to operate within 6 degrees of its average operating temperature at least 60% of the time. Given the data that you have taken, does the reactor meet these standards, or will you be pulling some 80 hour weeks in the near future trying to fix the process?

SOLUTION

The information given in this problem is as follows:

- Average: 30
- Standard Deviation: 3
- We want to find the probability of the temperature falling between 24 and 36 C

Using the PDF for a Normal Distribution, we can say that:

$$P(24 < T < 36) = \frac{1}{2} \left(\text{Erf} \left[\frac{36 - 30}{3\sqrt{2}} \right] - \text{Erf} \left[\frac{24 - 30}{3\sqrt{2}} \right] \right) = \frac{1}{2} \left(\text{Erf}(1.4142) - \text{Erf}(-1.4142) \right)$$

This expression can easily be solved using a [table of Erf\[\] values](#) as well as the property of the Erf function that states $\text{Erf}(-x) = -\text{Erf}(x)$. Another simple approach would be to use Mathematica with the syntax shown below.

```
In[4]:= NIntegrate[PDF[NormalDistribution[30, 3], x], {x, 24, 36}]
Out[4]= 0.9545
```

Solving for $P(24 < T < 36)$, we get the probability of the temperature falling within two standard deviations of the average to be about 95%. Since this value is much greater than the required 60%, you can be rest assured that your reactor is running well.

8.7 Worked out Example 2

You are an engineer at a plant producing a volatile fuel. In your first week on the job both the primary control and redundancy control fail in the same day, necessitating the significant inconvenience of shutting down the reactor in order to prevent a much more inconvenient explosion. Your boss wants you to decide whether to simply replace both sensors or add an additional sensor to ensure that such problems are avoided in the future. While adding another sensor would certainly help solve the problem there is an extra cost associated with purchasing and installing the sensor. A very helpful fellow engineer with a penchant for statistics helps you out by informing you that these dual instrument failures occur at the rate of one per 3.8×10^8 hours. What is the probability that this type of failure will happen again in the next 50 years (the estimated life of the plant)? What is your recommendation to your boss?

SOLUTION

Because you are given the probability of the event occurring and are interested in the amount of time separating two events using an exponential distribution is appropriate. To solve this you use the CDF expression:

$$CDF(x) = 1 - e^{-\lambda x}$$

In this case λ is given in hours and x in years, so you must first convert one of the units. Also the rate given is in events per hour. λ must be entered into the equation as the inverse (probability per time unit). Entering the appropriate numbers yields the following equation:

$$CDF(50) = 1 - e^{-50years * \frac{1}{4.34 * 10^4 years}}$$

There is a 0.115% chance of both sensors failing in the same day sometime in the next 50 years. Based in this data you can conclude that you are probably safe simply replacing the two sensors and not adding a third.

8.8 Worked Out Example 3

You work at a chemical plant that uses the famous reaction $A + B \rightarrow C$ to produce C. As part of your process you operate a mixing tank to dilute reactant A before sending it to the reactor. Reactant B is a byproduct from another process in the plant and comes in at a variable rate. This causes fluctuations in the level of the mixing tank for reactant A as the flow in and out of the tank has to be adjusted. In the past this has caused overflows in mixing tank A that your boss has tasked you with avoiding. You've decided the easiest way to avoid overflows is to simply buy a larger mixing tank. Currently the mixing tank is 50 gallons. After some experimentation you find the normal operating conditions of the tank are 45 gallons of reactant A with a 3 gallon standard deviation. However, to minimize costs the tank needs to be as small as possible. What is smallest tank you can buy that avoids overflows 99.99% of the time?

Solution:

Known values:

$$\mu = 45gal.$$

$$\sigma = 3gal.$$

Using a z-table you find that the smallest z-value that gives an $F(x)$ of 0.9999 is 3.71. You then rearrange the z equation given below to solve for x and plug in all known values.

$$z = \frac{x - \mu}{\sigma}$$

$$x = z * \sigma + \mu$$

$$x = 3.71 * 3 + 45 = 56.1$$

In order to prevent overflows 99.99% of the time the smallest tank that can be used is 56.1 gal.

8.9 Multiple Choice Question 1

Please briefly summarize the primary difference between continuous and discrete distributions, and their respective methods of analysis:

- a. Continuous distributions and discrete distributions are always both analyzed through calculus methods only. Continuous distributions are distinct from discrete distributions in that the sample size is too small to treat each individual event in a discrete manner.
- b. Continuous distributions are analyzed by applying calculus methods whereas discrete distributions are commonly addressed via arithmetic methods. Continuous distributions are distinct from discrete distributions in that the sample size is too large to treat each individual event in a discrete manner.
- c. By performing a standard z- transform, the interested student may begin the process of characterizing the probability of z falling between the specific range from $x = 'a'$ and $x = 'b'$.
- d. Error functions allow us to determine the likelihood of a data point falling within certain bounds without having to complete the rigorous of the probability distribution function. Continuous distributions may be addressed in this manner since their sample size is too confusing to be addressed in a discrete manner.

8.10 Multiple Choice Question 2

Please explain the primary philosophical difference between the parameters of the probability distribution function (PDF) and the cumulative distribution function (CDF).

- a. Who uses the word philosophical in a chemical engineering problem? The author of this question is most likely confused and trying too hard, so I will protest by not answering.

b. The PDF and CDF are identical in application, and as such, must also have identical parameters.

c. The PDF and CDF both commonly measure the probability of sensor noise being at or below a specific value. They are different in the fact that the CDF contains a specific range of use, ranging from k_1 to k_2 , whereas the PDF does not, as it rises from negative infinity to a value, k .

d. The major difference the PDF and CDF is that the PDF provides the probability of the variable x falling within a defined range. Alternatively, CDF gives the probability of the variable x falling at or below a certain limit, k .

8.11 Sage's Corner

Therapeutic Insulin Production

<http://www.youtube.com/v/b3aDqdOzP5I>

A Brief Problem on Continuous Exponential Distribution Functions

<http://video.google.com/googleplayer.swf?docId=6018713000402551106>

A copy of the slides can be found here: [Slides without narration](#)


Normal Distribution Functions in Excel

If YouTube doesn't work, click here [Normal Distribution Functions in Excel](#)

8.12 References

- Gernie, L. and W. Smith "Cartoon Guide to Statistics" Harper Perennial, c. 1993

Section 9. Discrete Distributions: hypergeometric, binomial, and poisson

Note:  [Video lecture](#) available for this section!

Authors: Tommy DiRaimondo, Rob Carr, Marc Palmer, Matt Pickvet

Stewards: Kaveh Saba, Arthur Edge, Kathryn Meintel, Renu Rao

Date Presented: 11/21/06; Date Revised: 11/14/07

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

9.1 What are Discrete Distributions?

In order to explain the meaning and utility of discrete distributions, it is necessary to first introduce the topic of **Random Variables**. The term *random* in Random Variable refers to the idea that each individual outcome has an equal chance of occurring. Therefore, each outcome is randomly determined. For example, a fair coin has an equal probability of flipping up heads as it does flipping up tails. Hence, the random variable is determined by the outcome of flipping a coin. However, it is frequently the case in chemical engineering that when a process is performed we are only interested in some function of the outcome rather than the outcome itself. For example, in a chemical reactor we might want to know the probability that two molecules collide and react to form a product at a certain temperature, however it is more useful to know the sum of these collisions that form product rather than the individual occurrences. This is analogous to rolling two dice and wanting to know the sum of the dice rather than the individual numbers rolled. These discrete values defined on some sample space compose what are called **Random Variables**.

9.1.1. Random Variable Example

Suppose that our experiment consists of tossing 4 fair coins. If we define a variable X and let it denote the number of heads flipped, then X is a random variable with possible discrete values of 0,1,2,3,4 with respective probabilities:

$$P\{X = 0\} = P\{T, T, T, T\} = \frac{1}{16}$$

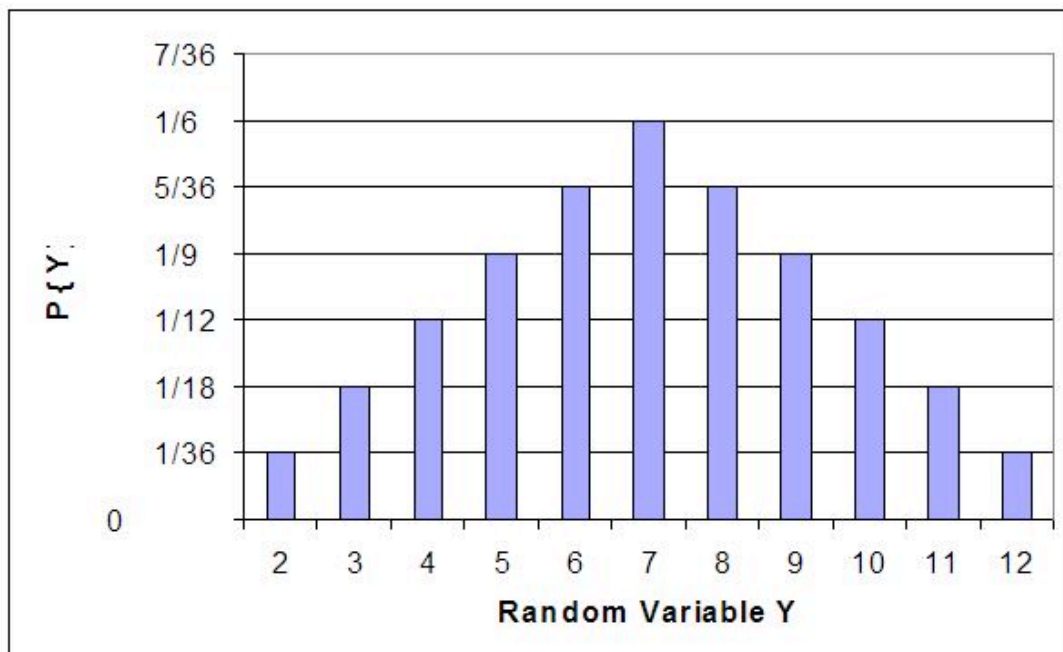
$$P\{X = 1\} = P\{T, T, T, H\}, P\{T, T, H, T\}, P\{T, H, T, T\}, P\{H, T, T, T\} = \frac{1}{4}$$

$$P\{X = 2\} = P\{T, T, H, H\}, P\{T, H, H, T\}, P\{H, T, H, T\}, P\{H, T, T, H\}, P\{T, H, T, H\}, P\{H, H, T, T\} = \frac{3}{8}$$

$$P\{X = 3\} = P\{T, H, H, H\}, P\{H, T, H, H\}, P\{H, H, T, H\}, P\{H, H, H, T\} = \frac{1}{4}$$

$$P\{X = 4\} = P\{H, H, H, H\} = \frac{1}{16}$$

We can do the same for the probability of rolling sums of two dice. If we let Y denote the sum, then it is a random variable that takes on the values of 2, 3, 4, 5, 6, 7, 8, 9, 10, & 12. Rather than writing out the probability statements we can represent Y graphically:



The graph plots the probability of the Y for each possible random value in the sample space (y-axis) versus the random value in the sample space (x-axis). From the graph one can infer that the sum with the greatest probability is $Y = 7$.

These are just two ways one can describe a random variable. What this leads into is representing these random variables as functions of probabilities. These are called the discrete distributions or probability mass functions. Furthermore, independent random events with known probabilities can be lumped into a discrete Random Variable. The Random Variable is defined by certain criteria, such as flipping up heads a certain number of times using a fair coin. The probability of a certain random variable equaling a discrete value can then be described by a discrete distribution. Therefore, a discrete distribution is useful in determining the probability of an outcome value without having to perform the actual trials. For example, if we wanted to know the probability of rolling a six 100 times out of 1000 rolls a distribution can be used rather than actually rolling the dice 1000 times.

Note: Here is a good way to think of the difference between discrete and continuous values or distributions. If there are two continuous values in a set, then there exists an infinite number of other continuous values between them. However, discrete values can only take on specific values rather than infinite divisions between them. For example, a valve that can only be completely open or completely closed is analogous to a discrete distribution, while a valve that can change the degree of openness is analogous to a continuous distribution.

The three discrete distributions we discuss in this article are the binomial distribution, hypergeometric distribution, and poisson distribution.

9.2 Binomial Distribution

This type of discrete distribution is used only when both of the following conditions are met:

1. The test has only two possible outcomes
2. The sample must be random

If both of the above conditions are met, then one is able to use this distribution function to predict the probability of a desired result. Common applications of this distribution range from scientific and engineering applications to military and medical ones. For example, a binomial distribution may be used in determining whether a new drug being tested has or has not contributed ("yes" or "no" labels) to alleviating symptoms of a disease.

Since only two outcomes are possible, they can be denoted as M_S and M_F for the number of successes and number of failures respectively. The term p is the frequency with which the desired number, M_S or M_F will occur. The probability of a collection of the two outcomes is determined by the following equation.

$$P(M_S, M_F) = kp^{M_S}(1 - p)^{M_F} \quad (1)$$

k in the above equation is simply a proportionality constant. For the binomial distribution it can be defined as the number of different combinations possible

$$k = C\left(\frac{M_S + M_F}{M_S}\right) = \frac{(M_S + M_F)!}{M_S!M_F!} \quad (2)$$

! is the factorial operator. For example, $4! = 4 * 3 * 2 * 1$ and $x! = x * (x - 1) * (x - 2) * \dots * 2 * 1$. In the above equation, the term $(M_S + M_F)!$ represents the number of ways one could arrange the total number of M_S and M_F terms and the denominator, $M_S!M_F!$, represents the number of ways one could arrange results containing M_S successes and M_F failures. Therefore, the total probability of a collection of the two outcomes can be

described by combining the two above equations to produce the binomial distribution function.

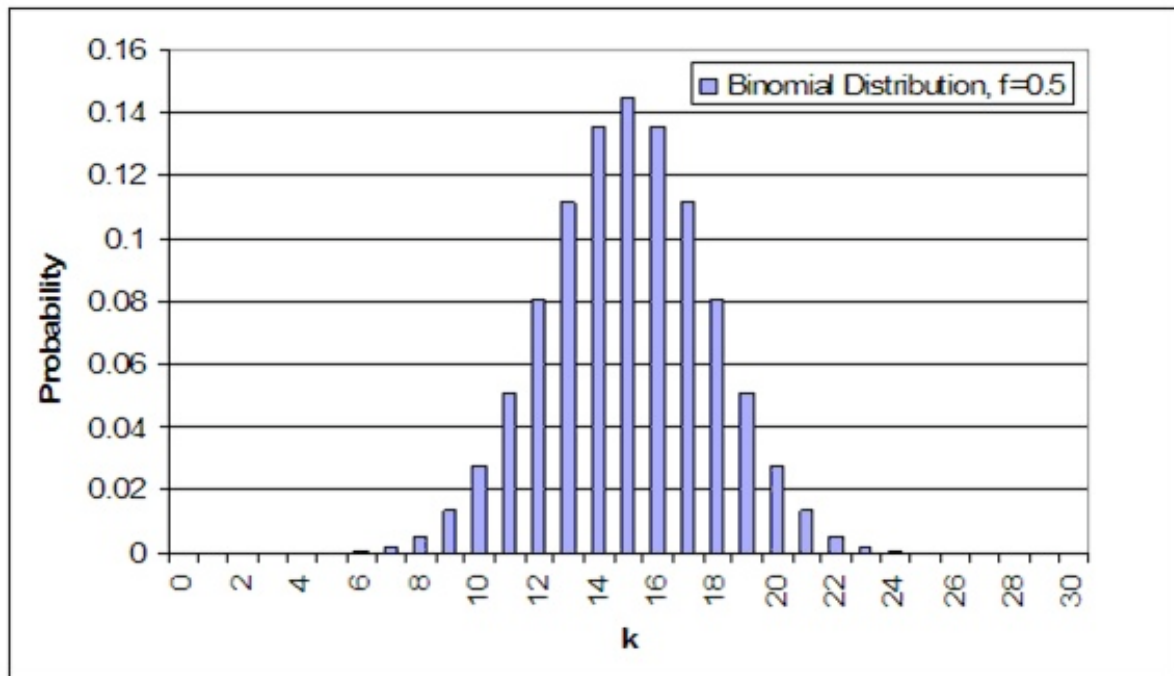
$$P(M_S, M_F) = \frac{(M_S + M_F)!}{M_S!M_F!} p^{M_S} (1 - p)^{M_F} \quad (3)$$

Which can be simplified as the equation

$$P\{X = k\} = \frac{n!}{(n - k)!k!} p^k (1 - p)^{n-k} \quad \text{for } k = 0, 1, 2, 3, \dots \quad (4)$$

In the above equation, n represents the total number of possibilities, or $M_S + M_F$, and k represents the number of desired outcomes, or M_S . These equations are valid for all non-negative integers of M_S , M_F , n , and k and also for p values between 0 and 1.

Below is a sample binomial distribution for 30 random samples with a frequency of occurrence being 0.5 for either result. This example is synonymous to flipping a coin 30 times with k being equal to the number of flips resulting in heads.



An important note about these distributions is that the area under the curve, or the

probability of each integer added together, always sums up to 1.

One is able to determine the mean and standard deviation, which is described in the [Basic Statistics](#) article, as shown below.

$$\mu = np \quad (5)$$

$$\sigma = \sqrt{np(1 - p)} \quad (6)$$

An example of a common question that may arise when dealing with binomial distributions is “What is the probability of a certain result occurring 33 – 66% of the time?” In the above case, it would be synonymous to the likelihood of heads turning up between 10 and 20 of the trials. This can be determined by summing the individual probabilities of each integer from 10 to 20.

$$P(66\% > X > 33\%) = \sum_{\text{possible values}} P(N_S) = P(10) + P(11) + \dots + P(19) + P(20) \\ = 0.0280 + 0.0509 + \dots + 0.0509 + 0.0280 = 0.9572$$

The probability of heads resulting in 33 – 66% of the trials when a coin is flipped 30 times is 95.72%.

The probability for binomial distribution can also be calculated using Mathematica. This will simplify the calculations, save time, and reduce the errors associated with calculating the probability using other methods such as a calculator. The syntax needed to calculate the probability in Mathematica is shown below in the screen shot. An example is also given for various probabilities based on 10 coin tosses.

```
In[22]:= (*Binomial Distribution*)
binom[nn_, kk_, pp_] := nn! / (kk! (nn - kk)!) * pp^kk * (1 - pp)^(nn - kk)

(*Example for Probability of getting 5 heads out of 10 tosses*)
binom[10, 5, 0.5]
Sum[binom[10, i, 0.5], {i, 0, 5}]
d = Table[binom[10, x, 0.50], {x, 0, 10}]

Out[23]= 0.246094 Probability of exactly 5 heads out of 10 tosses
Out[24]= 0.623047 Probability of 0-5 heads out of 10 tosses

Table of probabilities ranging from 0 to 10 heads out of 10 tosses
Out[25]= {0.000976563, 0.00976563, 0.0439453, 0.117188, 0.205078,
0.246094, 0.205078, 0.117188, 0.0439453, 0.00976563, 0.000976563}
```

where k is the number of events, n is the number of independent samples, and p is the known probability. The example above also generates a set of values for the probabilities of getting exactly 0 to 10 heads out of 10 total tosses. This will be useful because it simplifies calculating probabilities such as getting 0-6 heads, 0-7 heads, etc. out of 10 tosses because the probabilities just need to be summed according to the exact probabilities generated by the table.

In addition to calling the binomial function generated above, Mathematica also has a built in Binomial Distribution function that is displayed below:

`PDF[BinomialDistribution[n,p],k]` where n , p , and k still represent the same variables as before

This built in function can be applied to the same coin toss example.

```

In[11]: PDF[BinomialDistribution[10, 0.5], 5]
Out[11]: 0.246094

In[12]: Sum[PDF[BinomialDistribution[10, .5], k], {k, 0, 5}]
Out[12]: 0.623047

```

As expected, the probabilities calculated using the built in binomial function matches the probabilities derived from before. Both methods can be used to ensure accuracy of results.

9.3 Poisson Distribution

Note: The variables used in this section are defined the same way as seen above in the "Binomial Distribution" section.

A Poisson distribution has several applications, and is essentially a derived limiting case of the binomial distribution. It is most applicably relevant to a situation in which the total number of successes is known, but the number of trials is not. An example of such a situation would be if you know the mean expected number of cancer cells present per sample and wanted to determine the probability of finding 1.5 times that amount of cells in any given sample, you would use a Poisson distribution.

In order to derive the Poisson distribution, you must first start off with the binomial distribution function.

$$P\{X = k\} = \frac{n!}{(n - k)!k!} p^k (1 - p)^{n-k} \quad \text{for } k = 0, 1, 2, 3... \quad (4)$$

Due to the fact that the Poisson distribution does not require an explicit statement of the total number of trials, you must eliminate n out of the binomial distribution function. This is done by first introducing a new variable (μ), which is defined as the expected number of successes during the given interval and can be mathematically described as:

$$\mu = np \quad (5)$$

We can then solve this equation for p , substitute into equation 5, and obtain equation 7, which is a modified version of the binomial distribution function.

$$P\{X = k\} = \frac{n!}{(n-k)!k!} \left(\frac{\mu}{n}\right)^k \left(1 - \frac{\mu}{n}\right)^{n-k} \quad (7)$$

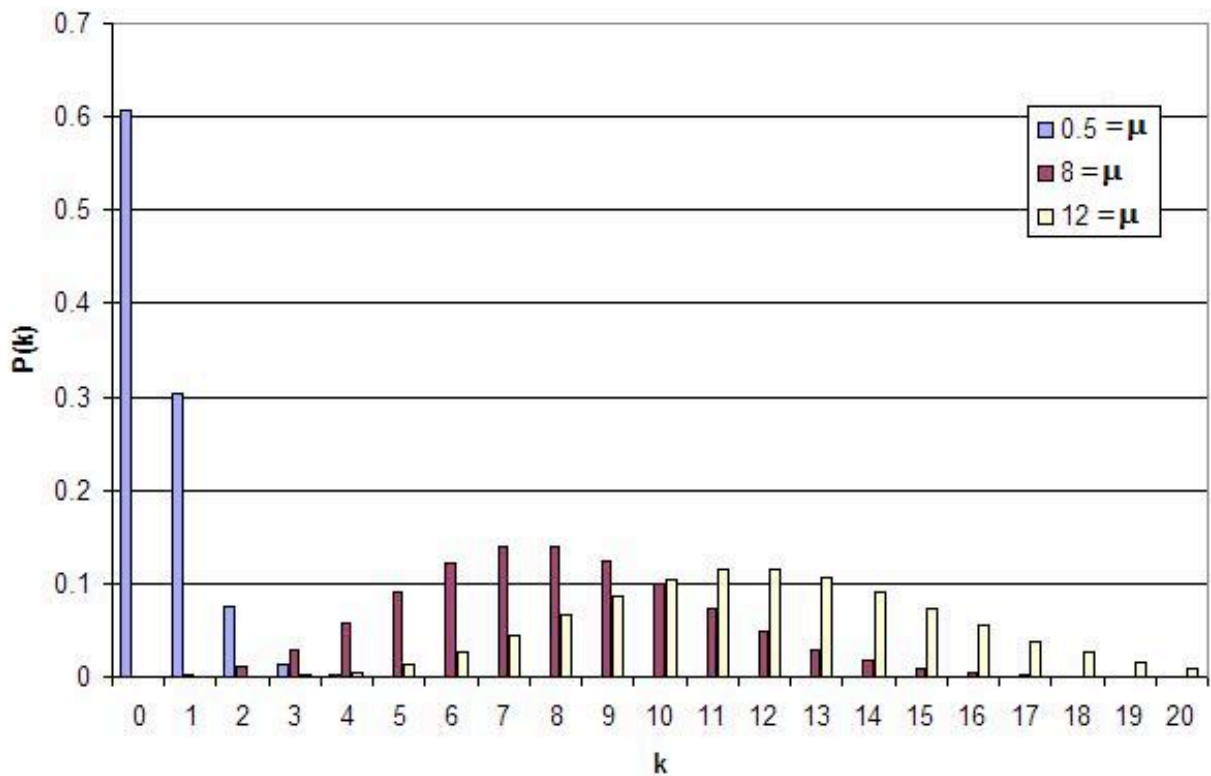
If we keep μ finite and allow the sample size to approach infinity we obtain equation 8, which is equal to the Poisson distribution function. (Notice to solve the Poisson distribution, you do not need to know the total number of trials)

$$P\{X = k\} = \frac{\mu^k e^{-\mu}}{k!} \quad (8)$$

In the above equation:

- e is the base of the natural logarithm ($e = 2.71828\dots$)
- k is the number of occurrences of an event
- $k!$ is the factorial of k
- μ is a positive real number, equal to the expected number of occurrences that occur during the given interval.

Using the Poisson distribution a probability versus number of successes plot can be made for several different numbers of successes.



This graph represents several key characteristics of a Poisson process.

1. The number of successes is independent of the time since the last event.
2. Probabilities, or outcomes, are discrete.
3. The probability of two or more successes in a short interval is extremely small (approximately zero).

These rules hint that the Poisson processes only model rare events, yet this is not true. What these characteristics say is that if you are limited to a small interval window, you will observe less than two events. It is important to know that the Poisson distribution is actually an approximation of the binomial distribution. As n increases and p decreases, the Poisson distribution becomes equal to the binomial distribution.

9.4 Hypergeometric Distribution

Note: The definitions of the variables in this section are different than the previous sections.

A hypergeometric distribution function is used only if the following three conditions can be met:

1. Only two outcomes are possible

2. The sample must be random
3. Selections are not replaced

Hypergeometric distributions are used to describe samples where the selections from a binary set of items are not replaced. This distribution applies in situations with a discrete number of elements in a group of N items where there are K items that are different. As a simple example imagine we are removing 10 balls from a jar of mixed red and green balls without replacing it. What is the chance of selecting 2 green balls? 5 red balls? In general terms, if there are K green balls and N total balls, the chance of selecting k green balls by selecting n balls is given by

$$P\{x = k\} = \frac{(\text{\# of ways to select } k \text{ green balls})(\text{\# of ways to select } n - k \text{ red balls})}{(\text{total number of ways to select})}$$

(9)

As another example, say there are two reactants sitting in a CSTR totaling to N molecules. The third reactant can either react with A or B to make one of two products. Say now that there are K molecules of reactant A, and $N-K$ molecules of reactant B. If we let n denote the number of molecules consumed, then the probability that k molecules of reactant of A were consumed can be described by the hypergeometric distribution. Note: This assumes that there is no reverse or side reactions with the products.

In mathematical terms this becomes

$$P\{X = k\} = \frac{(N - K)!K!n!(N - n)!}{k!(K - k)!(N - K + k - n)!(n - k)!N!}$$

where,

- N = total number of items
- K = total number of items with desired trait
- n = number of items in the sample
- k = number of items with desired trait in the sample

This can be written in shorthand as

$$P\{X = k\} = \frac{\binom{K}{k} \binom{N - K}{n - k}}{\binom{N}{n}} \quad (11)$$

Where

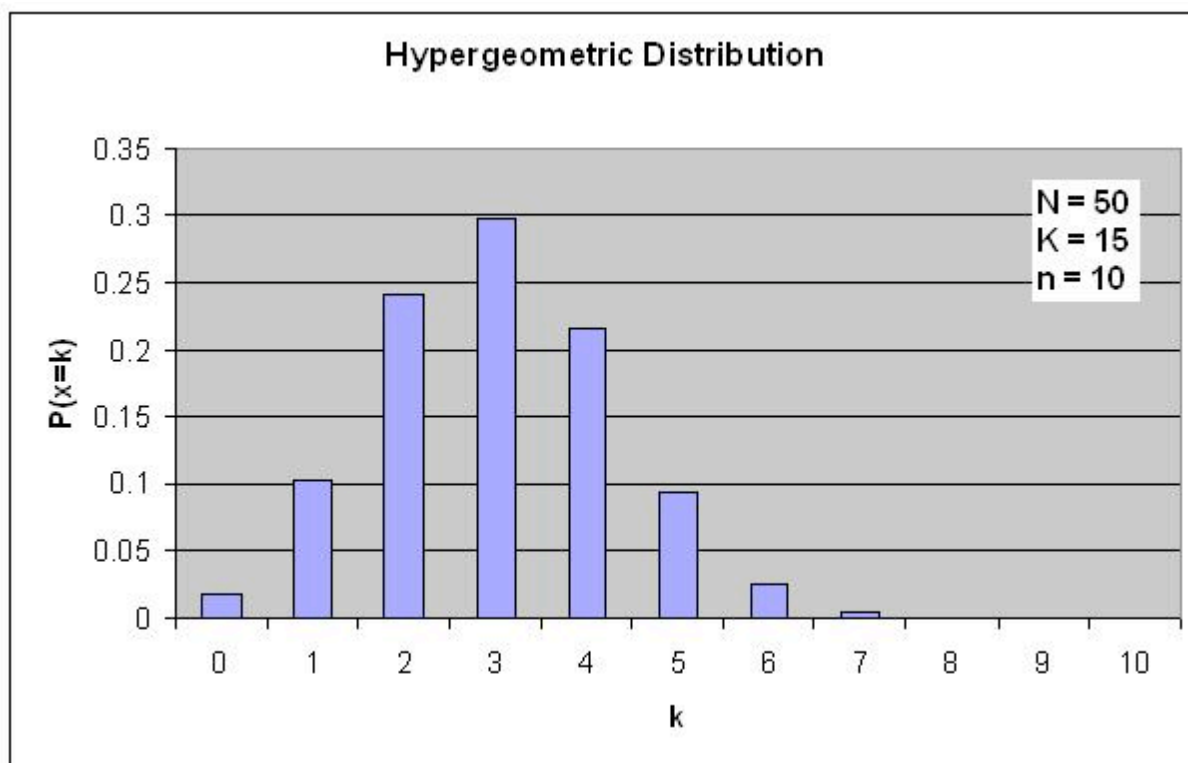
$$\binom{A}{B} = \frac{A!}{(A - B)!B!} \quad (12)$$

The formula can be simplified as follows: There are $\binom{N}{n}$ possible samples (without

replacement). There are $\binom{K}{k}$ ways to obtain k green balls and there are

$\binom{N - k}{n - k}$ ways to fill out the rest of the sample with red balls.

If the probabilities P are plotted versus k , then a distribution plot similar to the other types of distributions is seen.



Question:

Suppose that you have a bag filled with 50 marbles, 15 of which are green. What is the probability of choosing exactly 3 green marbles if a total of 10 marbles are selected?

Answer:

$$P\{X = 3\} = \frac{\binom{15}{3} \binom{50 - 15}{10 - 3}}{\binom{50}{10}}$$

$$P\{X = 3\} = \frac{(50 - 15)!15!10!(50 - 10)!}{3!(15 - 3)!(50 - 15 + 3 - 10)!(10 - 3)!50!}$$

$$P\{X = 3\} = 0.2979$$

9.4.1 Fisher's exact

A special case of the hypergeometric distribution is the Fisher's exact method. Fisher's exact is the probability of sampling a specific configuration of a 2 by 2 table with constrained marginals. Marginals in this case refer to the sums for each row and each column. Therefore, every Fisher's exact will have 4 marginals, those 4 being the sum of the first column, the sum of the second column, the sum of the first row, and the sum of the second row. Since these values are constant, that also means that the sum of **all** the elements in the table will always equal the same thing. This is clarified with the image below:

	Column 1	Column 2	
Row 1	A	B	E = A + B
Row 2	C	D	F = C + D
	G = A + C	H = B + D	I = A + B + C + D

In the image above, constant marginals would mean that E, F, G, and H would be held constant. Since those values would be constant, I would also be constant as I can be thought of as the sum of E and F or G and H are of which are constants.

In theory this test can be used for any 2 by 2 table, but most commonly, it is used when necessary sample size conditions for using the z-test or chi-square test are violated. The table below shows such a situation:

From this p_{fisher} can be calculated:

$$p_{fisher} = \frac{(a + b)!(c + d)!(a + c)!(b + d)!}{(a + b + c + d)!a!b!c!d!}$$

where the numerator is the number of ways the marginals can be arranged, the first term in the denominator is the number of ways the total can be arranged, and the remaining terms in the denominator are the number of ways each observation can be arranged.

As stated before, this calculated value is only the probability of creating the specific 2x2 from which the p_{fisher} value was calculated.

Another way to calculate p_{fisher} is to use Mathematica. The syntax as well as an example with numbers can be found in the screen shot below of the Mathematica notebook. For further clarification, the screen shot below also shows the calculated value of p_{fisher} with numbers. This is useful to know because it reduces the chances of making a simple algebra error.


```

In[8]:= (*Fisher's Exact*)
fishd[a_, b_, c_, d_] :=
  (a + b)! (c + d)! (a + c)! (b + d)! / ((a + b + c + d)! a! b! c! d!)

(*Fisher's Exact Example with Numbers where a=5,b=1,c=1,and d=18*)
Pfisher = N[fishd[5, 1, 1, 18]]

Out[9]= 0.000643704

```

Another useful tool to calculate p_{fisher} is using available online tools. The following link provides a helpful online calculator to quickly calculate p_{fisher} . [\[1\]](#)

Using Mathematica or a similar calculating tool will greatly simplify the process of solving for p_{fisher} .

After the value of p_{fisher} is found, the p-value is the summation of the Fisher exact value(s) for the more extreme case(s), if applicable. The p-value determines whether the null hypothesis is true or false. An example of this can be found in the worked out hypergeometric distribution example below.

Finding the p-value

As elaborated further here: [\[2\]](#), the p-value allows one to either reject the null hypothesis or not reject the null hypothesis. Just because the null hypothesis isn't rejected doesn't mean that it is advocated, it just means that there isn't currently enough evidence to reject the null hypothesis.

In order to find the p-value, it is necessary to find the probabilities of not only a specific table of results, but of results considered even more "extreme" and then sum those calculated probabilities. An example of this is shown below in example 2.

What is considered "more extreme" depends on the situation. In the most general sense, more extreme means further from the expected or random result.

Once the more extreme tables have been created and the probability for each value obtained, they can be added together to find the p-value corresponding to the least extreme table.

It is important to note that if the probabilities for every possible table were summed, the result would invariably be one. This should be expected as the probability of a table being included in the entire population of tables is 1.

- **Example 1**

The example table below correlates the the amount of time that one spent studying for an exam with how well one did on an exam.

	Does not study	Does Study	Totals
Score Poorly on Exam	1	3	4
Score Well on Exam	4	3	7
Totals	5	6	11

There are 5 possible configurations for the table above, which is listed in the Mathematica code below. All the p_{fisher} for each configuration is shown in the Mathematica code below.

```
(*Problem 2c*)
(*Fishers Exact*)
fishd[a_, b_, c_, d_] := (a + b)! (c + d)! (a + c)! (b + d)! / ((a + b + c + d)! a! b! c! d!)
x1 = N[fishd[1, 3, 4, 3]]
x2 = N[fishd[0, 4, 5, 2]]
x3 = N[fishd[2, 2, 3, 4]]
x4 = N[fishd[3, 1, 2, 5]]
x5 = N[fishd[4, 0, 1, 6]]
x1 + x2 + x3 + x4 + x5 (*all possible cases, should sum to 1*)
0.30303
0.0454545
0.454545
0.181818
0.0151515
1.
```

- **Example 2**

What are the odds of choosing the samples described in the table below with these marginals in this configuration or a more extreme one?

	catalyst A	catalyst B	Totals
Bad product	5	1	6
Good product	1	18	19
Totals	6	19	25

Solution

First calculate the probability for the initial configuration.

$$P_{fisher} = \frac{6!19!6!19!}{25!5!1!1!18!} = 0.000643704$$

Then create a new table that shows the most extreme case that also maintains the same marginals that were in the original table.

	catalyst A	catalyst B	Totals
Bad product	6	0	6
Good product	0	19	19
Totals	6	19	25

Then calculate the probability for the most extreme case.

$$P_{fisher} = \frac{6!19!6!19!}{25!6!0!0!19!} = 0.00000564653$$

Finally add the two probabilities together.

$$P_{fisher} = 0.000643704 + 0.00000564653 = 0.00064$$

9.5 Maximum Entropy Function

The maximum entropy principle uses all the testable information about multiple given probability distributions to describe the true probability distribution by maximizing the information entropy. To derive a distribution with the maximum entropy principle, you obtain some testable information I about some quantity x . This information is expressed as m constraints on the expectation values of the functions f_k . This makes the Bayesian probability distribution to satisfy:

$$F_k = \sum_{i=1}^n \Pr(x_i|I) f_k(x_i) \quad k = 1, \dots, m$$

We also know that all of these probabilities must sum to 1, so the following constraint is introduced:

$$\sum_{i=1}^n \Pr(x_i|I) = 1$$

Then the probability distribution with maximum information entropy that satisfies all these constraints is:

$$\Pr(x_i|I) = \frac{1}{Z(\lambda_1, \dots, \lambda_m)} \exp [\lambda_1 f_1(x_i) + \dots + \lambda_m f_m(x_i)]$$

The normalization constant is determined by the classical partition function:

$$Z(\lambda_1, \dots, \lambda_m) = \sum_{i=1}^n \exp [\lambda_1 f_1(x_i) + \dots + \lambda_m f_m(x_i)]$$

The λ_k parameters are Lagrange multipliers with values determined by:

$$F_k = \frac{\partial}{\partial \lambda_k} \log Z(\lambda_1, \dots, \lambda_m)$$

All of the well-known distributions in statistics are maximum entropy distributions given appropriate moment constraints. For example, if we assume that the above was constrained by the second moment, and then one would derive the Gaussian distribution with a mean of 0 and a variance of the second moment.

The use of the maximum entropy distribution function will soon become more predominant. In 2007 it had been shown that Bayes' Rule and the Principle of Maximum Entropy were compatible. It was also shown that maximum entropy reproduces every aspect of orthodox Bayesian inference methods. This enables engineers to tackle problems that could not be simply addressed by the principle of maximum entropy or Bayesian methods, individually, in the past.

9.6 Summary

The three discrete distributions that are discussed in this article include the Binomial, Hypergeometric, and Poisson distributions. These distributions are useful in finding the chances that a certain random variable will produce a desired outcome.

9.6.1 Binomial Distribution Function

The Binomial distribution function is used when there are only two possible outcomes, a *success* or a *failure*. A success occurs with the probability \mathbf{p} and a failure with the probability $\mathbf{1-p}$. Suppose now that in \mathbf{n} independent trials the *binomial* random variable \mathbf{X} represents the number of successes. The following equation applies to binomial random variables:

$$P\{X = k\} = \frac{n!}{(n-k)!k!} p^k (1-p)^{n-k} \quad \text{for } k = 0, 1, 2, \dots, n$$

$$P\{X \leq i\} = \sum_{k=0}^i \frac{n!}{(n-k)!k!} p^k (1-p)^{n-k}$$

9.6.2 Poisson Distribution Function

The Poisson distribution can be used in a large variety of situations. It can also be used to approximate the Binomial Distribution when \mathbf{n} is large and \mathbf{p} is small yielding a moderate \mathbf{np} .

The following example is a situation in which the Poisson Distribution applies: Suppose a CSTR is full of molecules and the probability of any one molecule reacting to form product is small (say due to a low temperature) while the number of molecules is large, then the probability distribution function would fit the Poisson Distribution well (Note: all the molecules are the same here, unlike in the hypergeometric example to follow). Other examples include, the number of wrong telephone numbers that are dialed each day or the number of people in a community that live to 100 years of age. The following equation is the Poisson Distribution function:

$$P\{X = k\} = \frac{\mu^k e^{-\mu}}{k!} \quad \text{for } k = 0, 1, 2, \dots, n$$

$$P\{X \leq i\} = \sum_{k=0}^i \frac{\mu^k e^{-\mu}}{k!}$$

9.6.3 Summary of Key Distributions

Distribution	Requirements	Distribution Function
Binomial	<ul style="list-style-type: none"> Only two outcomes are possible Sample is random 	$P\{X = k\} = \frac{n!}{(n-k)!k!} p^k (1-p)^{n-k}$
Poisson	<ul style="list-style-type: none"> Success is independent of the interval The probability of two consecutive successes is small 	$P\{X = k\} = \frac{\mu^k e^{-\mu}}{k!}$
Hypergeometric	<ul style="list-style-type: none"> Selections are not replaced 	$P\{X = k\} = \frac{\binom{K}{k} \binom{N-K}{n-k}}{\binom{N}{n}}$

9.6.4 Summary of Distribution Approximations

There are many useful approximations for discrete random variables. An important approximation is that which yields a normal distribution because it allows for confidence intervals and probabilities to be continuous. Additionally, since the normal distribution is so well understood it is used for convenience when speaking to those who have yet to study probability theory. Below is a table of useful approximations. The majority of the theory behind these approximations is in the application of the Central Limit Theorem and Large Number Law but these are outside the scope of this text.

The Following Distribution	Is Approximately A...	When the Following Are Met...
Hypergeometric(n, K, N)	A continuous Normal random variable where $\mu = nK/N$ and $\sigma^2 = n(K/N)(1-K/N)$, Normal ($nK/N, n(K/N)(1-K/N)$)	1) Satisfies requirements for approximating a Binomial below. 2) There are a large number of samples, n. At least 100*.
	A Binomial random variable where $n = n$ and $p = K/N$ Binomial (n, K/N)	1) Both K, N large in comparison to n (an order of magnitude or larger)
Binomial(n,p)	A continuous Normal random variable where $\mu = np$ and $\sigma^2 = np(1-p)$, Normal ($np, np(1-p)$)	1) Large number of samples, n. At least 100*.
	A Poisson random variable where $\lambda = np$ Poisson (np)	1) Large number of samples n. 2) Small Probability, p. 3) Moderate size $\lambda = np$
Poisson(λ)	A continuous Normal random variable where $\mu = \lambda$ and $\sigma^2 = \lambda$, Normal (λ, λ)	1) Large number of samples, n. At least 100*.

The above chart can be read as "A random variable under the following distribution can be approximately a <blank> random variable when the following requirements are met." For example, the final line of the table can be read: "A random variable following a Poisson distribution with parameter λ is approximately a continuous Normal random variable where the mean is λ and the variance is λ assuming that there are at least 100 samples that have been taken."

9.7 Worked out Binomial Distribution Example

In order for a vaccination of Polio to be efficient, the shot must contain at least 67% of the appropriate molecule, VPOLIO. To ensure efficacy, a large pharmaceutical company manufactured a batch of vaccines with each syringe containing 75% VPOLIO. Your doctor draws a syringe from this batch which should contain 75% VPOLIO. What is the probability that your shot, will successfully prevent you from acquiring Polio? Assume the syringe contains 100 molecules and that all molecules are able to be delivered from the syringe to your blood stream.

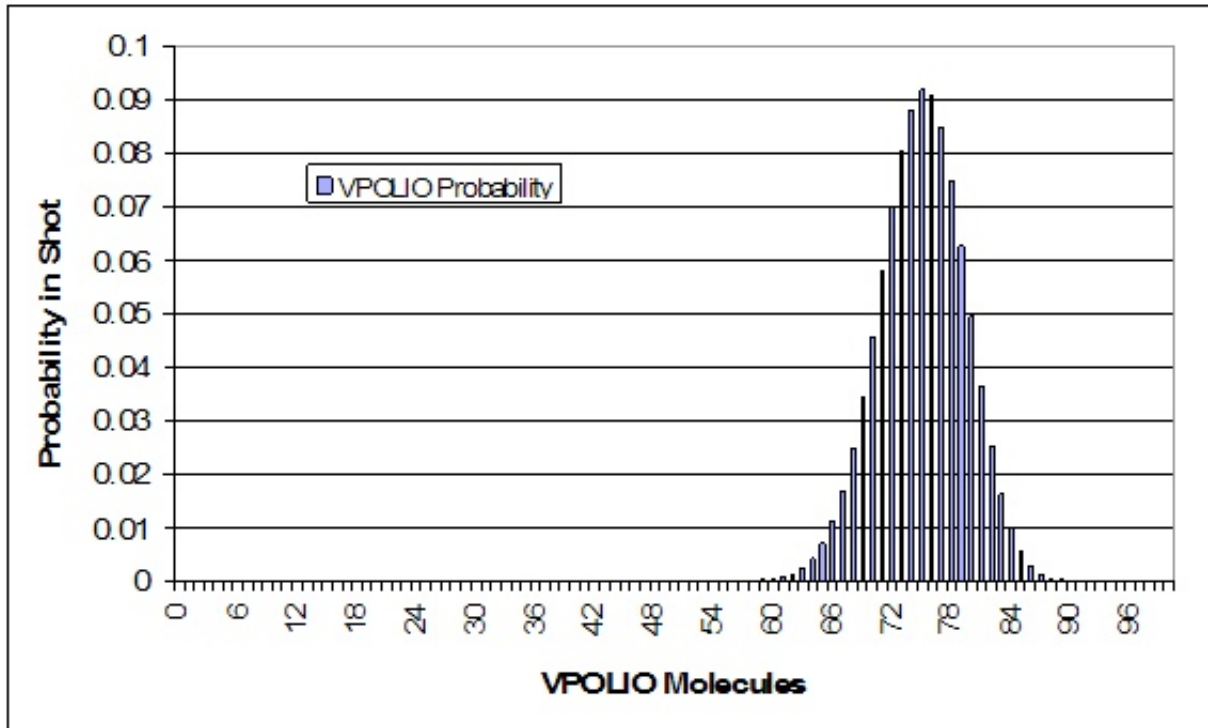
9.7.1 Solution

This can be done by first setting up the binomial distribution function. In order to do this, it is best to set up an Excel spreadsheet with values of k from 0 to 100, including each integer. The frequency of pulling a VPOLIO molecule is 0.75. Randomly drawing any molecule, the probability that this molecule will never be VPOLIO, or in other words, the probability of your shot containing 0 VPOLIO molecules is

$$P = \frac{100!}{(100 - 0)!0!} (0.75)^0 (1 - 0.75)^{100-0}$$

Note that $0! = 1$

Your spreadsheet should contain probabilities for all off the possible values of VPOLIO in the shot. A link to our spreadsheet can be seen at the end of this article. A graph of our distribution is shown below.



The next step is to sum the probabilities from 67 to 100 of the molecules being VPOLIO. This calculation is shown in the sample spreadsheet. The total probability of at least 67 of the molecules being VPOLIO is 0.9724. Thus, there is a 97.24% chance that you will be protected from Polio.

[Media:Binomial Distribution Example1.xls](#)

9.8 Gaussian Approximation Of A Binomial Distribution Example

Calculation of the binomial function with n greater than 20 can be tedious, whereas calculation of the Gauss function is always simple. To illustrate this, consider the following example.

Suppose we want to know the probability of getting 23 heads in 36 tosses of a coin. This probability is given by the following binomial distribution:

$$P = \frac{36!}{23!13!} (0.5)^{36} = 3.36\%$$

To use a Gaussian Approximation, we must first calculate the mean and standard deviation.

$$\mu = np = 18$$

$$\sigma = \sqrt{np(1-p)} = 3$$

Now we can approximate the probability by the Gauss function below.

$$P = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-X)^2}{2\sigma^2}} = 3.32\%$$

This approximation is very close and requires much less calculation due to the lack of factorials. The usefulness of the Gaussian approximation is even more apparent when n is very large and the factorials involve very intensive calculation.

9.9 Worked out Hypergeometric Distribution Example

A teacher has 12 students in her class. On her most recent exam, 7 students failed while the other 5 students passed. Curious as to why so many students failed the exam, she took a survey, asking the students whether or not they studied the night before. Of the students who failed, 4 students did study and 3 did not. Of the students who passed, 1 student did study and 4 did not. After seeing the results of this survey, the teacher concludes that those who study will almost always fail, and she proceeds to enforce a "no-studying" policy. Was this the correct conclusion and action?

9.9.1 Solution

This is a perfect situation to apply the Fisher's exact test to determine if there is any association between studying and performance on the exam. First, create a 2 by 2 table describing this particular outcome for the class, and then calculate the probability of seeing this exact configuration. This is shown below.

	Did Study	Did Not Study	Totals
Failed Exam	4	3	7
Passed Exam	1	4	5
Totals	5	7	12

$$p_{fisher,1} = \frac{(4 + 3)!(1 + 4)!(4 + 1)!(3 + 4)!}{(4 + 3 + 1 + 4)!4!3!1!4!} = 0.221$$

Next, create 2 by 2 tables describing any configurations with the exact same marginals that are more extreme than the one shown above, and then calculate the probability of seeing each configuration. Fortunately, for this example, there is only one configuration that is more extreme, which is shown below.

	Did Study	Did Not Study	Totals
Failed Exam	5	2	7
Passed Exam	0	5	5
Totals	5	7	12

$$p_{fisher,2} = \frac{(5 + 2)!(0 + 5)!(5 + 0)!(2 + 5)!}{(5 + 2 + 0 + 5)!5!2!0!5!} = 0.0265$$

Finally, test the significance by calculating the p-value for the problem statement. This is done by adding up all the previously calculated probabilities.

$$p = p_{fisher,1} + p_{fisher,2} = 0.221 + 0.0265 = 0.248$$

Thus, the p-value is greater than 0.05, which is the standard accepted level of confidence. Therefore, the null hypothesis cannot be rejected, which means there is no significant association between studying and performance on the exam. Unfortunately, the teacher was wrong to enforce a "no-studying" policy.

9.10 Worked out Poisson Example

The hormone PREGO is only found in the female human body during the onset of pregnancy. There is only 1 hormone molecule per 10,000 found in the urine of a pregnant woman. If we are given a sample of 5,000 hormone molecules what is the probability of finding exactly 1 PREGO? If we need at least 10 PREGO molecules to be 95% positive that a woman is pregnant, how many total hormone molecules must we collect? If the concentration of hormone molecules in the urine is 100,000 molecules/mL of urine, what is the minimum amount of urine (in mL) necessary to insure an accurate test (95% positive for pregnancy)?

9.10.1 Solution

This satisfies the characteristics of a Poisson process because

- 1.) PREGO hormone molecules are randomly distributed in the urine
- 2.) Hormone molecule numbers are discrete
- 3.) If the interval size is made smaller (i.e. our sample size is reduced), the probability of finding a PREGO hormone molecule goes to zero

Therefore we will assume that the number of PREGO hormone molecules is distributed according to a Poisson distribution.

To answer the first question, we begin by finding the expected number of PREGO hormone molecules:

$$\mu = np \qquad \mu = (5,000) \left(\frac{1}{10,000} \right) = 0.5$$

Next we use the Poisson distribution to calculate the probability of finding exactly one PREGO hormone molecule:

$$P\{X = k\} = \frac{\mu^k e^{-\mu}}{k!} = 0.303 \qquad \text{where } k = 1 \quad \mu = 0.5$$

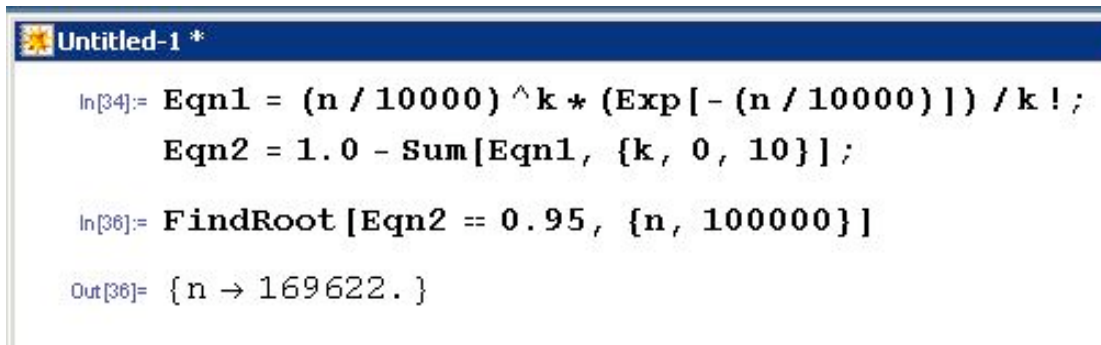
The second problem is more difficult because we are calculating **n**. We begin as before by calculating the expected number of PREGO hormone molecules:

$$\mu = np = \frac{n}{10,000}$$

Now we apply the Poisson Distribution Function equation:

$$P\{X \geq 10\} = 0.95 = \sum_{k=10}^{\infty} \frac{\mu^k e^{-\mu}}{k!} = 1.0 - \sum_{k=0}^{10} \frac{\mu^k e^{-\mu}}{k!} = 1.0 - \sum_{k=0}^{10} \left(\left(\frac{n}{10,000} \right)^k \frac{e^{-\left(\frac{n}{10,000}\right)}}{k!} \right)$$

It is easiest to solve this in Mathematica:



```

Untitled-1 *
In[34]:= Eqn1 = (n / 10000) ^ k * (Exp[-(n / 10000)]) / k! ;
          Eqn2 = 1.0 - Sum[Eqn1, {k, 0, 10}];

In[36]:= FindRoot [Eqn2 == 0.95, {n, 100000}]

Out[36]= {n -> 169622.}

```

The function **FindRoot[]** was used in Mathematica because the **Solve[]** function has problems solving polynomials of degree order greater than 4 as well as exponential functions. However, **FindRoot[]** requires an initial guess for the variable trying to be solved, in this case **n** was estimated to be around 100,000. As you can see from the Mathematica screen shot the total number of hormone molecules necessary to be 95% sure of pregnancy (or 95% chance of having atleast 10 PREGO molecules) was 169,622 molecules.

For the last step we use the concentration of total hormone molecules found in the urine and calculate the volume of urine required to contain 169,622 total hormone molecules as this will yield a 95% chance of an accurate test:

$$\text{Concentration} = \frac{100,000 \text{ molecules}}{\text{mL urine}}$$

$$\text{Volume of urine} = \frac{169,622}{100,000} = 1.69622 \text{ mL}$$

9.11 Example: Gaussian Approximation to a Poisson Distribution

To illustrate the Gaussian approximation to the Poisson distribution, consider a distribution where the mean (μ) is 64 and the number of observations in a definite interval (N) is 72. Determine the probability of these 72 observations?

Using the Poisson Distribution

$$P(N) = e^{-\mu} \cdot \frac{\mu^N}{N!}$$

$$P(72) = e^{-64} \cdot \frac{64^{72}}{72!} = 2.9\%$$

This can be difficult to solve when the parameters N and μ are large. An easier approximation can be done with the Gauss function:

$$P(72) = G_{64,8} = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-X)^2}{2\sigma^2}} = 3.0\%$$

where, $X=\mu$ and $\sigma = \sqrt{\mu}$.

9.12 Multiple Choice Question 1

All of the following are characteristics of the Poisson distribution **EXCEPT**:

- a) The number of successes is independent of the interval
- b) There are imaginary numbers
- c) Probabilities, or outcomes, are discrete
- d) Two or more success in a short interval is extremely small

9.13 Multiple Choice Question 2

If there are **K** blue balls and **N** total balls, the chance of selecting **k** blue balls by selecting **n** balls in shorthand notation is given by:

$$P\{X = k\} = \frac{\binom{N}{n} \binom{K - k}{N - n}}{\binom{K}{n}}$$

a)

$$P\{X = k\} = \frac{\binom{n}{k} \binom{n - K}{N - k}}{\binom{K}{n}}$$

b)

$$P\{X = k\} = \frac{\binom{K}{k} \binom{N - K}{n - k}}{\binom{N}{n}}$$

c)

$$P\{X = k\} = \frac{\binom{K}{n} \binom{N - n}{K - N}}{\binom{N}{n}}$$

d)

9.14 Discrete Distribution Presentation: Clown Time

<http://www.youtube.com/v/6WOieU664Ew>

9.15 References

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Section 10. Multinomial distributions

Note: [Video lecture](#) available for this section!

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10.1 Introduction

Statistical events generate two types of outcomes: continuous or discrete. Continuous outcomes can take an infinite number of values; for instance, a person's height can take any real number, so there are infinite possibilities. Typical events generating continuous outcomes may follow a normal, exponential, or geometric distribution. Discrete outcomes can only take prescribed values; for instance, a dice roll can only generate an integer between 1 to 6. Discrete outcomes are typically distributed either binomially or multinomially. It is with multinomial distribution that this article is concerned.

10.2 Multinomial Distributions: Mathematical Representation

Multinomial distributions specifically deal with events that have **multiple discrete outcomes**. The [Binomial distribution](#) is a specific subset of multinomial distributions in which there are only two possible outcomes to an event.

Multinomial distributions are not limited to events only having discrete outcomes. It is possible to categorize outcomes with continuous distributions to different degrees (high, medium, low). For instance, the water level - a continuous entity - in a storage tank can be made discrete by categorizing them into either "desirable" or "not desirable."

Multinomial distributions, therefore, have expansive applications in process control.

10.2.1 Probability Density Function

One way of describing the probability of an outcome occurring in a trial is the probability density function. The probability density function (PDF) mathematically represents the probability of having a specified outcome. The probability density function is a useful way to find the probability of simultaneous occurrence of specific results (i.e. having $n_1 = 1$, $n_2 = 1$, and $n_3 = 1$ with 3 trials as opposed to other outcomes, such as $n_1 = 3$, $n_2 = 0$, $n_3 = 0$ or $n_1 = 0$, $n_2 = 1$, $n_3 = 2$).

$$P(n_1, n_2, \dots, n_k) = \frac{N!}{(n_1!n_2!\dots n_k!)} \prod_{i=1}^k p_i^{n_i} = \frac{N!}{(n_1!n_2!\dots n_k!)} * (p_1^{n_1} p_2^{n_2} \dots p_k^{n_k})$$

where

N is the number of trials
 k is the number of possible outcomes
 n_i is the number of occurrences of outcome i
 p_i is the probability of observing outcome i

We know that the the sum of the probabilities of all possible outcomes that can occur in a trial must be unity (since one outcome must occur). The probability density function yields this result for both continuous and discrete outcomes. However, it is important to note that to get this result for continuous outcomes, one must take the integral of the probability density function over all possible outcomes. To get this unity result for discrete outcomes, one must sum the probabilities of each outcome (similar to taking Riemann sums).

10.2.2 Cumulative Distribution Function

While the probability density function calculates the probability of a single outcome, the cumulative distribution function (CDF) is a useful way to find the probability that an outcome lies within a given range of values.

$$P(n_1 \leq c_1, n_2 \leq c_2, \dots, N - n_1 - n_2 - \dots) = \sum_{n_1=0}^{c_1} \sum_{n_2=0}^{c_2} \dots \sum_{n_{k-1}=0}^{c_{k-1}} \frac{N!}{n_1!n_2!\dots(N - n_1 - n_2 - \dots)!} \prod_{i=1}^k p_i^{n_i}$$

where

N is the number of trials
 k is the number of possible outcomes
 n_i is the number of occurrences of outcome i
 p_i is the probability of seeing outcome i
 c_i is the maximum number of occurrences of outcome i

10.2.3 Visualizing Probability Density Function with Mathematica

Before using the functions for multinomial probability distributions, a special package must be loaded using the following command (depending on the version of Mathematica):

```
<< Needs["MultivariateStatistics`"] (Mathematica 6.0)
```

```
<< Statistics`MultiDiscreteDistributions` (Mathematica 5.2)
```

Note that the ``` (tilde) is the key next to 1 and not the single quote character `'`.

Table of pertinent Mathematica commands:

Command	Description
PDF[multinomial,x]	probability density function at x, where x is scalar-, vector-, or matrix-valued depending on distribution
CDF[multinomial,x]	cumulative distribution function at x
Mean[multinomial]	mean
Variance[multinomial]	variance
StandardDeviation[multinomial]	standard deviation

To plot the multinomial distribution probability density function (PDF) in Mathematica, follow three simple steps:

Defining the Multinomial Distribution

multinomial = MultinomialDistribution[n,{p1,p2,...pk}] where k is the number of possible outcomes, n is the number of outcomes, and p1 to pk are the probabilities of that outcome occurring. n and p1 to pk are usually given as numbers but can be given as symbols as long as they are defined before the command.

Defining the PDF of the Multinomial Distribution

pdf=PDF[multinomial, {x1,x2,...,xk}]; The x here simply refers to the variable so this command can be typed as is, and leave the x as a variable not a number.

Plotting the PDF

Plot3D[pdf, {x1, 0, 6}, {x2, 0, 5}, AxesLabel -> {x1, x2, probability}] the 0,6 and 0,5 are the ranges of x1 and x2 on the plot respectively, and the AxesLabel argument is to help us see which is which on the plot created. This command can also be typed as is, by leaving all the x's as variables.

- Note that this will only work if you have 2 variables. If there are more variables, constraints can be set so that it can be plotted. For 3 variables, set the third variable x3 as n-x1-x2. See the attached Mathematica notebook for more information.

[Media:Multinomial.nb](#)

10.2.4 Other Characteristics

Statistics have historically been useful in descriptive and inferential analysis of data. Likewise, multinomial distribution is also applicable to the aforementioned areas:

descriptive statistics, inferential statistics, and six-sigma. Several key variables are used in these applications:

The expected value below describes the mean of the data. Discrete random variables can take on a range of values; the mean of the data describes the location of the data within this range.

$$E(X_i) = np_i.$$

The data's standard deviation describes the variance of the data. The standard deviation of the data describes the spread of the data with respect to the center value (the mean of the data).

$$\text{var}(X_i) = np_i(1 - p_i).$$

Using the above parameters, it is possible to find the probability of data lying within n standard deviations of the mean. By setting n equal to 6, six sigma quality control can be implemented on the event and outcomes in question.

10.2.5 Derivation of Binomial Distribution

As was stated above, the binomial distribution is simply a special case of the multinomial distribution. Using the multinomial distribution, the probability of obtaining two events n_1 and n_2 with respective probabilities p_1 and p_2 from N total is given by:

$$P(n_1, n_2) = \frac{N!}{n_1!n_2!} (p_1^{n_1} p_2^{n_2})$$

If we label the event of interest, say n_1 in this case, as " k ," then, since only two outcomes are possible, n_2 must equal $N-k$. Finally, If we label the probability of obtaining k as simply " p ," then the probability of obtaining event n_2 (p_2) must be $1-p$, because again only two outcomes are possible. With these substitutions, the above equation simplifies to

$$P(k, N, p) = \frac{N!}{k!(N - k)!} p^k (1 - p)^{N-k}$$

Which is the familiar binomial distribution, where k is the number of events of interest, N is the total number of events, and p is the probability of attaining the event of interest.

10.3 Applications of Multinomial Distributions

As mentioned before, multinomial distributions are a generalized version of binomial distributions. In chemical engineering applications, multinomial distributions are relevant to situations where there are more than two possible outcomes (temperature = {high, med, low}). Multinomial systems are a useful analysis tool when a “success-failure” description is insufficient to understand the system. A continuous form of the multinomial distribution is the [Dirichlet distribution](#).

Using Bayes' Rule is one of the major applications of multinomial distributions. For example, Bayes' Rule can be used to predict the pressure of a system given the temperature and statistical data for the system. Bayes' Rule can be used to determine the probability of an event or outcome as mentioned above. Additional details on Bayes' Rule can be found at [Bayes' Rule, conditional probability, independence](#).

10.3.1 Bayes' Rule Example

In case you've forgotten how to use Bayes' Rule, here is an example that shows how to use it to solve a problem with a multinomial outcome which results from combining dual possibilities (such as desired flow vs. undesired flow and configuration A vs. configuration B).

You are given a flow apparatus with two possible specific valve configurations, A and B. For specific valve configuration A, desired flow rates are achieved 98.5% of the time. And for specific valve configuration B, the desired flow rates are achieved 89.3% of the time. An operator might use the configuration from A 79% of the time when desired flow rates are achieved. Can you determine the probability that a randomly chosen configuration is the same as the one in specific valve configuration B and produces undesirable flow rates?

Worked Out Solution

We'll be using the following symbols:

F_U : {undesirable flow rates}

F_D : {desirable flow rates}

C_B : {configuration from Apparatus B}

Thus we want to find : $P(F_U \cap C_B)$, which is the probability of undesirable flow rates and valve configuration B.

If we use Apparatus A 79% of the time then the probability of using Apparatus B would be 21% or : $P(F_D \cap C_B) = 0.21$, which is the probability of using configuration B and getting desired flow rates.

Additionally, we are given : $P(F_D | C_B) = 0.893$, which is the probability of a desired flow rate, given that configuration B is used.

Then

$P(F_U | C_B) = 1 - P(F_D | C_B) = 1 - 0.893 = 0.107$
, which is the probability that an undesirable flow rate is obtained, given that configuration B is used.

The information from above is then used below:

$P(F_U \cap C_B) = P(F_U | C_B) * P(C_B) = (0.107)(0.21) = 0.0225 = 2.25\%$
, which is the probability of getting an undesirable flow rate and configuration B which is found by taking the probability of getting an undesirable flow rate given that configuration B is used and multiplying that by the probability of a desirable flow rate and configuration B.

10.4 Worked Out Example 1

from Perry's, page 3-72

Consider the scenario in which you toss a fair die 12 times. What is the probability that each face value (1-6) will occur exactly twice?

10.4.1 Solutions to Example 1

The probability can be determined using a multinomial distribution in which 6 outcomes are possible. The individual probabilities are all equal given that it is a fair die, $p = 1/6$. The total number of trials N is 12, and the individual number of occurrences in each category n is 2.

$$P(2, 2, 2, 2, 2, 2) = \frac{12!}{2!2!2!2!2!2!} * \left(\frac{1}{6}\right)^2 \left(\frac{1}{6}\right)^2 \left(\frac{1}{6}\right)^2 \left(\frac{1}{6}\right)^2 \left(\frac{1}{6}\right)^2 \left(\frac{1}{6}\right)^2 = 0.003488$$

Therefore, the probability of rolling exactly 2 of each face value on a fair die is about 0.35%.

10.5 Worked Out Example 2

A bowl has 2 maize marbles, 3 blue marbles and 5 white marbles. A marble is randomly selected and then placed back in the bowl. You do this 5 times. What is the probability of choosing 1 maize marble, 1 blue marble and 3 white marbles?

10.5.1 Solutions to Example 2

N is the number of trials = 5

k is the number of possible outcomes = 3

n_i is the number of occurrences of outcome i

p_i is the probability of seeing outcome i

The three possible outcomes are choosing a maize marble, a blue marble or a white marble.

We must determine n_i and p_i to solve the multinomial distribution.

The number of occurrences of the outcome are the number of times we wish to see each outcome. These are given in the problem statement.

$$n_{maize} = 1$$

$$n_{blue} = 1$$

$$n_{white} = 3$$

The probability of seeing each outcome is easy to find. For example, there are two maize marbles in the bowl of 10, so the probability of choosing a maize marble is $\frac{2}{10}$.

$$p_{maize} = \frac{2}{10}$$

$$p_{blue} = \frac{3}{10}$$

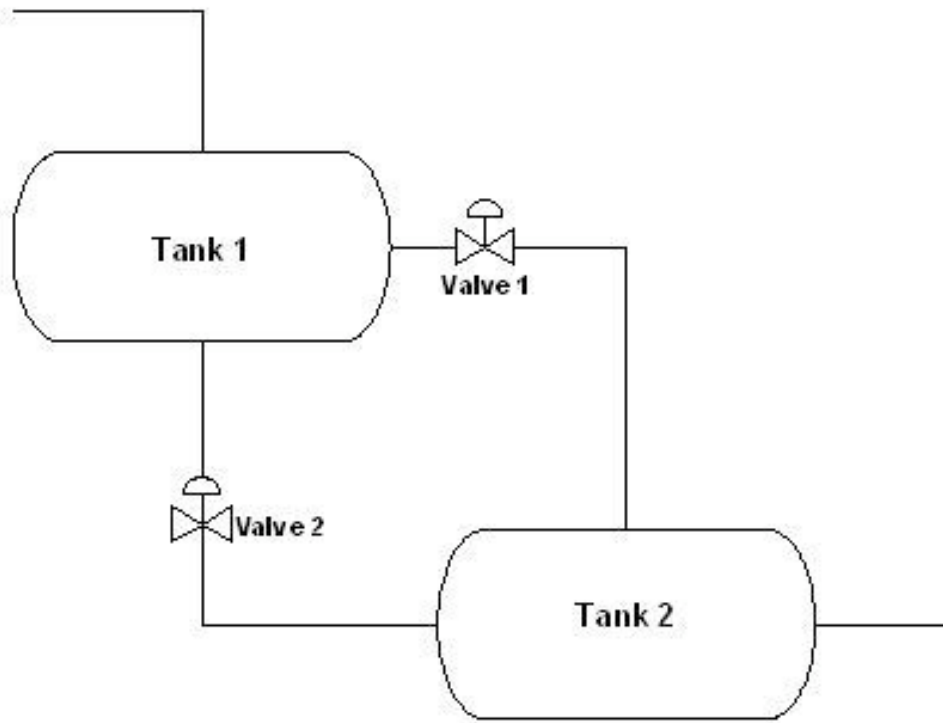
$$p_{white} = \frac{5}{10}$$

We can now solve the multinomial distribution as shown below. The probability of choosing 1 maize marble, 1 blue marble and 3 white marbles is 0.15.

$$P(1, 1, 3) = \frac{5!}{1!1!3!} * \left(\frac{2}{10}\right)^1 \left(\frac{3}{10}\right)^1 \left(\frac{5}{10}\right)^3 = 0.15$$

10.6 Worked Out Example 3

Two valves are used to control the flow of liquid out of a storage tank (Tank 1) in to another storage tank (Tank 2) and controlled by Valves 1 and 2 as seen below. The valves exist in two states: open and closed.



The following table describes the four different valve configurations and the frequency of the desired flow for each valve configuration based on experimental data.

Configuration	Valve 1	Valve 2	Probability of that configuration having the best flow
1	Open	Closed	0.305
2	Open	Open	0.476
3	Closed	Open	0.218
4	Closed	Closed	0.001

To reduce costs, two different apparatuses with a similar configuration, but with different pipe dimensions are being considered to replace the original apparatus. Below are data tables for each potential replacement apparatus with different valve configurations and the number of times out of 100 measurements that the valve configuration gave the desired flow.

Apparatus 1

Configuration	Valve 1	Valve 2	# of Best Flow
1	Open	Closed	42
2	Open	Open	37
3	Closed	Open	21
4	Closed	Closed	0

Apparatus 2

Configuration	Valve 1	Valve 2	# of Best Flow
1	Open	Closed	20
2	Open	Open	22
3	Closed	Open	56
4	Closed	Closed	2

Based on the information above, which apparatus is more like the desired model? By how much?

10.6.1 Solution to Example 3

With the 4 different valve configurations, multinomial distribution can be utilized to calculate the probability of a measurement. The goal here is to find the model with the highest probability density function, because that one is more like the desired model.

The probability of a measurement can be calculated as follows given that there are 4 different possible valve configurations (see section on pdf for more information on where this equation came from):

$$P(n_1, n_2, n_3, n_4) = \frac{N!}{n_1! n_2! n_3! n_4!} p_1^{n_1} p_2^{n_2} p_3^{n_3} p_4^{n_4}$$

n_i = total number of measurements with the best flow rate from each valve configuration

i = configuration

p_i = probability of that configuration having the best flow

N = Total # of observations

The calculation for the probability of each apparatus can be done similarly:

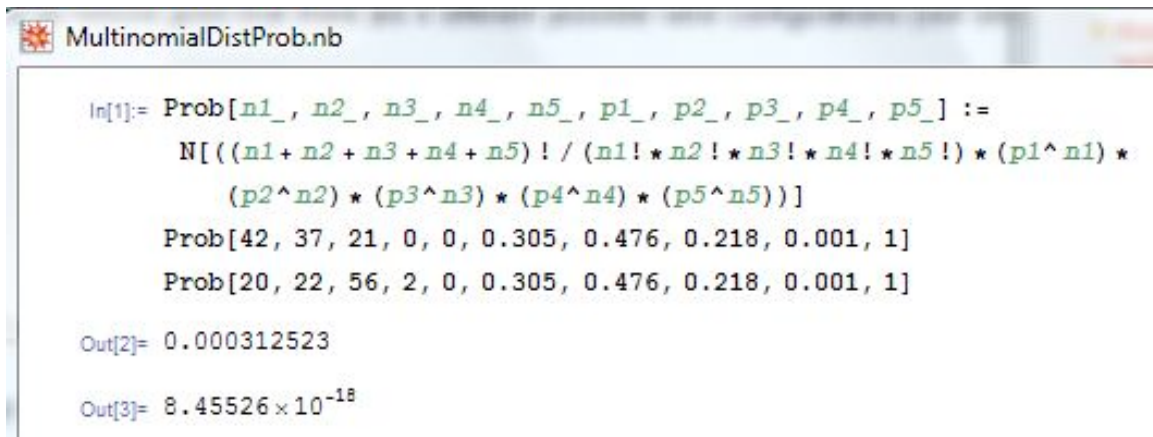
Apparatus 1:

$$P(42,37,21,0) = \frac{100!}{42! 37! 21! 0!} 0.305^{42} 0.476^{37} 0.218^{21} 0.001^0$$
$$P(42,37,21,0) = 3.125 \times 10^{-4}$$

Apparatus 2:

$$P(20,22,56,2) = \frac{100!}{20! 22! 56! 2!} 0.305^{20} 0.476^{22} 0.218^{56} 0.001^2$$
$$P(20,22,56,2) = 8.455 \times 10^{-18}$$

Based on the calculations above for both apparatuses, Apparatus 1 is more like the desired model. Apparatus 1 has a higher probability density function, based on the relative likelihood of each configuration flow.



```
MultinomialDistProb.nb

In[1]:= Prob[n1_, n2_, n3_, n4_, n5_, p1_, p2_, p3_, p4_, p5_] :=
  N[ ((n1 + n2 + n3 + n4 + n5)! / (n1! * n2! * n3! * n4! * n5!)) * (p1^n1) *
    (p2^n2) * (p3^n3) * (p4^n4) * (p5^n5) ]
  Prob[42, 37, 21, 0, 0, 0.305, 0.476, 0.218, 0.001, 1]
  Prob[20, 22, 56, 2, 0, 0.305, 0.476, 0.218, 0.001, 1]

Out[2]= 0.000312523

Out[3]= 8.45526 × 10-18
```

This figure shows Mathematica code that can be used in order to solve the probability of a multinomial distribution. The n values are the number of occurrences of each outcome and the p values are the probabilities of each outcome. The function is set for a multinomial distribution with five different outcomes. However, it can be used for multinomial distributions with fewer outcomes by setting the unused n values to 0 and the unused p values to any number other than 0. This figure also shows the probabilities calculated from Apparatus 1 and Apparatus 2.

10.7 Worked out Example 4

A runaway reaction occurs when the heat generation from an exothermic reaction exceeds the heat loss. Elevated temperature increases reaction rate, further increasing heat generation and pressure buildup inside the reactor. Together, the uncontrolled escalation of temperature and pressure inside a reactor may cause an explosion.

The precursors to a runaway reaction - high temperature and pressure - can be detected by the installation of reliable temperature and pressure sensors inside the reactor. Runaway reactions can be prevented by lowering the temperature and/or pressure inside the reactor before they reach dangerous levels. This task can be accomplished by sending a cold inert stream into the reactor or venting the reactor.

Les Lloyd is a process engineer at the Miles Reactor Company that has been assigned to work on a new reaction process. Using historical data from all the similar reactions that have been run before, Les has estimated the probabilities of each outcome occurring during the new process. The potential outcomes of the process include all permutations of the possible reaction temperatures (low and high) and pressures (low and high). He has combined this information into the table below:

Outcome	Temperature	Pressure	Probability
1	high	high	0.013
2	high	low	0.267
3	low	high	0.031
4	low	low	0.689

Worried about risk of runaway reactions, the Miles Reactor Company is implementing a new program to assess the safety of their reaction processes. The program consists of running each reaction process 100 times over the next year and recording the reactor conditions during the process every time. In order for the process to be considered safe, the process outcomes must be within the following limits:

Outcome	Temperature	Pressure	Frequency
1	high	high	$n_1 = 0$
2	high	low	$n_2 \leq 20$
3	low	high	$n_3 \leq 2$
4	low	low	$n_4 = 100 - n_1 - n_2 - n_3$

Help Les predict whether or not the new process is safe by answering the following question: What is the probability that the new process will meet the specifications of the new safety program?

10.7.1 Solution to Example 4

The probability of the safety guidelines being met is given by the following CDF expression:

$$P(n_1 = 0, n_2 \leq 20, n_3 \leq 2, n_4 = 100 - n_1 - n_2 - n_3) = \sum_{n_1=0}^0 \sum_{n_2=0}^{20} \sum_{n_3=0}^2 \frac{100!}{n_1!n_2!n_3!(100 - n_1 - n_2 - n_3)!} p_1^0 p_2^{n_2} p_3^{n_3} p_4^{100 - n_1 - n_2 - n_3}$$

where

- N is the number of trials
- k is the number of possible outcomes
- n_i is the number of occurrence of outcome i
- p_i is the probability of seeing outcome i
- c_i is the maximum number of occurrence of outcome i

This CDF expression can be evaluated using the following commands in Mathematica:

```
<< Needs["MultivariateStatistics`"]
<< multinomial = MultinomialDistribution[100, {0.013, 0.267, 0.031, 0.689}]
<< CDF[multinomial, {0, 20, 2, 78}]
```

The result is:

$$P(n_1 = 0, n_2 \leq 20, n_3 \leq 2, n_4 = 1000 - n_1 - n_2 - n_3) = 0.00132705$$

Based on this probability calculation, it appears unlikely that this new process will pass the new safety guidelines.

10.8 Sage's Corner

<http://www.youtube.com/v/aA1QpREhy5c>


For slides of this presentation by Group Si: [Media:Multinomial Distribution.ppt](#)

10.9 References

- Woolf, Peter, Amy Keating, Christopher Burge, and Michael Yaffe. (2004). *Statistics and Probability Primer for Computational Biologists*. Massachusetts Institute of Technology.
- "Multinomial Distribution." Wikipedia. http://en.wikipedia.org/wiki/Multinomial_distribution.
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- *Multinomial Calculator: Online Statistical Calculator*. Accessed 27 Nov. 2007.
<http://stattrek.com/Tables/multinomial.aspx#calculator>

Section 11. Comparisons of two means

Note:  [Video lecture](#) available for this section!

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Date Revised: 11/15/07

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

11.1 Introduction

Engineers often must compare data sets to determine whether the results of their analyses are statistically equivalent. A sensor outputs a series of values and the engineer must both determine whether the sensor is precise and whether the values are accurate according to a standard. To make this evaluation, statistical methods are used. One method compares the probability distributions and another uses the Students t-test on two data sets. Microsoft Excel also has functions that perform the t-test that output a fractional probability to evaluate the null hypothesis ([Basic Statistics](#)).

11.2 Distributions

11.2.1 General Distributions

Distributions are governed by the [probability density function](#):

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x - \mu}{\sigma}\right)^2\right)$$

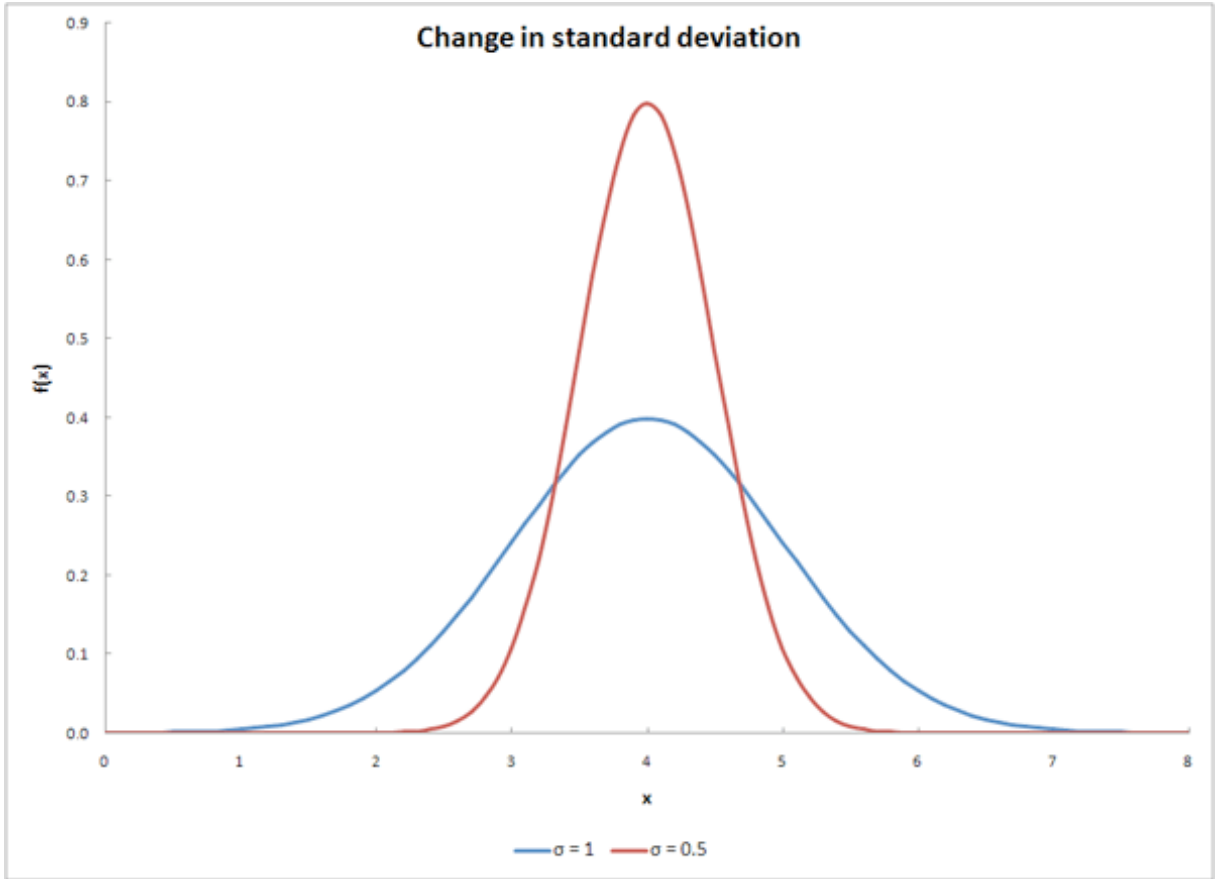
where

σ is the standard deviation of a data set

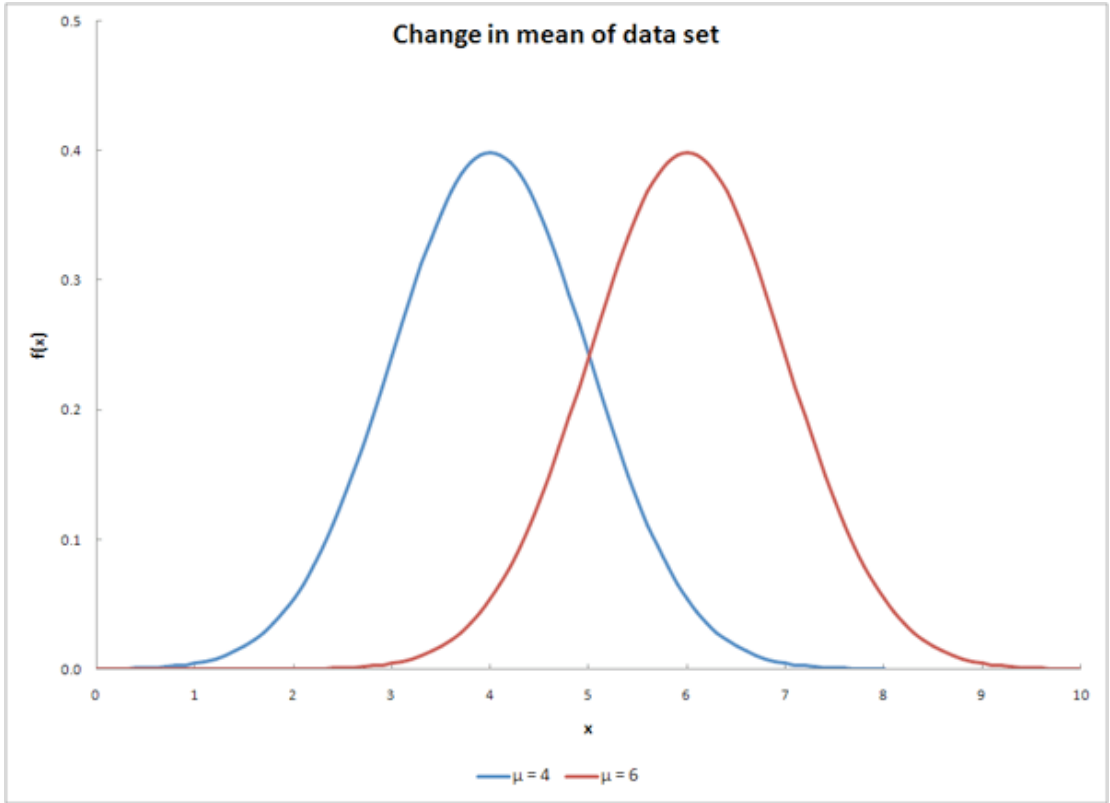
μ is the mean of the data set

x is the input value

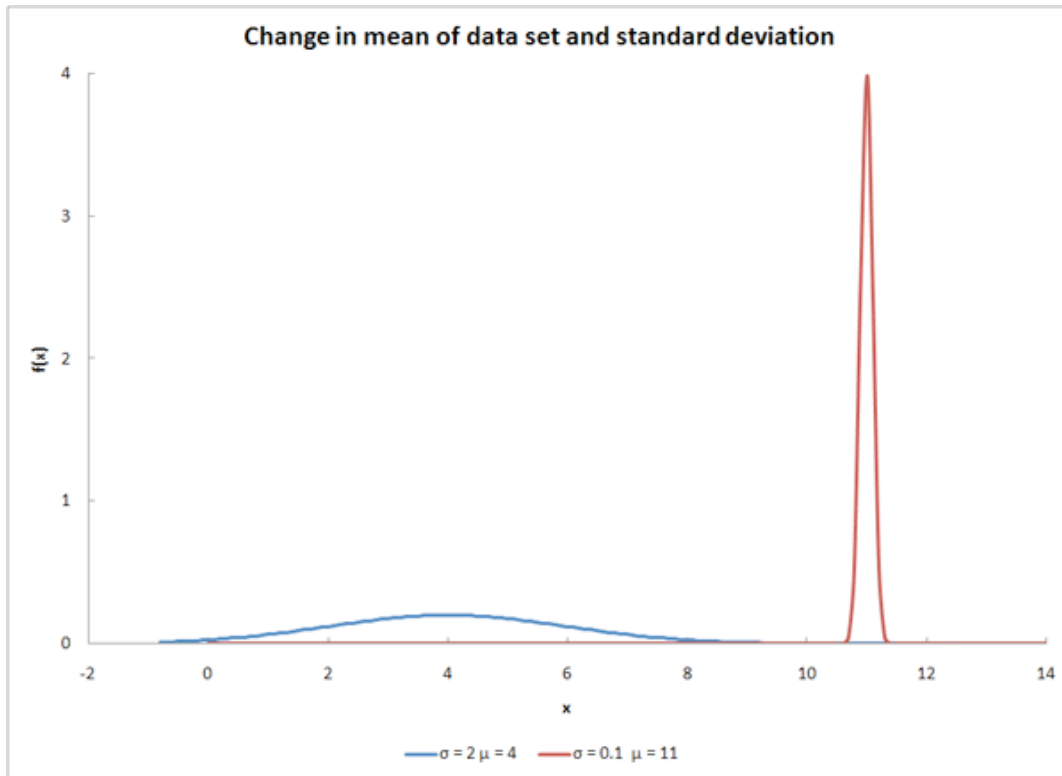
This equation gives a typical bell curve. Changing σ will alter the shape of the curve, as shown in the graph below.



Changing μ will shift the curve along the x-axis, as shown below.



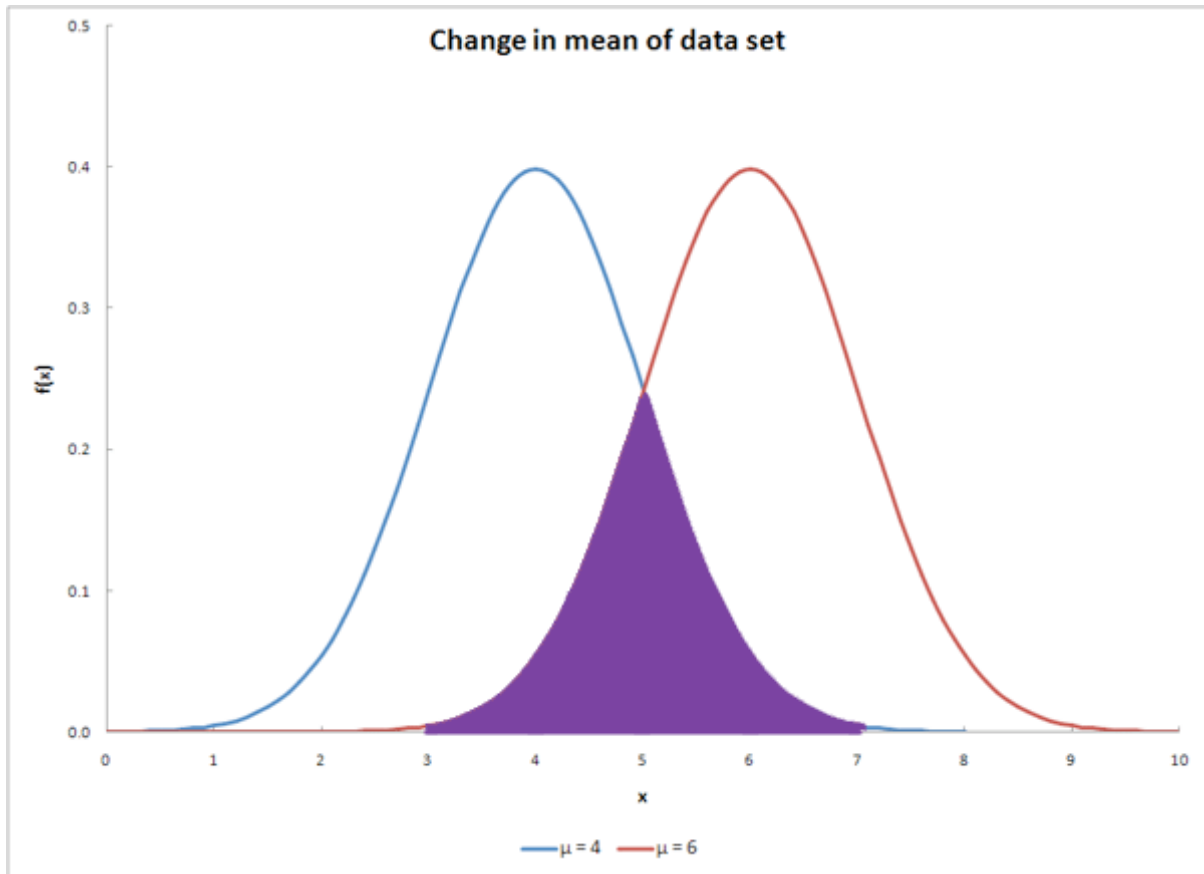
Changing both variables will have a result similar to the graph below.



For a more indepth look at distributions, go to ([Distributions](#)).

11.2.2 Overlapping Distributions

The overlap between two distribution curves helps determine the probability of the two data sets being from the same distribution. The probability value increases as overlapping increases. The overlap is shown as the purple region in the graph below.



11.3 Comparison of Two Means

11.3.1 Probability

The similarity of two data sets can be determined by finding the probability of overlap. This is illustrated by the following equation:

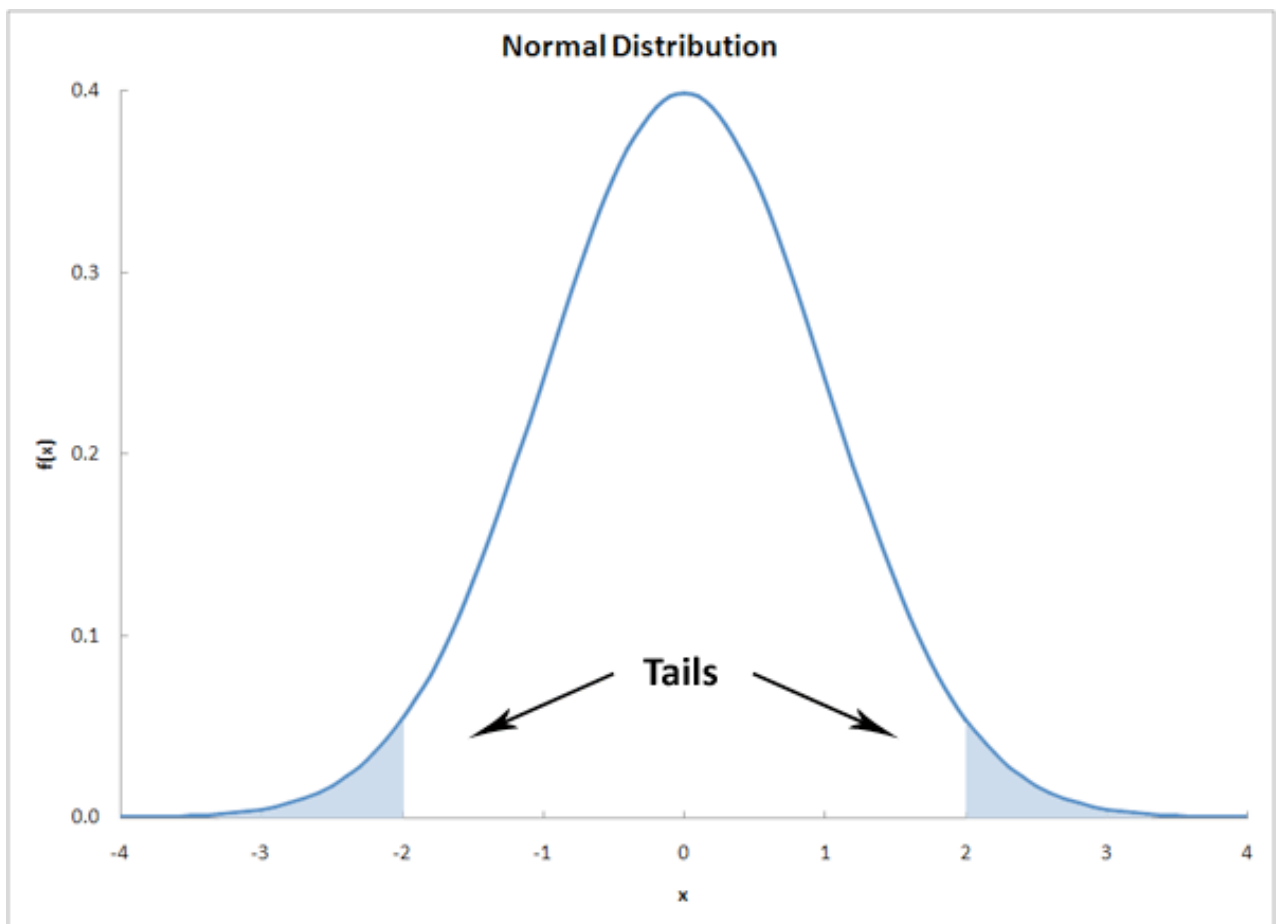
$$P(\text{overlap}) = \int_{-\infty}^{\infty} \min \begin{cases} p_s(k|\theta_s) \\ p_o(k|\theta_o) \end{cases}$$

The functions contained within the integral are the probability distributions of each respective data set. The equation sums the lesser probability distribution from each data set. After using this equation, the solution will be a value with a range between 0 and 1 indicating the magnitude of overlapping probability. A value of 0 demonstrates that the two data sets do not overlap at all. A value of 1 demonstrates that the two data sets completely overlap. Values between 0 and 1 give the extent of overlap between the two data sets. This probability is not the same as the confidence interval that can be computed with t-tests.

11.3.2 Student's T-Test

The Student's t-test is extremely useful for comparing two means. There are various versions of the student t-test, depending on the context of the problem. Generally, the test quantifies the signal to noise ratio - where the signal is the difference of means and the noise is a function of the error around the means. If the signal is large and the noise is small, one can be more confident that the difference between the means is "real" or significant. To prove a significant difference, we need to disprove the null hypothesis. The "null hypothesis" (H_0) is that there is no difference between the two means. If we are able to disprove the "null hypothesis" then we will be able to say that the two groups are statistically different within a known level of confidence.

The extremities at either ends of a probability distribution are referred to as the "tails" of the distribution. The assessment of the significance of a calculated t-value will depend upon whether or not both tails of the distribution need to be considered. This will depend on the form of the null hypothesis. If your null hypothesis is an equality, then the case where one mean is larger *and* smaller must be considered; i.e. only one tail of the distribution should be accounted for. Conversely, if the null hypothesis is an inequality, then you are only concerned with the domain of values for a mean either less than *or* greater than the other mean; i.e. both tails of the distribution should be accounted for.

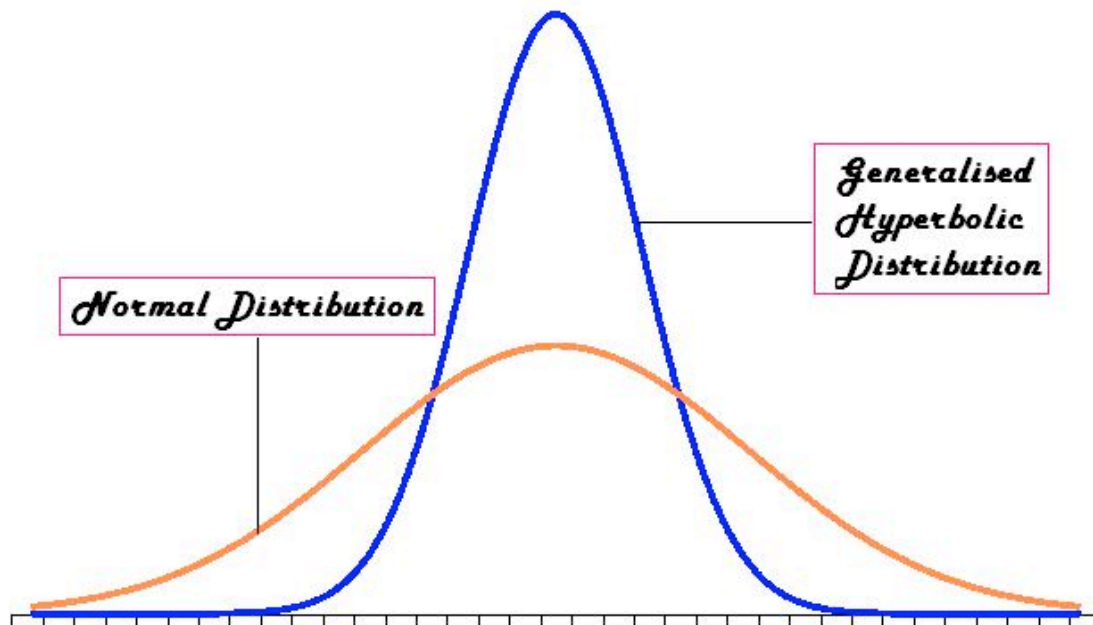


More Info: the student t-distribution

The t-distribution is the resulting probability distribution with a small sample population. This distribution is the basis for the t-test, in order to find the statistical significance between two means of data. This distribution is in the form of a generalised hyperbolic function (Which goes into details that would only clutter here. For more information, the wikipedia site holds a lot of information on the subject:

http://en.wikipedia.org/wiki/Generalised_hyperbolic_distribution).

The t-distribution is commonly used when the standard deviation is unknown, or cannot be known (ie: a very small population set). When the data sets are large, or a standard deviation is assumed, the t-distribution is not very useful for a statistical analysis, and other methods of analysis should be used. An example of the t-distribution can be seen below:



Comparing Two Unknown True Means when Sample Standard Deviations are approximately Equal

The first accepted assumption is that when two sample means are being compared, the standard deviations are approximately equal. This method requires the average, standard deviation, and the number of measurements taken for each data set. The deviations are then pooled into one standard deviation. The equation for this t-test is as follows:

$$t = \frac{\text{Signal}}{\text{Noise}} = \frac{\bar{x}_1 - \bar{x}_2}{S_{pooled}} \sqrt{\frac{n_1 n_2}{n_1 + n_2}}$$

Where:

$$S_{pooled} = \sqrt{\frac{s_1^2 (n_1 - 1) + s_2^2 (n_2 - 1)}{n_1 + n_2 - 2}}$$

Where:

\bar{x}_1 is the average of the first data set

\bar{x}_2 is the average of the second data set

n_1 is the number of measurements in the first data set

n_2 is the number of measurements in the second data set

s_1 is the standard deviation of the first data set

s_2 is the standard deviation of the second data set

t is a result of the t-test; it relates to values from the Student's t-distribution

Also note that the variance is defined as the square of the standard deviation.

Using t-distribution tables (sample shown below), the confidence level for the two means can then be determined. This confidence level determines whether the two means are significantly different. The confidence level can be found with the degrees of freedom for the measurements and the t-value computed above. The degree of freedom is equal to two less than the total number of measurements from the two data sets, as shown below:

$$DOF = n_1 + n_2 - 2$$

The following table is an image of a t value table, which can also be found ([here](#)):

Degrees of Freedom	Confidence Level %			
	50	90	95	98
1	1.000	6.314	12.706	31.821
2	0.816	2.920	4.303	6.965
3	0.756	2.353	3.182	4.541
4	0.741	2.132	2.776	3.747
5	0.727	2.015	2.571	3.365
6	0.718	1.943	2.447	3.143
7	0.711	1.895	2.365	2.998
8	0.706	1.860	2.306	2.896
9	0.703	1.833	2.262	2.821
10	0.700	1.812	2.228	2.764
15	0.691	1.753	2.131	2.602
20	0.687	1.725	2.086	2.528
25	0.684	1.708	2.060	2.485
30	0.683	1.697	2.042	2.457
40	0.681	1.684	2.021	2.423
60	0.679	1.671	2.000	2.390
120	0.677	1.658	1.980	2.358
∞	0.674	1.645	1.960	2.326

For example, if you had two data sets totaling 10 measurements and you calculated a t-value of 2.305 the confidence level would be 95%. This means that there is a 95% chance that the two data sets are statistically different and only a 5% chance that the two data sets are statistically similar. Also, degrees of freedom between the values listed on the table can be found by interpolating between those two values.

Note that there are some drawbacks when evaluating two means to see if they are significant or not. This problem mainly stems from the standard deviation. If say a set of values has a certain mean x , but the standard deviation was high due to the fact that some numbers in may have been greatly out of the range of the mean. This standard deviation may imply, from the student's t-test, that the mean x is significantly different from the mean of another set of data, when in actuality it may not seem that different. Hence, this must be taken into account when comparing two means using the student's t-test.

Comparing Two Unknown True Means ($\mu_1 = ?$ and $\mu_2 = ?$) with Known True Unequal Standard Deviations ($\sigma_1 \neq \sigma_2$)

The z-test is used when the difference between a sample mean and the population mean is large enough to be statistically significant. The t-test and z-test are essentially the same but in the z-test the actual population means (μ) and standard deviations (σ) are known. Since the estimate for difference in standard deviation used here is biased, two sample z-tests are rarely used.

The two sample z-statistic is described by:

$$z = \frac{\text{Signal}}{\text{Noise}} = \frac{\bar{x}_1 - \bar{x}_2}{\sqrt{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}}}$$

Where:

\bar{x}_1 is the average of the first data set

\bar{x}_2 is the average of the second data set

n_1 is the number of measurements in the first data set

n_2 is the number of measurements in the second data set

σ_1 is the known standard deviation of the first population

σ_2 is the known standard deviation of the second population

A different table is used to look up the probability of significance, please refer to [Z-score table](#). If $p < 0.05$ (using a 95% confidence interval), we can declare a significant difference exists. The p-value is the probability that the observed difference between the means is caused by sampling variation, or the probability that these two samples came from the same population.

Comparing Two Unknown True Means ($\mu_1 = ?$ and $\mu_2 = ?$) with Unknown True Standard Deviations ($\sigma_1 = ?$ and $\sigma_2 = ?$)

This is known as the two sample t-statistic, which is used in statistical inference for comparing the means of two independent, normally distributed populations with unknown true standard deviations. The two sample t-statistic is described by:

$$t = \frac{\text{Signal}}{\text{Noise}} = \frac{\bar{x}_1 - \bar{x}_2}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}}$$

Where:

\bar{x}_1 is the average of the first data set

\bar{x}_2 is the average of the second data set

n_1 is the number of measurements in the first data set

n_2 is the number of measurements in the second data set

s_1 is the standard deviation of the first data set

s_2 is the standard deviation of the second data set

Comparing the Mean of Differences for Paired Data

This is used in statistical analysis for the case where a single mean of a population occurs when two quantitative variables are collected in pairs, and the information we desire from these pairs is the difference between the two variables.

Two examples of paired data:

1. Each unit is measured twice. The two measurements of the same data are taken under varied conditions.
2. Similar units are paired prior to the experiment or run. During the experiment or run each unit is placed into different conditions.

The mean of differences t-statistic is described by:

$$t = \frac{\bar{d}}{\frac{s_d}{\sqrt{n}}}$$

Where:

\bar{d} is the the mean of the differences for a sample of the two measurements

s_d is the standard deviation of the sampled differences

n is the number of measurements in the sample

Summary of Two Sample Mean Tests

Tests of Two Population Means			
Case	USE	Test Statistic	Formula
I	known σ 's , and normal populations	z_0	$z = \frac{\bar{x} - \bar{y} - \Delta_0}{\sqrt{\frac{\sigma_1^2}{m} + \frac{\sigma_2^2}{n}}}$
II	unknown σ 's , and normal populations (unequal variances)	t_0	$t = \frac{\bar{x} - \bar{y} - \Delta_0}{\sqrt{\frac{s_1^2}{m} + \frac{s_2^2}{n}}}$
III	unknown σ 's , and normal populations (equal variances)	t_0	$t = \frac{\bar{x} - \bar{y} - \Delta_0}{\sqrt{s_p^2 \left(\frac{1}{m} + \frac{1}{n} \right)}}$
IV	Paired t-test	t_0	$t = \frac{\bar{d} - \Delta_0}{s_d / \sqrt{n}}$

11.3.3 Excel Method

Instead of using the t-distribution tables to interpolate values, it is often easier to use built-in tools in Excel. The following three functions can be used for most of the common situations encountered when comparing two means:

- The TDIST function is useful when you have calculated a t-value and you want to know the probability that the t-value is significant.

- The TINV function is useful when you know the probability of significance you are interested in, and you desire the t-value (essentially the reverse of the TDIST function). This is helpful if you are designing an experiment and would like to determine the number of experimental runs needed to test for the difference of two means.
- The TTEST function is useful if you have two sets of data and you would like to know the probability that the mean of the two data sets are significantly different.

TDIST Function

The TDIST function has the syntax "`=TDIST(x,deg_freedom,tails)`"

Where:

- **x** is the t-value of the statistic
- **deg_freedom** is the number of degrees of freedom of the t-statistic. For comparing sample means \bar{x}_o and \bar{x}_s , with sample sizes n_o and n_s respectively, has $n_o + n_s - 2$ degrees of freedom.
- **tails** is the number of tails to be summed for probability. If null hypothesis is an equality, 2 tails will be used. If the null hypothesis is an inequality, 1 tail will be used.

The output of the function is the fractional probability of the Students t-distribution. For example, if the function returned a value of 0.05, this would correspond to a 95% or equivalently (1 - 0.05) confidence level for rejecting the null hypothesis.

TINV Function

The TINV function has the syntax "`=TINV(probability, deg_freedom)`"

Where:

- **probability** is the fractional probability of the Students t-distribution. This is identical to the output of the "TDIST" function.
- **deg_freedom** is the number of degrees of freedom of the t-statistic. For comparing sample means \bar{x}_o and \bar{x}_s , with sample sizes n_o and n_s respectively, has $n_o + n_s - 2$ degrees of freedom.

The output of the function is the t-value of the Student's t-distribution.

TTEST Function

The TTEST function has the syntax "`=TTEST(array 1, array 2, tails, type)`"

Where:

- **array 1** is the first data set
- **array 2** is the second data set
- **tails** is the number of tails to be summed for probability (1 or 2). If null hypothesis is an equality 2 tails will be used, if the null hypothesis is an inequality 1 tail will be used.
- **type** is the type of t-test to be performed the values that correspond to each type of test are listed below.

	If type equals		This test is performed		
1		Paired	2		Two-
sample equal variance (homoscedastic)				3	
	Two-sample unequal variance (heteroscedastic)				

For our purposes we will only be concerned with type = 3. This corresponds to unequal variance (independent data sets). The other two types are useful and may prove interesting for the curious, but are beyond our scope.

Alternatively if you are not fond of Excel, a website located [here](#) will do the TTEST calculation for you.

The output of the function is the fractional probability of the Student's t-distribution. For example, if the function returned a value of 0.05, this would correspond to a 95% or equivalently (1 - 0.05) confidence level for rejecting the null hypothesis.

This function is very useful when the data-sets of the two means to be compared are known.

11.4 Worked out Example 1

You are a product quality engineer at a company that manufactures powdered laundry detergent in 100 ounce boxes. You are in charge of determining whether the product meets the specifications the company promises the customer. In the past, 100 samples

(n_o) of the process established normal process conditions. The data is given below. Note that weighing samples using an imprecise scale does not affect your results. Also assume that the standard deviations are close enough to pool them.

Sample	Mass (oz)	Sample	Mass (oz)	Sample	Mass (oz)	Sample	Mass (oz)
1	101.5323	26	103.6760	51	102.8321	76	102.2068
2	102.6114	27	99.4326	52	103.1561	77	100.0458
3	98.5144	28	101.0811	53	104.9740	78	99.1730
4	102.5376	29	103.0467	54	102.8182	79	101.1648
5	99.6549	30	104.5012	55	104.6667	80	102.7247
6	103.2026	31	103.3905	56	102.7701	81	104.5956
7	102.9082	32	103.3171	57	100.3976	82	100.5764
8	103.5021	33	102.4609	58	104.4545	83	101.6134
9	102.3490	34	100.2123	59	101.3030	84	104.6165
10	104.0031	35	102.0465	60	103.6512	85	101.5386
11	98.9170	36	104.3919	61	101.2811	86	102.2764
12	103.1442	37	104.3028	62	104.8338	87	99.8757
13	103.9829	38	104.7788	63	100.0149	88	102.9348
14	102.0530	39	99.9478	64	101.5113	89	104.2985
15	100.8094	40	102.4054	65	103.6051	90	99.1000
16	102.4637	41	100.5217	66	104.5143	91	104.3817
17	100.1330	42	99.2822	67	100.6274	92	100.0774
18	101.1803	43	100.0083	68	104.7486	93	103.3923
19	102.4206	44	103.0967	69	103.0690	94	103.1890
20	99.2446	45	104.3340	70	101.9572	95	104.2288
21	101.1265	46	99.4872	71	102.6948	96	104.7568
22	104.5352	47	102.7668	72	104.4613	97	99.7750
23	103.0829	48	104.0406	73	102.1133	98	103.7144
24	101.3206	49	103.9086	74	99.6126	99	104.7967
25	104.7705	50	103.6373	75	104.3923	100	101.8893

You randomly sample 25 (n_s) of the products and you get the following data:

Sample	Mass (oz)
1	103.0484
2	103.2938
3	102.0150
4	100.2619
5	97.5217
6	97.8343
7	100.5561
8	101.7700
9	97.5080
10	99.6632
11	98.4071
12	98.6208
13	99.9031
14	97.6498
15	98.9091
16	98.0822
17	99.1118
18	102.5405
19	103.7024
20	102.6328
21	97.4841
22	99.9671
23	100.7755
24	99.9557
25	98.7856

The data can also be found in the first tab of this Excel file: [Data File](#)

Is the process running significantly different from normal with 95% confidence? In this example, do not use built-in Excel functions.

11.4.1 Solution

Using the data, the normal process produces an average (\bar{x}_o) product mass of 102.37 and a variance (s_o^2) of 3.17.

The sample has an average mass (\bar{x}_s) of 100.00 with a variance (s_s^2) of 4.00.

These were calculated using the AVERAGE function and VAR function in Excel. See the second tab of this Excel file for further explanation: [Example 1](#)

The null hypothesis is that the means are identical and the difference between the two means is due purely to chance.

Using the t-test:

$$t = \frac{\bar{x}_o - \bar{x}_s}{\sqrt{\frac{s_o^2(n_o-1) + s_s^2(n_s-1)}{n_o + n_s - 2}}} \sqrt{\frac{n_o n_s}{n_o + n_s}}$$

$$t = \frac{102 - 100}{\sqrt{\frac{3(100-1) + 4(25-1)}{100+25-2}}} \sqrt{\frac{25 * 100}{25 + 100}} = 5.00$$

Looking at the table that is reprinted below for reference:

Degrees of Freedom	Confidence Level %			
	50	90	95	98
120	0.677	1.658	1.980	2.358
∞	0.674	1.645	1.960	2.326

The number of degrees of freedom is:

$$DOF = n_o + n_s - 2$$

$$DOF = 25 + 100 - 2 = 123$$

The t-value corresponding to 95% confidence level at 123 degrees of freedom is between 1.960 and 1.980. Since the calculated t-value, 5.00, is much greater than 1.980, the null hypothesis is rejected at the 95% confidence level.

We conclude that the two means are significantly different. Thus, the process is not running normally and it is time to troubleshoot to find the problems occurring in the system.

11.5 Worked out Example 2

Same problem as "Worked Out Example 1." Instead, use the TTEST function in Excel.

11.5.1 Solution

The solution can also be seen in the third tab of this Excel file: [Example 2](#)

Using the TTEST function, with tails = 2 and test type = 3, the function gives a T-test value of 4.78×10^{-6} .

Since 4.78×10^{-6} is less than 0.05 (from our 95% confidence level) we can once again conclude that we can reject the null hypothesis.

11.6 Multiple Choice Question 1

If there are two sets of data, one with 15 measurements and another with 47 measurements, how many degrees of freedom would you enter in the Excel functions?

a. 20

b. 47

c. 15

d. 60

11.6.1 Answer

The number of degrees of freedom is calculated as follows:

$$DOF = n_1 + n_2 - 2$$

where n_1 is the number of measurements in the first data set and n_2 is the number of measurements in the second data set.

Therefore,

$$DOF = 15 + 47 - 2 = 60$$

the answer is **d**.

11.7 Multiple Choice Question 2

What does the statement "Accurate within 95% confidence" mean?

a. The average of the data set is statistically equal to the true value within 95%

b. The value is the average plus or minus 95%

c. The average is statistically equal to the true value within 5%

11.7.1 Answer

The answer is **c**.

11.8 Sage's Corner

PowerPoint Presentation #1


<http://video.google.com/googleplayer.swf?docId=4694719892575996020>

For slides of this presentation: [Media:Comparison of Two Means.ppt](#)

11.9 References

- "Comparison of Two Means." State.Yale.Edu. Yale. 19 Nov. 2006 <<http://www.stat.yale.edu/Courses/1997-98/101/meancomp.htm>>.
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Section 12. Factor analysis and ANOVA

Note:  [Video lecture](#) available for this section!

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12.1 Introduction

First invented in the early 1900s by psychologist Charles Spearman, factor analysis is the process by which a complicated system of many variables is simplified by completely defining it with a smaller number of "factors." If these factors can be studied and determined, they can be used to predict the value of the variables in a system. A simple example would be using a person's intelligence (a factor) to predict their verbal, quantitative, writing, and analytical scores on the GRE (variables).

Analysis of variance (ANOVA) is the method used to compare continuous measurements to determine if the measurements are sampled from the same or different distributions. It is an analytical tool used to determine the significance of factors on measurements by looking at the relationship between a quantitative "response variable" and a proposed explanatory "factor." This method is similar to the process of comparing the statistical difference between two samples, in that it invokes the concept of hypothesis testing. Instead of comparing two samples, however, a variable is correlated with one or more explanatory factors, typically using the F-statistic. From this F-statistic, the P-value can be calculated to see if the difference is significant. For example, if the P-value is low (P-value < 0.05 or P-value < 0.01 - this depends on desired level of significance), then there is a low probability that the two groups are the same. The method is highly versatile in that it can be used to analyze complicated systems, with numerous variables and factors. In this article, we will discuss the computation involved in *Single-Factor*, *Two-Factor: Without Replicates*, and *Two-Factor: With Replicates* ANOVA. Below, is a brief overview of the different types of ANOVA and some examples of when they can be applied.

12.1.1 Overview and Examples of ANOVA Types

ANOVA Types

Single-Factor ANOVA (One-Way):

One-way ANOVA is used to test for variance among two or more independent groups of data, in the instance that the variance depends on a single factor. It is most often employed when there are at least three groups of data, otherwise a t-test would be a sufficient statistical analysis.

Two-Factor ANOVA (Two-Way):

Two-way ANOVA is used in the instance that the variance depends on two factors. There are two cases in which two-way ANOVA can be employed:

- Data *without replicates*: used when collecting a single data point for a specified condition
- Data *with replicates*: used when collecting multiple data points for a specified condition (the number of replicates must be specified and must be the same among data groups)

When to Use Each ANOVA Type

- Example: There are three identical reactors (R1, R2, R3) that generate the same product.
 - One-way ANOVA: You want to analyze the variance of the product yield as a function of the reactor number.
 - Two-way ANOVA without replicates: You want to analyze the variance of the product yield as a function of the reactor number and the catalyst concentration.
 - Two-way ANOVA with replicates: For each catalyst concentration, triplicate data were taken. You want to analyze the variance of the product yield as a function of the reactor number and the catalyst concentration.

ANOVA is a Linear Model

Though ANOVA will tell you if factors are significantly different, it will do so according to a linear model. ANOVA will always assume a linear model, it is important to consider strong nonlinear interactions that ANOVA may not incorporate when determining significance. ANOVA works by assuming each observation as overall mean + mean effect + noise. If there are non-linear relationships between these (for example, if the difference between column 1 and column 2 on the same row is that $\text{column2} = \text{column1}^2$), then there is the chance that ANOVA will not catch it.

12.2 Key Terms

Before further explanation, please review the terms below, which are used throughout this Wiki.

Term or Variable	Description
Factor	Characteristics differentiating populations from one another
Group	Sample set that is influenced by the same factor
Levels	Populations (or treatments)
n_j	Number of elements in group j
x_{ji}	Element within group j
s_j^2	Variance within group j
N	Total number of samples
k	Total number of groups
\bar{x}_j	Mean of group j
\bar{x}	Mean of all samples within all groups
SSGroups	Sum of squares between groups
SSE	Sum of squared errors within groups
MSGroups	Mean square between groups
MSE	Mean square error within groups
SSTotal	Total sum of squares
df	Degrees of freedom

12.3 Comparison of Sample Means Using the F-Test

The F-Test is the ratio of the sample variances. The F-statistic and the corresponding F-Test are used in single-factor ANOVA for purposes of hypothesis testing.

Null hypothesis (H_o): all sample means arising from different factors are equal

Alternative hypothesis (H_a): the sample means are not all equal

Several assumptions are necessary to use the F-test:

- The samples are independent and random
- The distribution of the response variable is a normal curve within each population
- The different populations may have different means
- All populations have the same standard deviation

12.3.1 Introduction to the F-Statistic

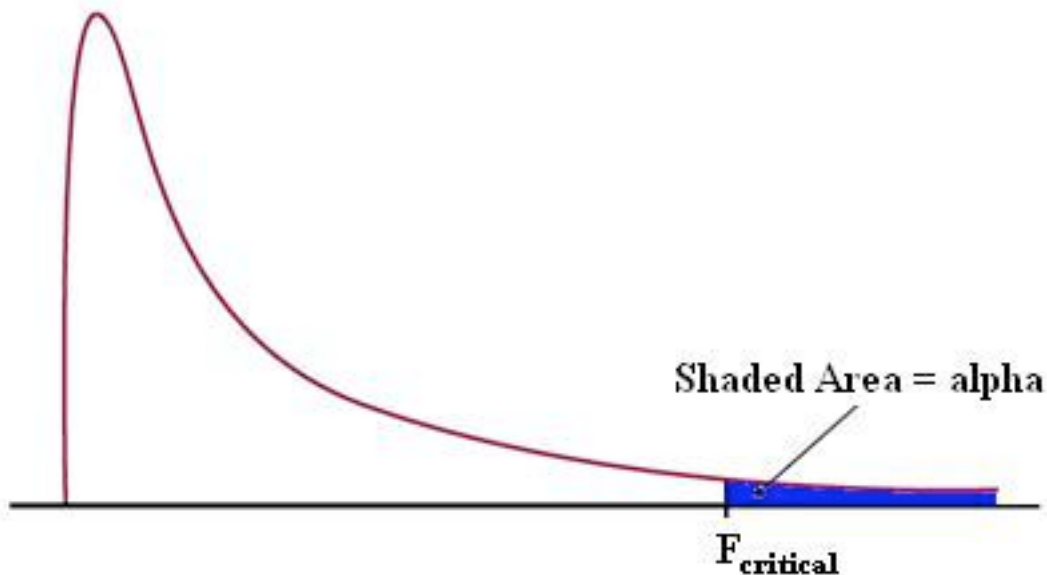
The F-statistic is the ratio of two variance estimates: the variance between groups divided by the variance within groups. The larger the F-statistic, the more likely it is that the difference between samples is due to the factor being tested, and not just the natural variation within a group. A standardized table can be used to find $F_{critical}$ for any system. $F_{critical}$ will depend on alpha, which is a measure of the confidence level. Typically, a value of alpha = 0.05 is used, which corresponds to 95% confidence. If $F_{observed} > F_{critical}$, we conclude with 95% confidence that the null hypothesis is false. For an explanation of how to read an F-Table, see *Interpreting the F-statistic* (below). In a similar manner, F

tables can also be used to determine the p-value for a given data set. The p-value for a given data set is the probability that you could obtain this data set if the null hypothesis were true: that is, if the results were strictly due to chance. When H_0 is true, the F-statistic has an F distribution.

12.3.2 F-Distributions

The F-distribution is important to ANOVA, because it is used to find the p-value for an ANOVA F-test. The F-distribution arises from the ratio of two Chi squared distributions. Thus, this family has a numerator and denominator degrees of freedom. (For information on the Chi squared test, click [here](#).) Every function of this family has a skewed distribution and minimum value of zero.

Figure 1 - F distribution with alpha and $F_{critical}$ indicated



12.4 Single-Factor Analysis of Variance

In the case of single-factor analysis, also called single classification or one-way, a factor is varied while observing the result on the set of dependent variables. These dependent variables belong to a specific related set of values and hence, the results are expected to be related.

This section will describe some of the computational details for the F-statistic in one-way ANOVA. Although these equations provide insight into the concept of analysis of variance and how the F-test is constructed, it is not necessary to learn formulas or to do this analysis by hand. In practice, computers are always used to do one-way ANOVA

12.4.1 Setting up an Analysis of Variance Table

The fundamental concept in one-way analysis of variance is that the variation among data points in all samples can be divided into two categories: variation between group means and variation between data points in a group. The theory for analysis of variance stems from a simple equation, stating that the total variance is equal to the sum of the variance between groups and the variation within groups –

Total variation = variation between groups + variation within groups

An analysis of variance table is used to organize data points, indicating the value of a response variable, into groups according to the factor used in each case. For example, Table 1 is an ANOVA table for comparing the amount of weight lost over a three month period by dieters on various weight-loss programs.

Table 1 - Amount of weight lost by dieters on various programs over a 3 month period

Program 1	Program 2	Program 3
7	9	15
9	11	12
5	7	18
7		

A reasonable question is, can the type of program (a factor) be used to predict the amount of weight a dieter would lose on that program (a response variable)? Or, in other words, is any one program superior to the others?

12.4.2 Measuring Variation Between Groups

The variation between group means is measured with a weighted sum of squared differences between the sample means and the overall mean of all the data. Each squared difference is multiplied by the appropriate group sample size, n_i , in this sum. This quantity is called **sum of squares between groups** or **SS Groups**.

$$SSGroups = n_1(x_1 - \bar{x})^2 + n_2(x_2 - \bar{x})^2 + \dots + n_k(x_k - \bar{x})^2 = \sum_{groups} n_j(\bar{x}_j - \bar{x})^2$$

The numerator of the F-statistic for comparing means is called the **mean square between groups** or **MS Groups**, and it is calculated as -

$$MSGroups = \frac{SSGroups}{k - 1}$$

12.4.3 Measuring Variation Within Groups

To measure the variation among data points within the groups, find the sum of squared deviations between data values and the sample mean in each group, and then add these quantities. This is called the **sum of squared errors, SSE**, or **sum of squares within groups**.

$$SSE = (n_1 - 1)s_1^2 + (n_2 - 1)s_2^2 + \dots + (n_k - 1)s_k^2 = \sum_{\text{all groups}} (n_j - 1)s_j^2$$

$$s_j^2 = \sum_{\text{group } j} \frac{(x_{ij} - \bar{x}_j)^2}{n_j - 1}$$

Where s_j^2 = variance within each group

The denominator of the F-statistic is called the **mean square error, MSE**, or **mean squares within groups**. It is calculated as

$$MSE = \frac{SSE}{N - k} = \frac{(n_1 - 1)s_1^2 + (n_2 - 1)s_2^2 + \dots + (n_k - 1)s_k^2}{n_1 + n_2 + \dots + n_k - k}$$

MSE is simply a weighted average of the sample variances for the k groups. Therefore, if all n_i are equal, MSE is simply the average of the k sample variances. The square root of MSE (s_p), called the **pooled standard deviation**, estimates the population standard deviation of the response variable (keep in mind that all of the samples being compared are assumed to have the same standard deviation σ).

12.4.4 Measuring the Total Variation

The total variation in all samples combined is measured by computing the sum of squared deviations between data values and the mean of all data points. This quantity is referred to as the **total sum of squares** or SS Total. The total sum of squares may also be referred to as SSTO. A formula for the sum of squared differences from the overall mean is

$$SSTotal = \sum_{\text{values}} (x_{ij} - \bar{x})^2$$

where x_{ij} represents the jth observation within the ith group, and \bar{x} is the mean of all observed data values. Finally, the relationship between SS Total, SS Groups, and SS Error is

$$SS\ Total = SS\ Groups + SS\ Error$$

Overall, the relationship between the total variation, the variation between groups, and the variation within a group is illustrated by Figure 2.

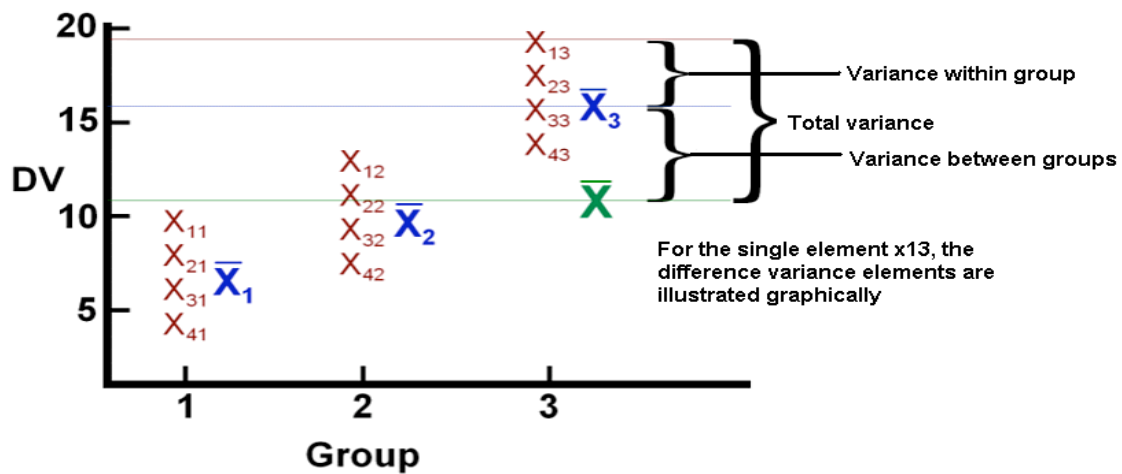


Figure 2: Visual illustration of variance in ANOVA, adapted from <http://www.uwsp.edu/psych/stat/12/anova-1w.htm>

A general table for performing the one-way ANOVA calculations required to compute the F-statistic is given below

Table 2 - One-Way ANOVA Table

Source	Degrees of Freedom	Sum of Squares	Mean Sum of Squares	F-Statistic
Between groups	k-1	$SS_{Groups} = \sum_{groups} n$	$\frac{SS_{Groups}}{k-1}$	$F = \frac{MSG_1}{MS}$
Within groups (error)	N-k	$SSE = \sum_{groups} (n_i - 1)$	$\frac{SSE}{N-k}$	
Total	N-1	$SSTO = \sum_{values} (x_{ij} -$		

12.4.5 Interpreting the F-statistic

Once the F-statistic has been found, it can be compared with a critical F value from a table, such as this one: [F Table](#). This F table is calculated for a value of alpha = 0.05, indicating a 95% confidence level. This means that if $F_{observed}$ is larger than $F_{critical}$ from the table, then we can reject the null hypothesis and say with 95% confidence that the variance between groups is not due to random chance, but rather due to the influence of a tested factor. Tables are also available for other values of alpha and can be used to find a more exact probability that the difference between groups is (or is not) caused by random chance.

12.4.6 Finding the Critical F value

In this [F Table](#), the first row of the F table is the number of degrees of between groups (number of groups - 1), and the first column is the number of degrees of freedom within groups (total number of samples - number of groups).

F_{α, n_1-1, n_2-1} F_{α, n_1-1, n_2-1}

Critical Values for F Distributions

$v_2 \backslash \alpha$		1	2	3	4	5	6	7	8	9	10	15	20
1	0.1	39.86	49.50	53.59	55.83	57.24	58.20	58.91	59.44	59.86	60.19	61.22	61.74
1	0.05	161.45	199.50	215.71	224.58	230.16	233.99	236.77	238.88	240.54	241.88	245.95	248.02
1	0.01	4052.2	4999.3	5403.5	5624.3	5764.0	5859.0	5928.3	5981.0	6022.4	6055.9	6157.0	6208.7
1	0.001	405311.6	499725.3	540256.5	562667.8	576496.1	586032.9	593185.4	597953.8	602245.3	605583.2	616073.6	620842.0
2	0.1	8.53	9.00	9.16	9.24	9.29	9.33	9.35	9.37	9.38	9.39	9.42	9.44
2	0.05	18.51	19.00	19.16	19.25	19.30	19.33	19.35	19.37	19.38	19.40	19.43	19.45
2	0.01	98.50	99.00	99.16	99.25	99.30	99.33	99.36	99.38	99.39	99.40	99.43	99.45
2	0.001	998.38	998.84	999.31	999.31	999.31	999.31	999.31	999.31	999.31	999.31	999.31	999.31
3	0.1	5.54	5.46	5.39	5.34	5.31	5.28	5.27	5.25	5.24	5.23	5.20	5.18
3	0.05	10.13	9.55	9.28	9.12	9.01	8.94	8.89	8.85	8.81	8.79	8.70	8.66
3	0.01	34.12	30.82	29.46	28.71	28.24	27.91	27.67	27.49	27.34	27.23	26.87	26.69
3	0.001	167.06	148.49	141.10	137.08	134.58	132.83	131.61	130.62	129.86	129.22	127.36	126.43
4	0.1	4.54	4.32	4.19	4.11	4.05	4.01	3.98	3.95	3.94	3.92	3.87	3.84
4	0.05	7.71	6.94	6.59	6.39	6.26	6.16	6.09	6.04	6.00	5.96	5.86	5.80
4	0.01	21.20	18.00	16.69	15.98	15.52	15.21	14.98	14.80	14.66	14.55	14.20	14.02
4	0.001	74.13	61.25	56.17	53.43	51.72	50.52	49.65	49.00	48.47	48.05	46.76	46.10

For the diet example in Table 1, the degree of freedom between groups is $(3-1) = 2$ and and the degree of freedom within groups is $(13-3) = 10$. Thus, the critical F value is 4.10.

12.4.7 Computing the 95% Confidence Interval for the Population Means

It is useful to know the confidence interval at which the means of the different groups are reported. The general formula for calculating a confidence interval is

sample mean \pm *Multiplier* * *Standard error* . Because it is assumed that all populations have the same standard deviation

$s_p = \sqrt{(MSE)}$ can be used to estimate the standard deviation within each group. Although the population standard deviation is assumed to be the same, the standard error and the multiplier may be different for each group, due to differences in group size and degrees of freedom. The standard error of a sample mean is inversely proportional to the square root of the number of data points within the sample. It is

$$SE(\bar{x}_i) = \frac{s_p}{\sqrt{(n_i)}}$$

calculated as . The multiplier is determined using a t-distribution where the degrees of freedom are calculated as $df = N - k$.

Therefore, *Insert formula here* the confidence interval for a population mean is

$$\bar{x}_i \pm t * \frac{s_p}{\sqrt{(n_i)}}$$

. More details on confidence intervals can be found in

[Comparison of two means](#)

An example for using factor analysis is the following:

You have two assembly lines. Suppose you sample 10 parts from the two assembly lines.

Ho: $s_1^2 = s_2^2$ Ha: variances are not equal Are the two lines producing similar outputs?

Assume $\alpha = 0.05$ $F_{0.025,9,9} = 4.03$ $F_{1-0.025,9,9} = ?$

Observation	Line1	Line2
1	0.61	-1.01
2	0.15	-0.36
3	-0.24	-0.34
4	-0.65	-0.54
5	-0.58	-0.13
6	-0.48	-0.78
7	-0.35	-0.90
8	-0.07	-0.22
9	-0.45	-0.72
10	-0.25	-0.88

n	10	10
Mean	-0.231	-0.588
StDev	0.380	0.312
Variance	0.144	0.097

Are variances different?

Test for Equal Variances

Bonferroni confidence intervals for standard deviations

Lower	Sigma	Upper	N	Factor Levels
0.248633	0.380101	0.765391	10	LINE 1
0.204071	0.311976	0.628211	10	LINE 2

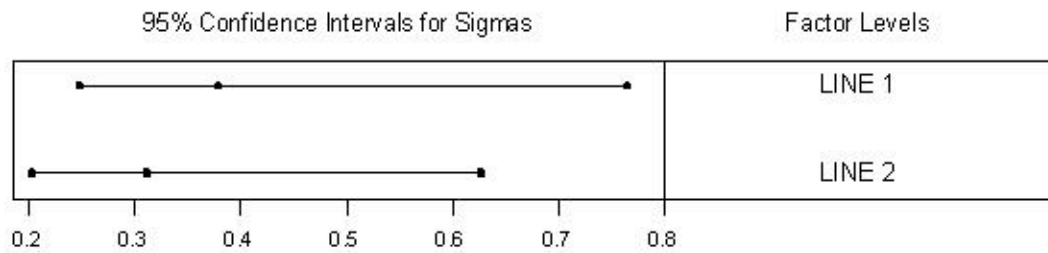
F-Test (normal distribution)

Test Statistic: 1.484

P-Value : 0.566

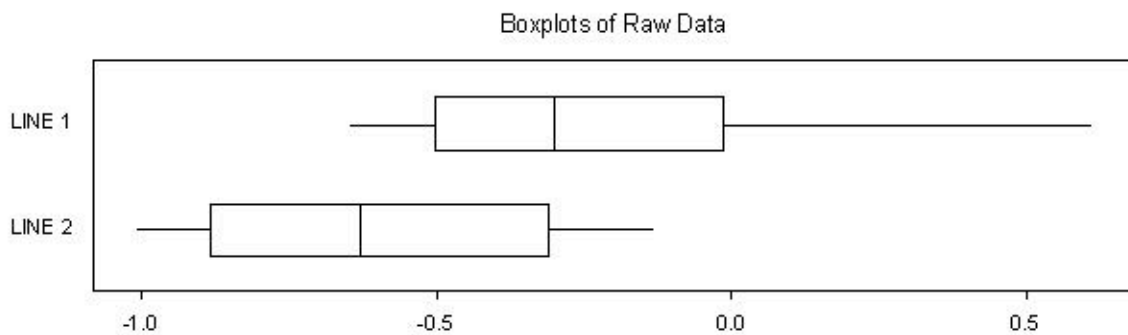
How would we test if the means are different?

Test for Equal Variances



F-Test
Test Statistic: 1.484
P-Value : 0.566

Levene's Test
Test Statistic: 0.000
P-Value : 0.992



12.5 Two-Factor Analysis of Variance

A two factor or two-way analysis of variance is used to examine how two qualitative categorical variables (male/female) affect the mean of a quantitative response variable. For example, a psychologist might want to study how the type and volume of background music affect worker productivity. Alternatively, an economist maybe be interested in determining the affect of gender and race on mean income. In both of these examples, there is interest in the effect of each separate explanatory factor, as well as the combined effect of both factors.

12.5.1 Assumptions

In order to use the two-way ANOVA, the following assumptions are required:

- Samples must be independent.
- Population variances must be equal.
- Groups must have same sample size. The populations from which the samples were obtained must be normally distributed (or at least approximately so).
- The null hypothesis is assumed to be true.

The null hypothesis is as follows:

- The population means for the first factor have to be equal. This is similar to the one-way ANOVA for the row factor.
- The population means for the second factor must also be equal. This is similar to the one-way ANOVA for the column factor.
- There isn't an interaction between the two factors. This is similar to performing an independence test using contingency tables.

More simply, the null hypothesis implies that the populations are all similar and any differences in the populations are caused by chance, not by the influence of a factor. After carrying out two-way ANOVA it will be possible to analyze the validity of this assumption.

12.5.2 Terms Used in Two-Way ANOVA

The **interaction** between two factors is the most unique part of a two-way analysis of variance problem. When two factors interact, the effect on the response variable depends on the value of the other factor. For example, the statement *being overweight caused greater increases in blood pressure for men than women* describes an interaction. In other words, the effect of weight (factor) on blood pressure (response) depends on gender (factor).

The term **main effect** is used to describe the overall effect of a single explanatory variable. In the music example, the main effect of the factor "music volume" is the effect

on productivity averaged over all types of music. Clearly, the main effect may not always be useful if the interaction is unknown.

In a two-way analysis of variance, three F-statistics are constructed. One is used to test the statistical significance of the interaction, while the other two are used to test the significance of the two separate main effects. The p-value for each F-statistic is also reported--a p-value of $<.05$ is usually used to indicate significance. When an F-factor is found to have statistical significance, it is considered a main effect. The p-value is also used as an indicator to determine if the two factors have a significant interaction when considered simultaneously. If one factor depends strongly on the other, the F-statistic for the interaction term will have a low p-value. An example output of two-way analysis of variance of restaurant tip data is given in Table 4.

Table 4 - Two-Way Analysis of Variance of Restaurant Tipping Data

Source	DF	Adj SS	Adj MS	F-Statistic	P-Value
Message	1	14.7	14.7	.13	.715
Sex	1	2602.0	2602.0	23.69	0.00
Interaction	1	438.7	438.7	3.99	.049
Error	85	9335.5	109.8		
Total	88	12407.9			

In this case, the factors being studied are sex (male or female) and message on the receipt (:-) or none). The p-values in the last column are the most important information contained in this table. A lower p-value indicates a higher level of significance. Message has a significance value of .715. This is much greater than .05, the 95% confidence interval, indicating that this factor has no significance (no strong correlation between presence of message and amount of tip). The reason this occurs is that there is a relationship between the message and the sex of the waiter. The interaction term, which was significant with a value of $p=0.049$, showed that drawing a happy face increased the tip for women but decreased it for men. The main effect of waiter sex (with a p-value of approximately 0) shows that there is a statistical difference in average tips for men and women.

12.5.3 Two-Way ANOVA Calculations

Like in one-way ANOVA analysis the main tool used is the square sums of each group. Two-way ANOVA can be split between two different types: with repetition and without repetition. With repetition means that every case is repeated a set number of times. For the above example that would mean that the :-) was given to females 10 times and males 10 times, and no message was given to females 10 times and males 10 times

Using the SS values as a start the F-statistics for two-way ANOVA with repetition are calculated using the chart below where a is the number of levels of main effect A, b is the number of levels of main effect B, and n is the number of repetitions.

Source	SS	DF	Adj MS	F-Statistic
Main Effect A	From data given	a-1	SS/df	MS(A)/MS(W)
Main Effect B	From data given	b-1	SS/df	MS(B)/MS(W)
Interaction Effect	From data given	(a-1)(b-1)	SS/df	MS(A*B)/MS(W)
Within	From data given	ab(n-1)	SS/df	
Total	sum of others	abn-1		

Without repetition means there is one reading for every case. For example is you were investigating whether or not difference in yield are more significant based on the day the readings were taken or the reactor that the readings were taken from you would have one reading for Reactor 1 on Monday, one reading for Reactor 2 on Monday etc... The results for two-way ANOVA without repetition is slightly different in that there is no interaction effect measured and the within row is replaced with a similar (but not equal) error row. The calculations needed are shown in the table below.

Source	SS	DF	MS	F-Statistic
Main Effect A	From data given	a-1	SS/df	MS(A)/MS(E)
Main Effect B	From data given	b-1	SS/df	MS(B)/MS(E)
Error	From data given	(a-1)(b-1)	SS/df	
Total	sum of others	ab-1		

These calculations are almost never done by hand. In this class you will usually use Excel or Mathematica to create these tables. Sections describing how to use these programs are found later in this chapter.

12.6 Other Methods of Comparison

Unfortunately, the conditions for using the ANOVA F-test do not hold in all situations. In this section, several other methods which do not rely on equal population standard deviations or normal distribution. It is important to realize that *no* method of factor analysis is appropriate if the data given is not representative of the group being studied.

12.6.1 Hypotheses About Medians

In general, it is best construct hypotheses about a population median, rather than the mean. Using the median accounts for the sample being skewed based on extreme outliers. Median hypotheses should also be used for dealing with ordinal variables (variables which are described only as being higher or lower than one other and do not have a precise value). When several populations are compared, the hypotheses are stated as -

H_0 : Population medians are equal

H_a : Population medians are not all equal

12.6.2 Kruskal-Wallis Test for Comparing Medians

The **Kruskal-Wallis Test** provides a method of comparing medians by comparing the relative rankings of data in the observed samples. This test is therefore referred to as a rank test or non-parametric test because the test does not make any assumptions about the distribution of data.

To conduct this test, the values in the total data set are first ranked from lowest to highest, with 1 being lowest and N being highest. The ranks of the values within each group are averaged, and the test statistic measures the variation among the average ranks for each group. A p-value can be determined by finding the probability that the variation among the set of rank averages for the groups would be as large or larger as it is if the null hypothesis is true. More information on the Kruskal-Wallis test can be found [\[here\]](#).

12.6.3 Mood's Median Test for Comparing Medians

Another nonparametric test used to compare population medians is **Mood's Median Test**. Also called the Sign Scores Test, this test involves multiple steps.

1. Calculate the median (M) using all data points from every group in the study
2. Create a contingency table as follows

	A	B	C	Total
Number of values greater than M				
Number of values less than or equal to M				

3. Calculate the expected value for each data set using the following formula:

$$expected = \frac{(rowtotal)(columntotal)}{grandtotal}$$

4. Calculate the chi-square value using the following formula

$$\chi = \frac{(actual - expected)^2}{expected}$$

A chi-square statistic for two-way tables is used to test the null hypothesis that the population medians are all the same. The test is equivalent to testing whether or not the two variables are related.

12.7 ANOVA and Factor Analysis in Process Control

ANOVA and factor analysis are typically used in process control for troubleshooting purposes. When a problem arises in a process control system, these techniques can be used to help solve it. A factor can be defined as a single variable or simple process that has an effect on the system. For example, a factor can be temperature of an inlet stream, flow rate of coolant, or the position of a specific valve. Each factor can be analyzed individually to determine the effect that changing the input has on the process control system as a whole. The input variable can have a large, small, or no effect on what is being analyzed. The amount that the input variable affects the system is called the “factor loading”, and is a numerical measure of how much a specific variable influences the system or the output variable. In general, the larger the factor loading is for a variable the more of an affect that it has on the output variable.

A simple equation for this would be:

$$Output = f_1 * input_1 + f_2 * input_2 + ... + f_n * input_n$$

Where f_n is the factor loading for the n^{th} input.

Factor analysis is used in this [case study](#) to determine the fouling in an alcohol plant reboiler. This article provides some additional insight as to how factor analysis is used in an industrial situation.

12.8 Using Mathematica to Conduct ANOVA

Mathematica can be used for one-way and two-way factor analyses. Before this can be done, the ANOVA package must be loaded into Mathematica using the following command:

```
Needs["ANOVA`"]
```

Once this command is executed, the 'ANOVA' command can be utilized.

12.8.1 One-Way Factor Analysis

The basic form of the 'ANOVA' command to perform a one-way factor analysis is as follows:

```
ANOVA[data]
```

An example set of data with five elements would look like:

```
ANOVA[[{1,2},{2,4},{2,5},{3,4},{3,1}]]
```

An output table that includes the degrees of freedom, sum of the squares, mean sum of the squares, F-statistic, and the P-value for the model, error, and total will be displayed when this line is executed. A list of cell means for each model will be displayed beneath the table.

12.8.2 Two-Way Factor Analysis

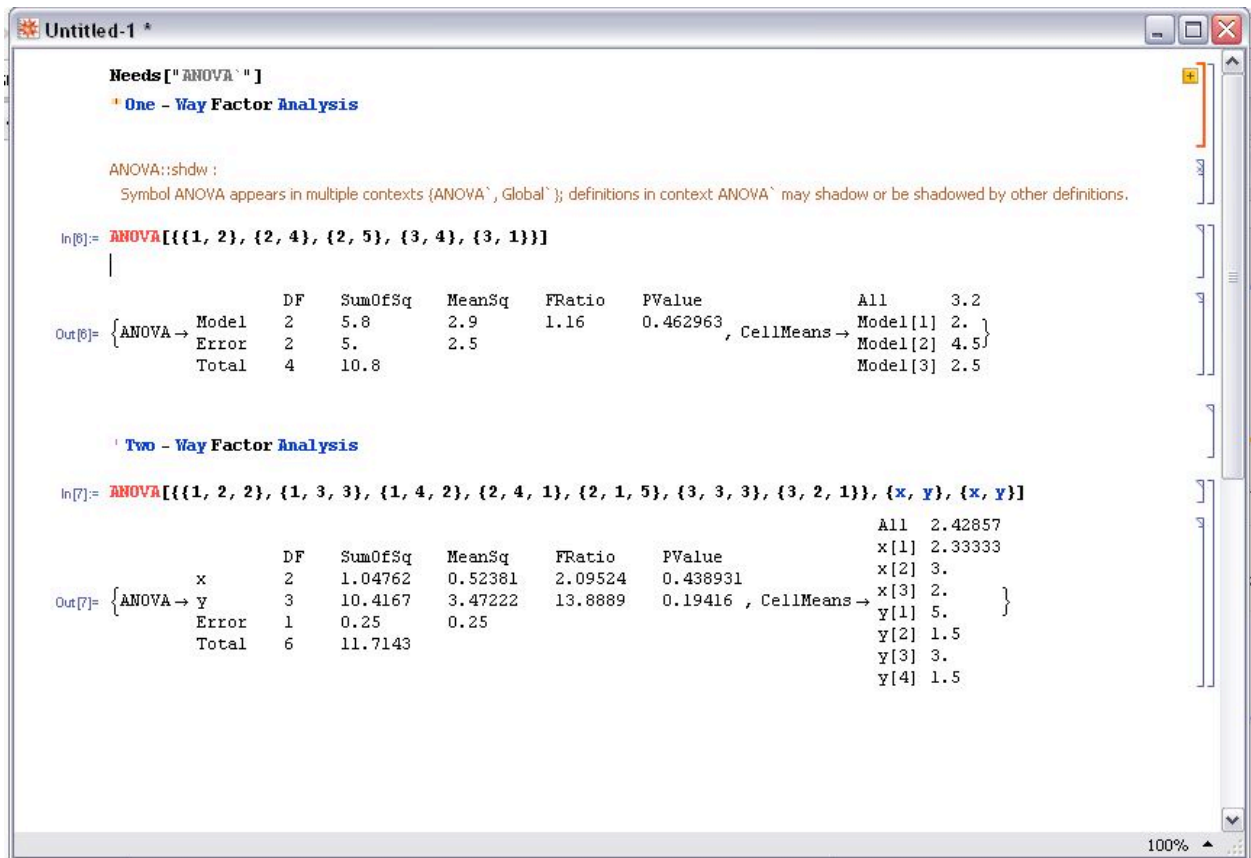
The basic form of the 'ANOVA' command to perform a two-way factor analysis is as follows:

```
ANOVA[data, model, vars]
```

An example set of data with seven elements would look like:

```
ANOVA[[{1,2,2},{1,3,3},{1,4,2},{2,4,1},{2,1,5},{3,3,3},{3,2,1}},{x,y},{x,y}]
```

An output table will appear similar to the one that is displayed in the one-way analysis except that there will be a row of statistics for each variable (i.e. x,y).



12.9 ANOVA in Microsoft Excel 2007

In order to access the ANOVA data analysis tool, install the package:

1. Click on the Microsoft Office button (big circle with office logo)
2. Click 'Excel Options'
3. Click 'Add-ins' on the left side
4. In the manage drop-down box at the bottom of the window, select 'Excel Add-ins'
5. Click 'Go...'
6. On the Add-Ins window, check the Analysis ToolPak box and click 'OK'

To use this package:

1. Click on the 'Data' tab and select 'Data Analysis'
2. Choose the desired ANOVA type- 'Anova: Single Factor', 'Anova: Two Factor with Replication', or 'Anova: Two Factor without Replication'(see note below for when to use replication)
3. Select the desired data points including data labels at top of the corresponding columns. Make sure the box is checked for 'Labels in first row' in the ANOVA parameter window.

4. Specify alpha in the ANOVA parameter window. Alpha represents the level of significance.
5. Output the results into a new worksheet.

NOTE: Anova: Two Factor with Replication is used in the cases where there are multiple readings for a single factor. For instance, the input below, there are 2 factors, control architecture and unit. This input shows how there are 3 readings corresponding to each control architecture (FB, MPC, and cascade). In this sense, the control architecture is replicated 3 times, each time providing different data relating to each unit. So, in this case, you would want to use the Anova Two Factor with Replication option.

control architecture				
	unit1	unit2	unit3	
FB	52.59	51.48	49.63	
FB	48.12	50.56	50.10	
FB	50.00	49.22	49.83	
MPC	49.67	50.61	50.67	
MPC	50.21	51.33	50.44	
MPC	49.84	51.81	51.41	
cascade	51.29	49.23	50.85	
cascade	50.91	48.47	49.95	
cascade	50.04	47.70	51.16	

Anova: Two Factor without Replication is used in cases where there is only one reading pertaining to a particular factor. For example, in the case below, each sample (row) is independent of the other samples since they are based on the day they were taken. Since multiple readings were not taken within the same day, the "without Replication" option should be chosen.

sample	Date	Reactor yield is kg of glycerin per run				
		Reactor 1	Reactor 2	Reactor 3	Reactor 4	Reactor 5
1	12/1/2007	107.173504	121.637341	94.427813	113.253739	100.40704
2	12/2/2007	111.720747	96.5692501	110.355107	126.534195	115.744327
3	12/3/2007	101.548829	108.285763	113.990532	102.178054	117.698256
4	12/4/2007	108.797073	113.160513	85.2385023	110.027039	96.109622
5	12/5/2007	96.3032079	111.141039	108.192291	118.733219	91.593933
6	12/6/2007	105.847343	91.3955177	88.5376488	102.178735	107.44279
7	12/7/2007	96.2074791	109.437155	120.697309	113.173557	109.97807
8	12/8/2007	111.926228	127.833877	100.12252	99.6354333	92.5296735
9	12/9/2007	97.6502824	97.7602335	108.549928	106.262861	84.4202995
10	12/10/2007	96.8221806	98.0003128	104.460937	115.837804	100.100045
11	12/11/2007	114.18772	87.6861313	109.119963	116.996506	103.318278

Excel outputs:

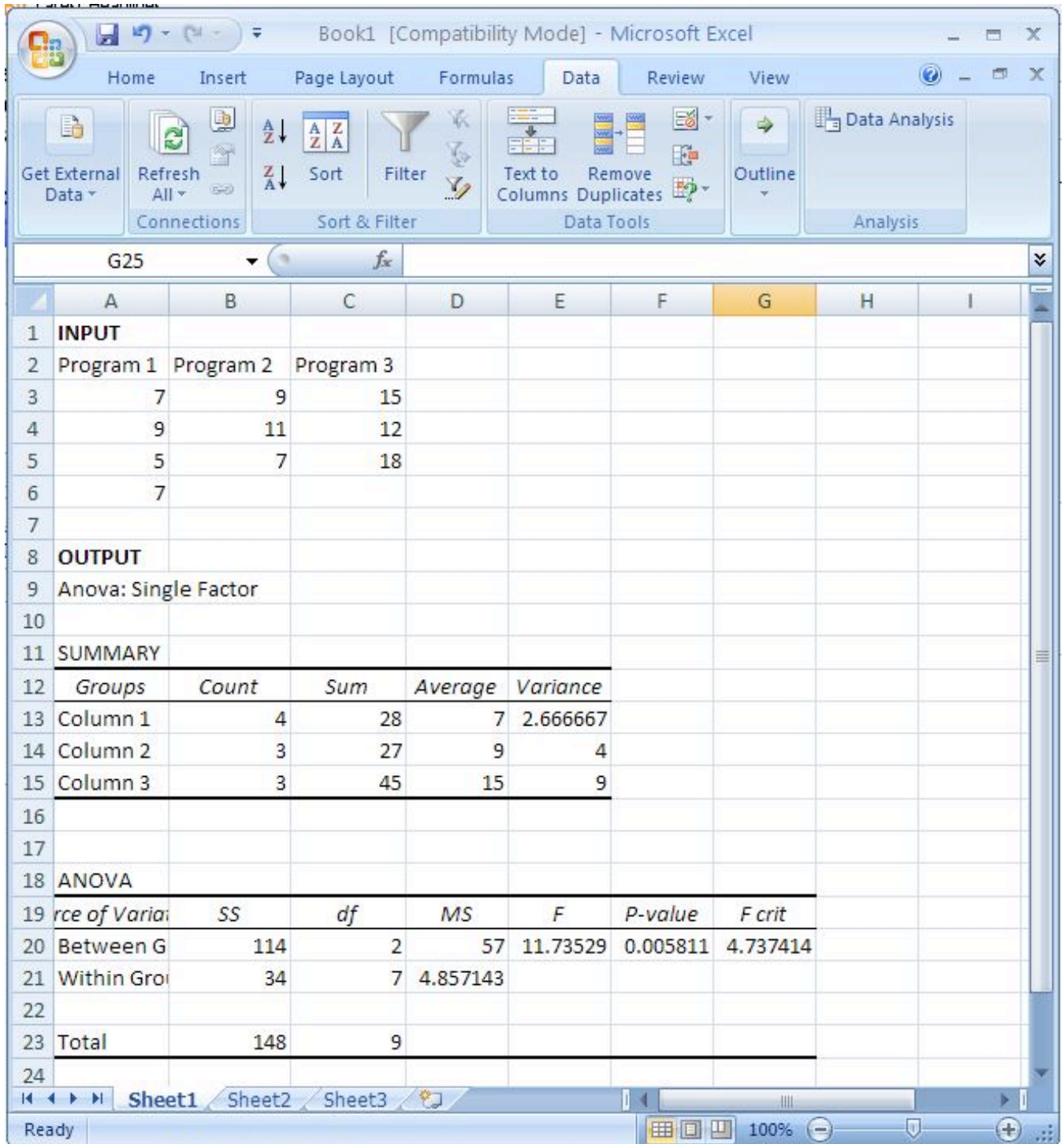
Summary:

1. Count- number of data points in a set
2. Sum- sum of the data points in a set
3. Average- mean of the data points in a set
4. Variance- standard deviation of the data points in a set

ANOVA:

1. Sum of squares (SS)
2. The degree of freedom (df)
3. The mean squares (MS)
4. F-statistic (F)
5. P-value
6. $F_{critical}$

See the figure below for an example of the inputs and outputs using Anova: Single Factor. Note the location of the Data Analysis tab. The data was obtained from the dieting programs described in Table 1. Since the F-statistic is greater than $F_{critical}$, the null hypothesis can be rejected at a 95% confidence level (since alpha was set at 0.05). Thus, weight loss was not random and in fact depends on diet type chosen.



12.10 Worked out Example 1

Determine the fouling rate of the reboiler at the following parameters:

$$T = 410K$$

$$C_c = 16.7g / L$$

$$R_T = 145min$$

Which process variable has the greatest effect (per unit) on the fouling rate of the reboiler?

Note that the tables below are made up data. The output data for a single input was gathered assuming that the other input variables provide a negligible output. Although the factors that affect the fouling of the reboiler are similar to the ones found in the article linked in the "ANOVA and Factor Analysis in Process Controls" section, the data is not.

Temperature of Reboiler (K)	400	450	500
Fouling Rate (mg/min)	0.8	0.86	0.95

Catalyst Concentration (g/L)	10	20	30
Fouling Rate (mg/min)	0.5	1.37	2.11

Residence Time (min)	60	120	180
Fouling Rate (mg/min)	0.95	2.3	3.81

Solution:

1) Determine the "factor loading" for each variable.

This can be done using any linearization tool. In this case, the factor loading is just the slope of the line for each set of data. Using Microsoft Excel, the equations for each set of data are the following:

Temperature of Reboiler

$$y = 0.0015 * x + 0.195$$

Factor loading: 0.0015

Catalyst Concentration

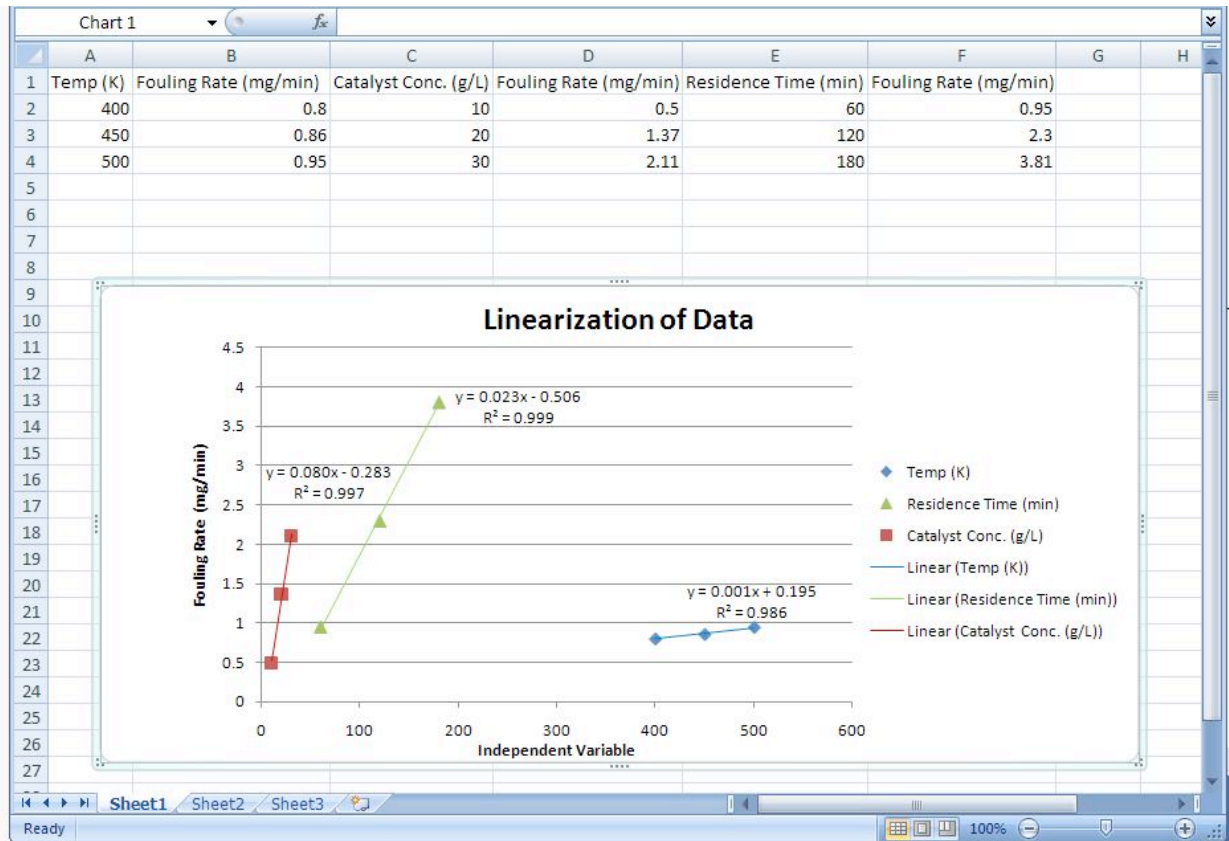
$$y = 0.0805 * x - 0.2833$$

Factor loading: 0.0805

Residence Time

$$y = 0.0238 * x - 0.5067$$

Factor loading: 0.0238



2) Determine the fouling rate for the given process conditions and which process variable affects the fouling rate the most (per unit). Note that the units of the factor loading value are **always** the units of the output divided by the units of the input.

Plug in the factor loading values into the following equation:

$$Output = f_1 * input_1 + f_2 * input_2 + \dots + f_n * input_n$$

You will end up with:

$$FoulingRate = 0.0015 * T + 0.0805 * C_c + 0.0238 * R_T$$

Now plug in the process variables:

$$FoulingRate = 0.0015 * 410 + 0.0805 * 16.7 + 0.0238 * 145$$

$$FoulingRate = 5.41 \text{ mg / min}$$

The process variable that affects the fouling rate the most (per unit) is the catalyst concentration because it has the largest factor loading value.

12.11 Worked out Example 2

Problem:

The exit flow rate leaving a tank is being tested for 3 cases. The first case is under the normal operating conditions, while the second (A) and the third (B) cases are for new conditions that are being tested. The flow value of 7 (gallons /hour) is desired with a maximum of 10. A total of 24 runs are tested with 8 runs for each case. The tests are run to determine whether any of the new conditions will result in a more accurate flow rate. First, we determine if the new conditions A and B affect the flow rate. The results are as follows:

	recorded reading							
Case 1	7	4	6	8	6	6	2	9
Case 2	5	5	3	4	4	7	2	2
Case 3	2	4	7	1	2	1	5	5
	x_1	x_1^2	x_2	x_2^2	x_3	x_3^2		
	7	49	5	25	2	4		
	4	16	5	25	4	16		
	6	36	3	9	7	49		
	8	64	4	16	1	1		
	6	36	4	16	2	4		
	6	36	7	49	1	1		
	2	4	2	4	5	25		
	9	81	2	4	5	25		
sum:	48	322	32	148	27	125		
sum ² :	2304		1024		729			
M	6		4		3.375			

$$SS\text{-total} = (322 + 148 + 125) - [(48 + 32 + 27)^2 / 24] = 117.96$$

$$SS\text{-among} = (2304/8 + 1024/8 + 729/8) - (48^2/24 + 32^2/8 + 27^2/8) = 30.08$$

$$SS\text{-within} = SS\text{-total} - SS\text{-among} = 87.88$$

Source	SS	df	MS	F
Among	30.08	2	15.04	3.59
Within	87.88	21	4.18	

The recorded values for the 3 cases are tabulated. Following this the values for each case are squared and the sums for all of these are taken. For the 3 cases, the sums are squared and then their means are found.

These values are used to help determine the table above (the equations give an idea as to how they are calculated). In the same way with the help of ANOVA, these values can be determined faster. This can be done using the mathematica explained above.

Conclusion:

$F_{critical}$ equals 3.4668, from an F-table. Since the calculated F value is greater than $F_{critical}$, we know that there is a statistically significant difference between 2 of the conditions. Thus, the null hypothesis can be rejected. However we do not know between which 2 conditions there is a difference. A post-hoc analysis will help us determine this. However we are able to confirm that there is a difference.

12.12 Worked out Example 3

As the new engineer on site, one of your assigned tasks is to install a new control architecture for three different units. You test three units in triplicate, each with 3 different control architectures: feedback (FB), model predictive control (MPC) and cascade control. In each case you measure the yield and organize the data as follows:

control architecture			
	unit1	unit2	unit3
FB	52.59	51.48	49.63
FB	48.12	50.56	50.10
FB	50.00	49.22	49.83
MPC	49.67	50.61	50.67
MPC	50.21	51.33	50.44
MPC	49.84	51.81	51.41
cascade	51.29	49.23	50.85
cascade	50.91	48.47	49.95
cascade	50.04	47.70	51.16

Do the units differ significantly? Do the control architectures differ significantly?

Answer: This problem can be solved using ANOVA Two factor with replication analysis.

	A	B	C	D	E	F	G
1	Anova: Two-Factor With Replication						
2							
3	SUMMARY	unit1	unit2	unit3	Total		
4	<i>FB</i>						
5	Count	3	3	3	9		
6	Sum	150.761011	148.937182	148.410265	448.562823		
7	Average	50.2536702	49.6457274	49.4700882	49.8403136		
8	Variance	0.29800293	1.67239644	0.20738831	0.5980637		
9							
10	<i>MPC</i>						
11	Count	3	3	3	9		
12	Sum	152.587461	151.579393	150.414035	459.408007		
13	Average	50.8624869	50.5264643	50.1380117	51.0453342		
14	Variance	1.15633649	0.39489561	1.22803466	1.04078844		
15							
16	<i>cascade</i>						
17	Count	3	3	3	9		
18	Sum	148.497691	149.009963	148.786968	451.806092		
19	Average	49.4992304	49.6699877	49.5956559	50.2006769		
20	Variance	0.39430412	1.9462112	0.28233969	1.42961206		
21							
22	<i>Total</i>						
23	Count	9	9	9			
24	Sum	451.846163	449.526538	447.611267			
25	Average	50.3945639	50.5272403	50.1274778			
26	Variance	2.21467697	1.68395885	0.74003268			
27							
28							
29	ANOVA						
30	<i>Source of Variation</i>	<i>SS</i>	<i>df</i>	<i>MS</i>	<i>F</i>	<i>p-value</i>	<i>F crit</i>
31	Sample	1089.68361	2	544.841807	27.0453226	3.7717E-06	3.55455715
32	Columns	0.9993799	2	0.49968995	0.02480404	0.97553434	3.55455715
33	Interaction	-1084.6194	4	-271.15486	-13.459816	#NUM!	2.92774417
34	Within	362.619174	18	20.1455097			
35							
36	Total	368.682737	26				

Units do not have a significant effect on the yield

Controllers do have a significant effect on the yield

12.13 Multiple Choice Question 1

ANOVA analysis works better for?

- A. Non-linear models
- B. Linear models
- C. Exponential models
- D. All of the above

12.14 Multiple Choice Question 2

Two-Way ANOVA analysis is used to compare?

- A. Any *two* sets of data
- B. Two One-Way ANOVA models to each other
- C. Two factors on their effect of the output
- D. B and C

12.15 Multiple Choice Answers

Question 1: B

Question 2: C

12.16 Sage's Corner

If you are a sage for this page, please link your narrated powerpoint presentation here.

For just the slides: <http://controls.engin.umich.edu/wiki/index.php/Image:Anchor2.ppt>

<http://video.google.com/googleplayer.swf?docId=-3237677123667838406>

<http://video.google.com/googleplayer.swf?docId=6201287739553253294>

For just the slides:

http://controls.engin.umich.edu/wiki/index.php/Image:ANOVA_Slides.ppt

<http://www.youtube.com/v/fA7xPxbM6NY>

For just the slides: <http://controls.engin.umich.edu/wiki/index.php/Image:Mn-anova-presentation.ppt>

<http://www.youtube.com/v/AEbYrMZEyac>

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Section 13. Correlation and mutual information

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Date Released: November 14, 2007

Date Revised: November 27, 2007 Stewards: Jeff Falta, Taylor Lebeis, Shawn Mayfield, Marc Stewart, Tom Welch

13.1 Introduction

The application of control networks to engineering processes requires an understanding of the relationships between system variables. One would expect, for example, to find a relationship between the steam flow rate to a heat exchanger and the outlet stream temperature. How, then, are engineers to quantify the degree of relation between a pair of variables? Often times, investigations into the correlation and mutual information of data sets can provide the answer. Correlation analysis provides a quantitative means of measuring the strength of a linear relationship between two vectors of data. Mutual information is essentially the measure of how much “knowledge” one can gain of a certain variable by knowing the value of another variable. By utilizing these techniques, engineers can increase the selectivity and accuracy of their control systems.

13.2 Correlation

13.2.1 Population Correlation Coefficient

The correlation coefficient is an important measure of the relationship between two random variables. Once calculated, it describes the validity of a linear fit. For two random variables, X and Y, the correlation coefficient, ρ_{xy} , is calculated as follows:

$$\rho_{xy} = \frac{\text{cov}(X, Y)}{\sigma_x \sigma_y}$$

That is, the covariance of the two variables divided by the product of their standard deviations. Covariance serves to measure how much the two random variables vary together. This will be a positive number if both variables consistently lie above the expected value and will be negative if one tends to lie above the anticipated value and the other tends to lie below. For a further description of covariance, as well as how to calculate this value, see [Covariance](#) on Wikipedia.

The correlation coefficient will take on values from 1 to -1. Values of 1 and -1 indicate perfect increasing and decreasing linear fits, respectively. As the population correlation coefficient approaches zero from either side, the strength of the linear fit diminishes.

Approximate ranges representing the relative strength of the correlation are shown below. See the [Correlation](#) article on wikipedia for more detailed information about the correlation theory establishing these ranges. The ranges also apply for negative values between 0 and -1.

Correlation

Small: 0.10 to 0.29

Medium: 0.30 to 0.49

Large: 0.50 to 1.00

13.2.2 Sample Correlation Coefficient

A modified form of the expression for the correlation coefficient describes the linearity of a data sample. For n measurements of variables X and Y , the sample correlation coefficient is calculated as follows:

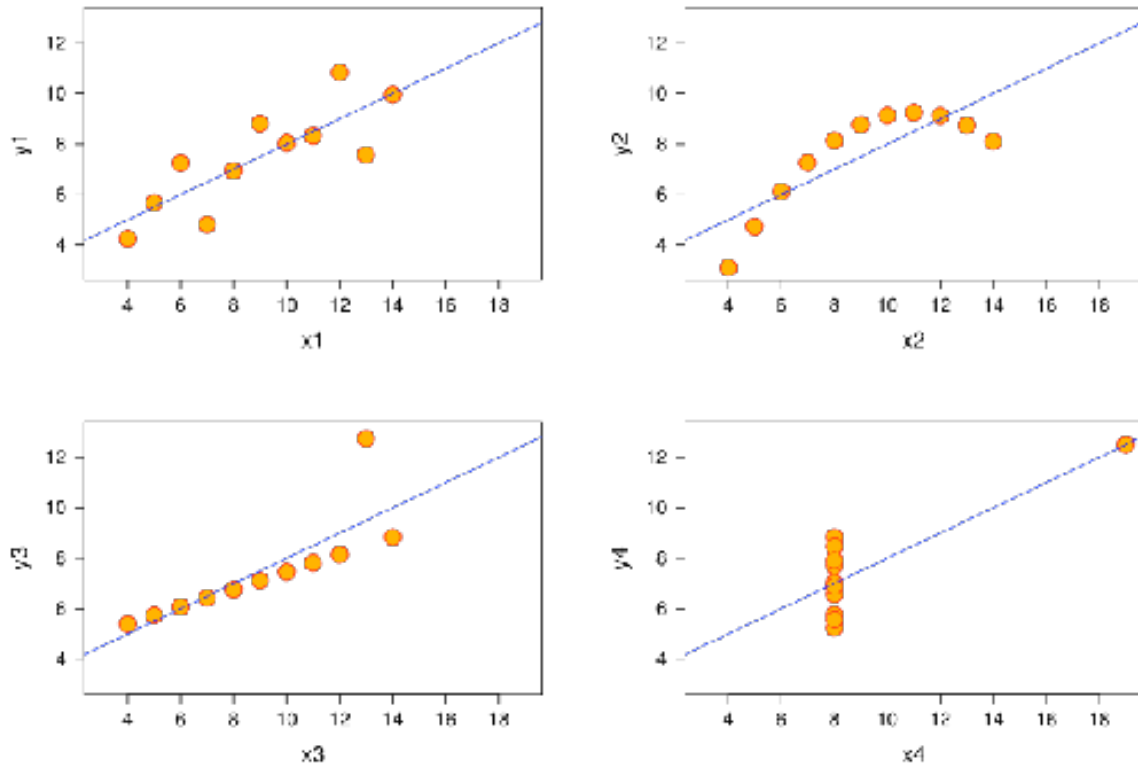
$$\rho_{xy} = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{(n - 1)s_x s_y}$$

where \bar{x} and \bar{y} are the sample averages, and s_x and s_y are the samples' standard deviations. This correlation coefficient will still take on values from 1 to -1, corresponding to the strength of linearity in the same way as the population correlation coefficient. This expression is often the more useful for process controls applications; an engineer can measure two variables, calculate their means and standard deviations, and ultimately determine the validity of a linear relationship between the two. This method is extremely useful when applied to a sample of experimental data that can be modeled by a normal distribution function. It is simpler and easier to use compared to the population correlation coefficient because it uses only well defined statistical inputs, mean and standard deviation, rather than the complex covariance function.

13.2.3 Correlation Coefficient Assumptions: Linearity, Normal Distribution

The correlation coefficient indicates the strength of a linear relationship between two variables with random distribution; this value alone may not be sufficient to evaluate a system where these assumptions are not valid.

The image below shows scatterplots of [Anscombe's quartet](#), a set of four different pairs of variables created by Francis Anscombe. The four y variables have the same mean (7.5), standard deviation (4.12), correlation coefficient (0.81) and regression line ($y = 3 + 0.5x$).



[Image from <http://en.wikipedia.org/wiki/Correlation> Correlation]

However, as can be seen on the plots, the distribution of the variables is very different.

The scatterplot of y_1 (top left) seems to exhibit random distribution. It corresponds to what one would expect when considering two variables linearly correlated and following normal distribution.

The scatterplot of y_2 (top right) does not exhibit random distribution; a plot of its residuals would not show random distribution. However, an obvious non-linear relationship between the two variables can be observed.

The scatterplot of y_3 (bottom left) seems to exhibit a near perfect linear relationship with the exception of one outlier. This outlier exerts enough influence to lower the correlation coefficient from 1 to 0.81. A [Q test](#) should be performed to determine if a data point should be retained or rejected.

The scatterplot of y_4 (bottom right) shows another example when one outlier is enough to produce a high correlation coefficient, even though the relationship between the two variables is not linear.

These examples indicate that the correlation coefficient alone should not be used to indicate the validity of a linear fit.

13.2.4 Engineering Applications

Measuring the correlation of system variables is important when selecting manipulated and measured control pairs. Say, for instance, that an engineer takes several measurements of the temperature and pressure within a reactor and notes that the data pairs have a correlation coefficient of approximately one. The engineer now understands that by applying a control system to maintain the temperature, he will also be controlling the reactor pressure by way of the linear relationship between the two variables.

Here we begin to see the role correlations play in defining MIMO versus SISO systems. Generally, engineers seek control systems with independent pairs of manipulated (u) and measured variables (x). If two inputs strongly influence a single output as measured by the correlation value, then the system will be difficult to decouple into a SISO controller. Correlation values closer to 0 for all but one manipulated variable means the system will be easier to decouple because here a single system input controls a single system output and there is limited effect on other process variables.

13.2.5 Correlation in Mathematica

Correlation coefficients can be quickly calculated with the aid of Mathematica. To illustrate by example, suppose that an engineer measures a series of temperatures inside a bacterial chemostat and the corresponding protein concentration in the product. She measures temperatures of 298, 309, 320, 333, and 345 K corresponding to protein concentrations of 0.4, 0.6, 0.7, 0.85, and 0.9 weight percent protein (these values are for illustrative purposes and do not reflect the performance of an actual chemostat). The engineer enters these measurements into Mathematica as a pair of vectors as follows:

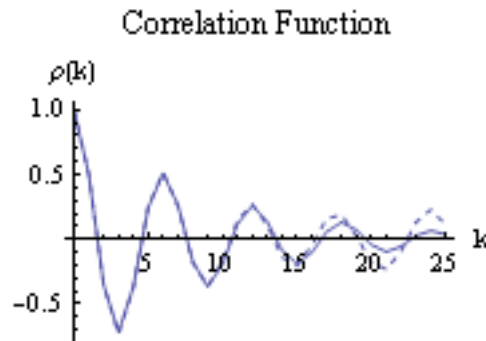
```
In[11]:= T = {{298}, {309}, {320}, {333}, {345}}
          W = {{0.4}, {0.6}, {0.7}, {0.85}, {0.9}}
```

where T is a vector containing the temperature measurements and C is a vector containing the concentration measurements. To determine the correlation coefficient, simply use the syntax below.

```
Correlation[T, W]
Out[13]= {0.978202}
```

In this case, the correlation coefficient of nearly 1 indicates a strong degree of linearity between the chemostat temperature and the protein concentration, informing the engineer that she can essentially control this concentration through temperature control. The sample correlation function in Mathematica uses an approximate solution with the mean and standard deviation of the data set, but the value is very close to the true correlation function value. This can be seen in the figure below as the dashed line represents the

sample correlation function, which deviates slightly from the true correlation function. As the sample becomes larger (i.e. higher n) the approximation gets closer to the true value. This represents a limitation of the sample correlation function and demonstrates how Mathematica can be used to determine multiple correlations between sets of data.



13.3 Mutual Information

Mutual information (also referred to as transinformation) is a quantitative measurement of how much one random variable (Y) tells us about another random variable (X). In this case, information is thought of as a reduction in the uncertainty of a variable. Thus, the more mutual information between X and Y, the less uncertainty there is in X knowing Y or Y knowing X. For our purposes, within any given process, several parameters must be selected in order to properly run the process. The relationship between variables is integral to correctly determine working values for the system. For example, adjusting the temperature in a reactor often causes the pressure to change as well. Mutual information is most commonly measured in logarithms of base 2 (bits) but is also found in base e (nats) and base 10 (bans).

13.3.1 Explanation of Mutual Information

The mathematical representation for mutual information of the random variables A and B are as follows:

$$I(A; B) = \sum_{b \in B} \sum_{a \in A} p(a, b) * \log \left(\frac{p(a, b)}{p(a)p(b)} \right)$$

where,

- $p(a, b)$ = joint probability distribution function of A and B.
- $p(a)$ = marginal probability distribution function of A.
- $p(b)$ = marginal probability distribution function of B.

For a review and discussion of probability distribution functions, please refer to [Probability Distribution \(Wikipedia\)](#).

When referring to continuous situations, a double integral replaces the double summation utilized above.

$$I(A; B, c) = \int_B \int_A p(a, b) * \log \left(\frac{p(a, b)}{p(a)p(b)} \right) da db$$

where,

- $p(a,b)$ = joint probability density function of A and B.
- $p(a)$ = marginal probability density function of A.
- $p(b)$ = marginal probability density function of B.

For a review and discussion of probability density functions, please refer to [Probability Density Function \(Wikipedia\)](#).

By performing the functions above, one measures the distance between the joint distribution/density functions of A and B. Since mutual information is always measuring a distance, the value obtained from this calculation will always be nonnegative and symmetric. Therefore,

$$I(A; B) \geq 0$$
$$I(A; B) = I(B; A)$$

In both cases, the information shared between both A and B is being measured. If A and B are independent of each other, then the difference between the two would be zero. In terms of chemical engineering processes, two independent variables would share no mutual information which means that one variable provides no information about the other variable. If A and B were identical, then all the information derived from obtaining variable A would supply the knowledge needed to get variable B.

By knowing the mutual information between two variables A and B, modeling of a multivariable system can be accomplished. If two or more variables provide the same information or have similar effects on one outcome, then this can be taken into

consideration while constructing a model. For example, if the level of a tank was observed to be too high, pressure and temperature could be plausible variables. If manipulating both of these variables causes a change in the fluid level in the tank, then there exists some mutual information between the pressure and temperature. It would then be important to establish the relationship between temperature and pressure to appropriately control the level of fluid in the tank.

13.3.2 Visual Representation of Mutual Information

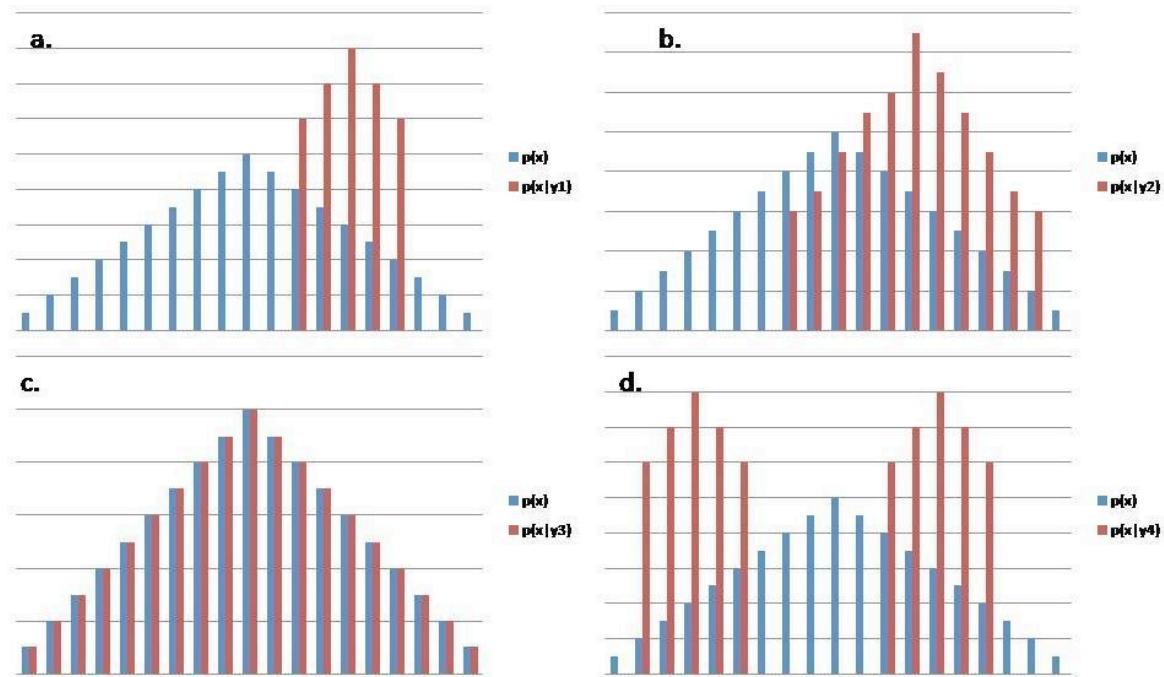


Figure 1. This figure demonstrates how y provides information for x . The blue is $p(x)$ and the red is $p(x|y)$ for a specific y .

A. y shares mutual information with x such that given a y_1 the values of x are now narrowed down to the five values.

B. y shares mutual information with x but it shares less information than A and therefore is not as helpful as A, as it does not eliminate as many potential x values.

C. y does not share any mutual information. Given the y_3 value, no x values are eliminated as potential values. Since y_3 does not provide any information there is no information between the two variables.

D. y shares mutual information with x . Because of the bimodal distribution, one more piece of information is required to describe which distribution lies within. Therefore, D gives as much information as part B. B gives 11 potential values while D gives 10 potential values. However, one additional bit of information is required to describe which of the two curves the x values lie on, thus there are 11 needed inputs.

13.3.3 Relating Mutual Information to Other Quantities/Concepts

Mutual information can be related to other concepts to gain a comprehensive understanding of the information obtained from any given parameter. Mutual information discussions are most commonly coupled with a discussion on Shannon entropy (See [Shannon Entropy](#) for more information on entropy).

Relative Entropy

In terms of probability theory, the relative entropy of a system measures the distance between two distinct probability functions. In chemical engineering applications, mutual information can be used to determine the entropy inherent in a system. Mutual information in this aspect can now be defined simply as:

$$I(A; B) = H(A) - H(A|B) = H(B) - H(B|A) = I(B; A) = H(A) + H(B) - H(A, B)$$

where,

- $H(A)$ = marginal entropy of A.
- $H(B)$ = marginal entropy of B.
- $H(A | B)$ = conditional entropy of A.
- $H(B | A)$ = conditional entropy of B.
- $H(A, B)$ = joint entropy of A and B.

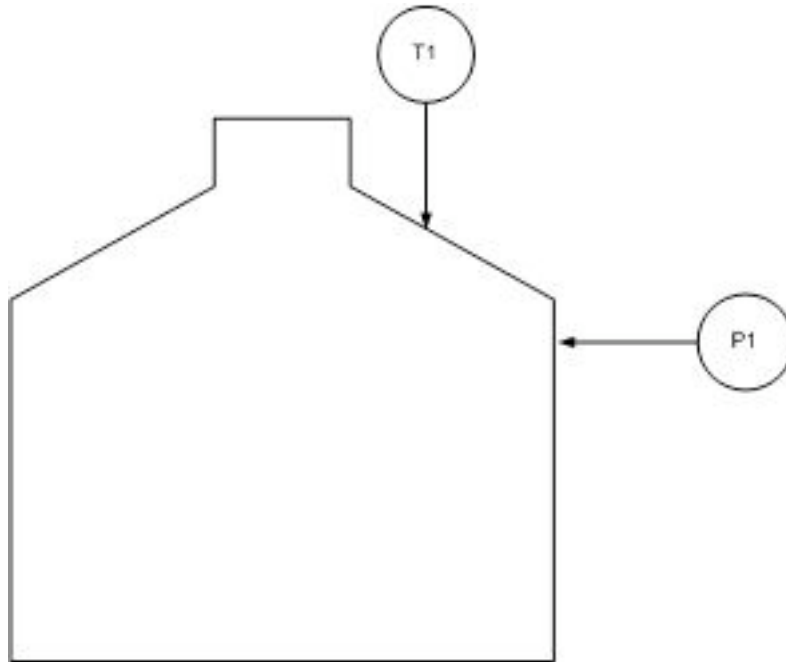
As described above, the marginal entropy still represents the uncertainty around a given variable A and B. Conditional entropy describes the uncertainty in the specified variable that remains after the other variable is known. In terms of mutual information, the conditional entropies of A and B tell us that a certain number of bits needs to be transferred from A in order to determine B and vice versa. Once again, these bits of information are determined by the logarithmic base chosen for analysis. One can determine the uncertainty in several different process parameters with respect to any other process variable.

Mutual Information and Boolean Models

Recall that via [Boolean Models](#), a complex series of sensors and valves can be modeled into a simple control system. A Boolean variable, however, will never return a value because it can only return True or False. This knowledge can be combined to determine a relationship between two different variables (from Boolean model) and then their dependency can be quantified (mutual information). Utilizing the same logic that goes into constructing truth tables, data can be input into tables to determine the mutual information value.

13.4 Correlation Example

Suppose an engineer wants to test the applicability of the ideal gas law to a closed tank containing a fixed amount of his company's gaseous product. Given that the vessel is of constant volume, and given that no change in moles will occur in this fixed system, one would hypothesize that the ideal gas law would predict a linear relationship between the temperature and pressure within the tank.



The engineer makes the following measurements and notes his findings in Excel.

T (K)	P (atm)
298	1.2
301	1.3
302	1.5
310	1.7
312	1.8
323	2
337	2.1
341	2.3
349	2.8

Before proceeding with his analysis, the engineer decides to calculate the correlation coefficient for these values in Mathematica.

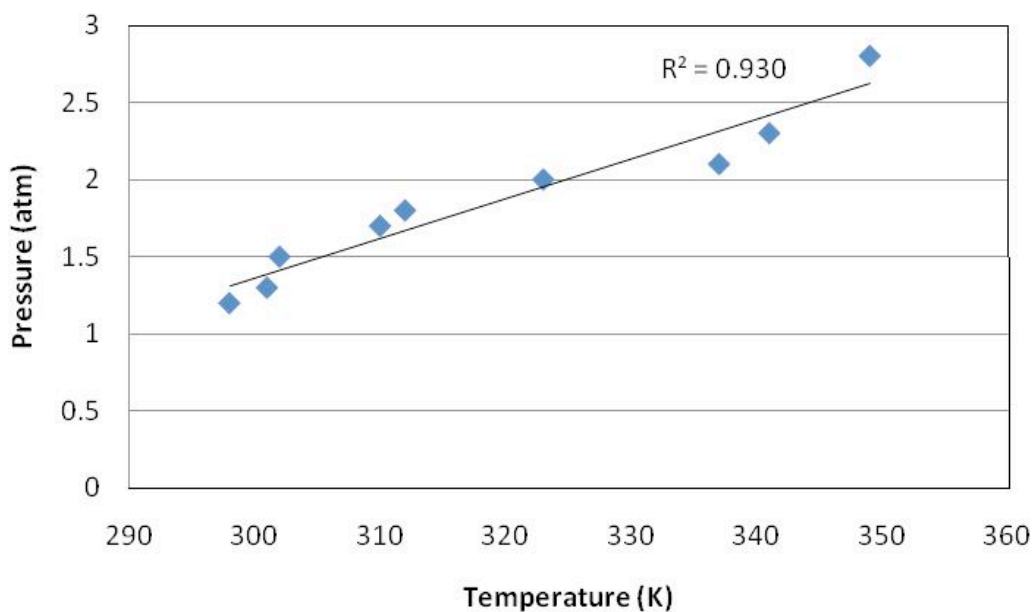
```
In[14]:= T = {{298}, {301}, {302}, {310}, {312}, {323}, {337}, {341}, {349}}
          P = {{1.2}, {1.3}, {1.5}, {1.7}, {1.8}, {2.0}, {2.1}, {2.3}, {2.8}}
          Correlation[T, P]
```

```
Out[14]= {{298}, {301}, {302}, {310}, {312}, {323}, {337}, {341}, {349}}
```

```
Out[15]= {{1.2}, {1.3}, {1.5}, {1.7}, {1.8}, {2.0}, {2.1}, {2.3}, {2.8}}
```

```
Out[16]= {{0.964549}}
```

Noting the correlation coefficient's approximate value of 1, the engineer proceeds by creating a linear fit of the data in Excel.



Indeed, the data are nearly linear.

13.5 Summary

If an engineer were trying to determine if two random variables are linearly related, calculating correlation coefficients would be the first step to determine this. If the mean and standard deviation for both variables are known values (i.e. calculated from

thousands of measurements), then the population correlation coefficient should be used. To determine the correlation coefficient for a smaller set of data, the sample correlation coefficient equations should be used. If the two variables were shown to have a high degree of correlation, the next step would be to plot the data and graphically check the linear relationship of this data. A high correlation coefficient does not necessarily mean the two variables are linearly related as shown by Anscombe's quartet, so this graphical check is necessary.

Mutual information helps reduce the range of the probability density function (reduction in the uncertainty) for a random variable X if the variable Y is known. The value of $I(X;Y)$ is relative, and the larger its value, the more information that is known of X . It is generally beneficial to try to maximize the value of $I(X;Y)$, thus minimizing uncertainty. The concept of mutual information is quite complex and is the basis of information theory.

13.6 Sage's Corner

The bigger your shoe size...

<http://video.google.com/googleplayer.swf?docId=6786850156215418037>
<http://video.google.com/googleplayer.swf?docId=-1774639730424023225>

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- Wikipedia [Correlation](#).
- Wikipedia [Mutual Information](#).
- Scholarpedia [Mutual Information](#).
- Kojadinovic, Ivan (no date) "On the use of mutual information in data analysis: an overview"

Section 14. Random sampling from a stationary Gaussian process

Title: Random Sampling From a Stationary Gaussian Process

Authors: Halley Crast, Andrew Laskowski, Maurice Telesford, Emily Yatch

Stewards: Matthew Kerry Braxton-Andrew, Josh Katzenstein, Soo Kim, Karen Staubach

Date Presented: November 30, 2006

Dates Revised: December 10, 2006; November 20, 2007

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

14.1 Introduction

Gaussian distributions are powerful tools for data analysis of randomly generated samples. Gaussian distributions are typically associated with a “Bell curve”, a graphical representation of a probability density function that is characterized by a peak at the data mean and a width determined by the standard deviation of the data set. The distribution of the curve around the mean is symmetric, with certain percentages of the data falling within one standard deviation of the mean. The probability that a data point exists within a certain range of values is equal to the area under the probability density curve between those two values. The total area under the curve is equal to one because all data points can be found to exist somewhere in that data set. For more detailed information on Gaussian distributions, consult the wiki article: [Continuous Distributions](#).

The random number sampler is a powerful tool and is very useful in process modeling. One example of a use for a random number samplers is to generate weather data from a model to simulate changing climate throughout the year, in order to properly maintain the temperature of a storage vessel. Another way it can be used is to create a control chart to monitor how well a process is controlled over time based on some information about normal system operation. The goal of random number generation is to be able to use large amounts of data based on limited experimentation to test a control scheme.

The objective of this article is to explain how random sampling to form a Gaussian data set is useful in process control. First is discussion of how to use a Gaussian distribution to analyze probability and compare the statistical similarities/differences between different data sets. Then is an explanation of how to use the Central Limit Theorem and show how to create a Gaussian distribution from non-Gaussian data using average values. Last are examples of how to use this theory in process controls, including how to generate and use control charts.

14.2 Random Number Sampler

The purpose of the random number sampler is to take randomly generated points and turn them into a Gaussian distribution (i.e. a PDF). It is important to use points distributed throughout the range of 0 to 1. This task is accomplished by assuming a random number (R) is equal to the 'y' value of the cumulative distribution function (CDF). The CDF is the cumulative area under the curve of the probability density function (PDF). By taking an integral from $-\infty$ to x in the PDF, this 'y' value of the CDF can be found. Since the value of R is already known, we can find the x values of the CDF and thus, the PDF. With the x values of the PDF known, we can find $P(x)$ and construct the Gaussian distribution. The relationship between R and x is shown below:

$$R = \int_{-\infty}^x \frac{1}{\sqrt{2\pi(\sigma)^2}} e^{-\frac{(X-\mu)^2}{2(\sigma)^2}} dX$$
$$R = \frac{1}{2} \left[\text{Erf} \left(\frac{x - \mu}{\sigma\sqrt{2}} \right) - \text{Erf} \left(\frac{-\infty - \mu}{\sigma\sqrt{2}} \right) \right]$$
$$R = \frac{1}{2} \left[\text{Erf} \left(\frac{x - \mu}{\sigma\sqrt{2}} \right) + 1 \right]$$
$$x = \sigma\sqrt{2} * \text{InverseErf}(2R - 1) + \mu$$

The process of choosing a random number and implementing it into the PDF can be done using Mathematica. Excel is not recommended because it cannot compute the Erf() of a negative number, so we cannot use it for data points below the mean in a CDF.

The first step for random sampling a stationary Gaussian process is to input the mean (μ) and the standard deviation (σ) into the equation below. Then, you can determine the random points either with Random[] function in Mathematica or via user input to develop a list of random numbers between 0 and 1. Using a random number input as R, Mathematica can be used to determine the corresponding data point x using the syntax below:

$$\text{Solve}[R == (1/2)*(Erf[(x - \mu)/(\sigma*\text{Sqrt}[2])]+1), x]$$

The syntax can be repeated to determine as many random numbers and their corresponding x values as is necessary for your problem. A CDF plot can be created by plotting all of the random R values versus their corresponding x values.

We will demonstrate how the procedure works in the following example. First, we chose 10 random numbers and found corresponding x values, given in Table 1 with $\mu = 10$ and $\sigma = 5$. See Figure 1 for the plot of the CDF.

Table 1: CDF Random Numbers and Corresponding x Values

Random Number, R	x
0	$-\infty$
0.1	3.59224
0.2	5.79189
0.3	7.378
0.4	8.73326
0.5	10
0.6	11.2667
0.7	12.622
0.8	14.2081
0.9	16.4078
1	∞

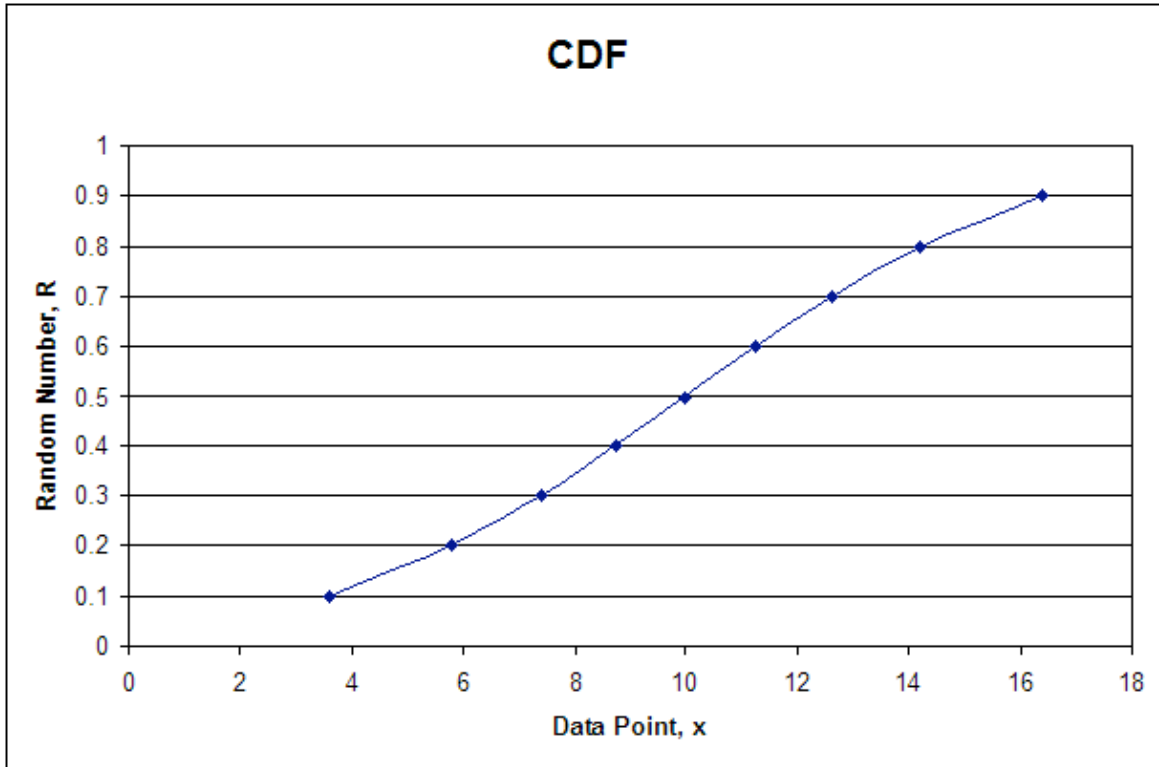


Figure 1: Continuous Distribution Function

In order to develop the PDF you would input the mean and standard deviation into the following PDF equation, and find $P(x)$ for each value of x .

$$P(\mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(X-\mu)^2}{2\sigma^2}}$$

The syntax used in Mathematica is:

$$\text{Solve}[P(x) == (1/\text{Sqrt}[2*\text{Pi}*\sigma^2])*e^{-(x-\mu)^2/(2*\sigma^2)}, P(x)]$$

The syntax outputs values for $P(x)$ which are then plotted against the x values calculated from the CDF. The following table shows the random numbers generated in

Mathematica, the corresponding x values, and the $P(x)$ values for the PDF. The plot of the PDF is also shown below.

Table 2: For Each R , x Values and Corresponding $P(x)$ Values

Random Number, R	x	$P(x)$
0	$-\infty$	0
0.1	3.59224	0.0351
0.2	5.79189	0.055992
0.3	7.378	0.069539
0.4	8.73326	0.077268
0.5	10	0.079788
0.6	11.2667	0.077269
0.7	12.622	0.069539
0.8	14.2081	0.055992
0.9	16.4078	0.035099
1	∞	0

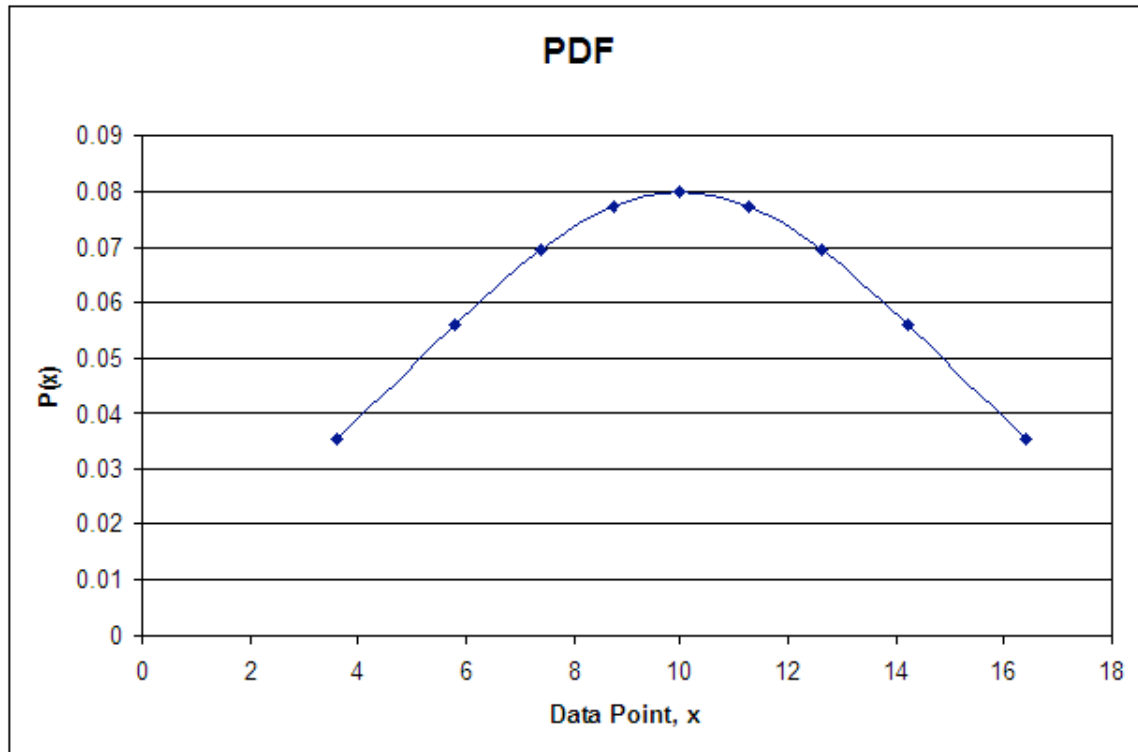


Figure 2: Probability Density Function

As you can see the plot is in fact Gaussian. The distribution will become more Gaussian as more random numbers are used. The take home message from the random number generator is that a data set with numbers ranging between 0 and 1, obtained through random number generation, can be converted into a Gaussian distribution.

14.3 Probability Primers

One major advantage of the random number sampler is the ability to generate different data sets without having to actually gather data. These data sets can be used to help you better understand the workings of many of the different statistical comparisons. For instance, if the sample size increases, does that lead to more or less significance in the difference of two means? Most of these analysis tools are the topics of other wikis, so we will revisit a few only briefly with the intent on asking more in-depth questions in example 1.

14.3.1 Probability

Recall that the area under any Gaussian function is related to the probability. Suppose we use our sampler to generate a random set of 100 data points with a mean of 10 and a

standard deviation of 5. The probability of creating an additional data point between ‘a’ and ‘b’ is the integral of the Gaussian distribution function from ‘a’ to ‘b’ as follows:

$$P(a \leq x \leq b) = \int_a^b \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx$$

Further information on probabilities can be found in this wiki article: [Continuous Distributions](#)

14.3.2 Error in the Mean

Assume we have the same data set as described above. Let’s say we wish to add a new data point and compute the probability that the new mean of the data set lies between ‘c’ and ‘d.’ This calculation is very similar to that described above with one difference. The standard deviation, which describes the variance in individual data points, is replaced with the standard error in the mean, which describes the variance in the mean as data sample size changes. The standard error in the mean is calculated as follows:

$$\sigma_{\mu} = \frac{\sigma}{\sqrt{n}}$$

Once this value is obtained, we can solve for the probability as follows:

$$P(a \leq \mu \leq b) = \int_c^d \frac{1}{\sqrt{2\pi\sigma_{\mu}^2}} e^{-\frac{(x-\mu)^2}{2\sigma_{\mu}^2}} dx$$

Further information on standard error can be found in this wiki article: [Comparison of Two Means](#)

14.3.3 Comparison of Two Data Sets

Now suppose we have two distinct data sets with different means and standard deviations and we wish to determine if one data set is statistically different from the second. To do this, we will compute a p-value. The p-value is computed as follows:

$$P(\mu_1 \rightarrow \mu_2, \mu_1 < \mu_2) = \int_{\mu_2}^{\infty} \frac{1}{\sqrt{2\pi\sigma_{\mu 1}^2}} e^{-\frac{(x-\mu_1)^2}{2\sigma_{\mu 1}^2}} dx$$
$$P(\mu_1 \rightarrow \mu_2, \mu_1 > \mu_2) = \int_{-\infty}^{\mu_2} \frac{1}{\sqrt{2\pi\sigma_{\mu 1}^2}} e^{-\frac{(x-\mu_1)^2}{2\sigma_{\mu 1}^2}} dx$$

Further information on p-values and mean comparisons can be found in these wiki articles: [Comparison of Two Means](#) and [P-Values](#)

14.4 Central Limit Theorem

Recall that one property of the random number sampler was that as the set of randomly generated numbers increased, errors became more random and the distribution became more Gaussian. The central limit theorem states that the sampling of a given distribution mean will approach a normal or Gaussian distribution as the sample size increases. This theorem is proven by the following example illustrated in the “Statistics for Experimenters: An Introduction to Design, Data Analysis, and Model Building.”

14.4.1 Rolling of Dice

The probability that a certain face will land upright when rolling a six-sided die is the same for each face. This is shown below in Figure 3 (a). The mean value of a roll can be calculated to be 3.5 by summing up the value of each face and dividing by 6. As the sample size is increased, this mean value will be shown to have the highest density of occurrence. When the sample size is increased to two dice you can notice in Figure 3 (b) that the density distribution of the average score begins to take the shape of a curve. The density distribution of the average score for sample size increases to three, five, and ten dice are shown in Figure 3 (c, d, and e respectively). For each increase it can be noted

that the density of the extreme values decreases and the overall density distribution appears more like a Gaussian distribution, as predicted by the central limit theorem.

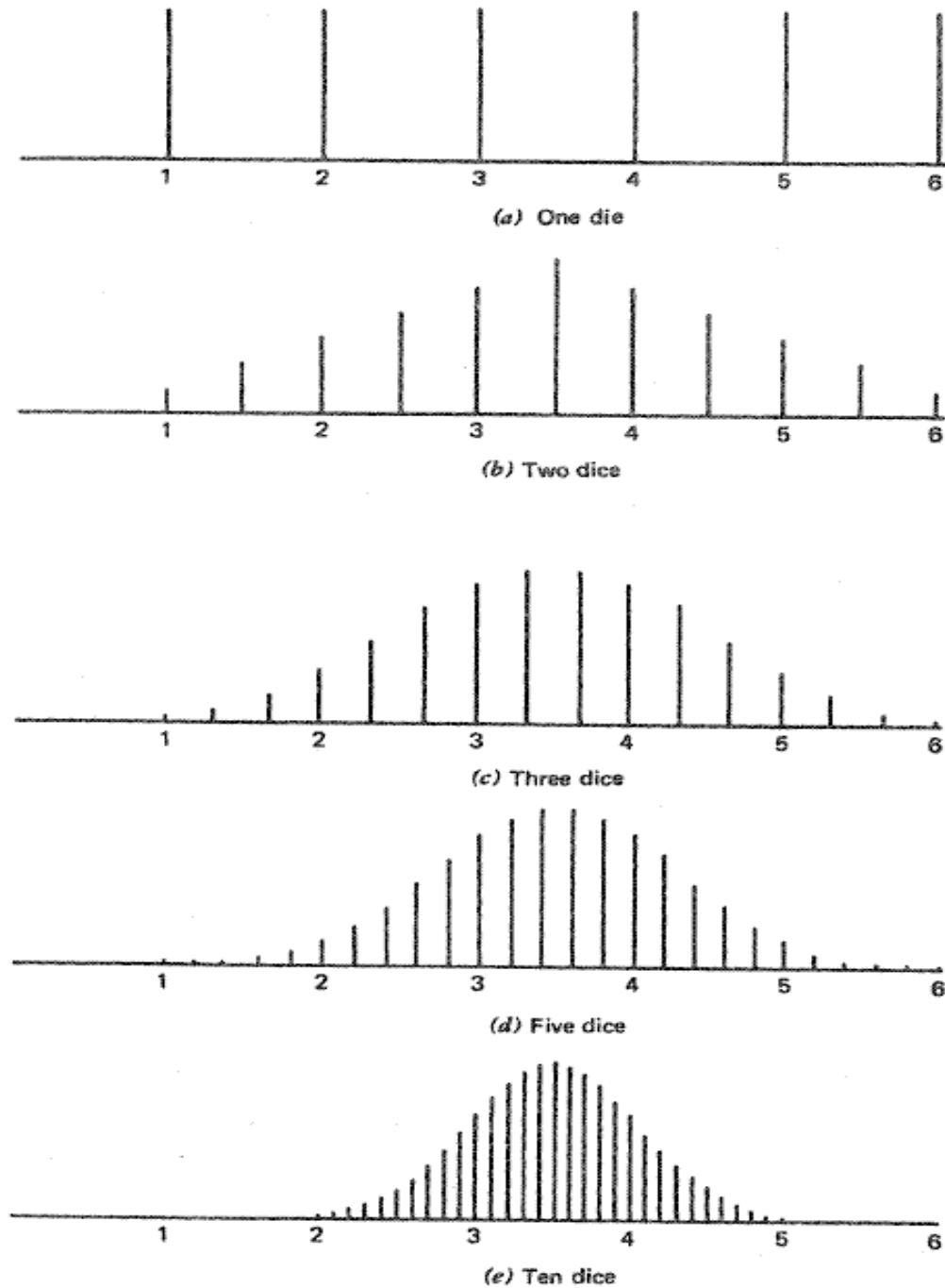


Figure 3: Distribution from Increasing Sample Size (Box, "Statistics for Experimenters")

14.4.2 Random Number Generation

The above dice example is analogous to random number generation. Consider a set of random numbers between 0 and 10. If these numbers were truly chosen randomly, then you would expect an even distribution of numbers between 0 and 10. The average of these numbers would be about 5, with a large standard deviation. However, let's suppose your data set now consists of an average of two random numbers. In this case, the data will be less evenly distributed, as averaging tends to lessen the contribution of terms further away from 5. The shape of the distribution will begin to appear Gaussian.

As you increase the number of random numbers averaged together ('n') to create each data point, the distribution becomes more Gaussian in nature. Please refer to figure 4. When $n=1$ (one random number is used to compute each data point), the density distribution is relatively even. As 'n' increases, the curves become more Gaussian in nature until we have a very smooth Gaussian distribution when $n=100$ (100 random numbers were averaged to obtain one data point).

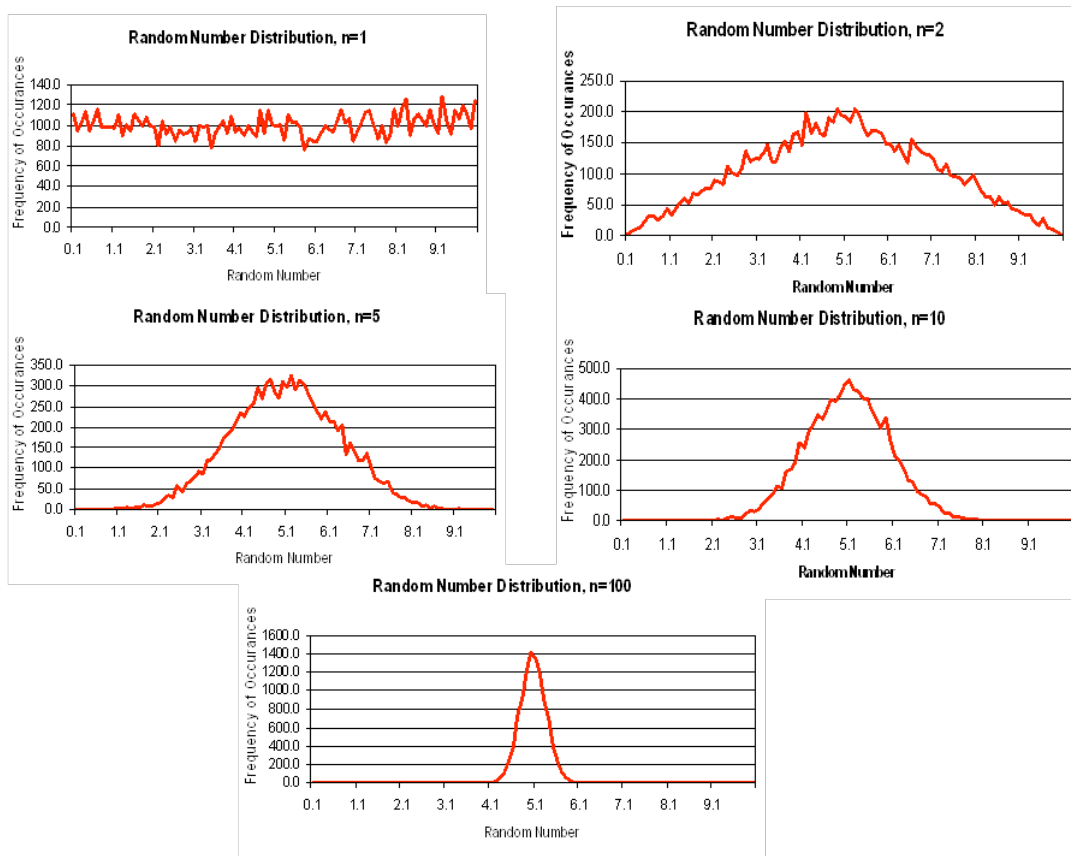


Figure 4: Distribution of data points generated by averaging random numbers

14.5 Example 1

In a healthy adult female, studies have shown that the mean fraction of deoxygenated blood leaving the lungs is 0.05 with a standard deviation 0.01. To obtain this data, 100 healthy females had been sampled using our random number sampler.

- a) Assuming this distribution is Gaussian, 95% of all healthy females will have deoxygenated blood fractions in what range (assume this range is centered over the mean of the data)?
- b) What is the expected error in the mean to a 95% level of confidence?
- c) A second study has been conducted on pregnant adult females. It was found that the mean fraction of deoxygenated blood leaving the lungs was 0.06 with a standard deviation of 0.02. Is the deoxygenated blood concentration in this population of women statistically different?
- d) Now assume that only 10 adult females had been sampled instead of 100. Analyze how the answer to part (c) may change.

14.5.1 Solution:

a) To solve this problem, recall the equation of a Gaussian distribution. Substitute in the value of the mean (0.05) and standard deviation (0.01). Next, recall that the area under the curve corresponds to probability, so we can set integrate this function to determine the range at which the probability equals 0.95. The bounds on this integral are $0.05 + k$ and $0.05 - k$, since we are assuming this data range is centered about the mean. This integral can be solved in integral form or in error function form, depending on the commands you choose to use in inputting the function into a computer algebra system solver. Maple, Excel, and Mathematics can be used to solve the expression simply by entering the last line of math text shown in the solution below.

$$P(\mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

$$P(\mu, \sigma) = \frac{1}{\sqrt{2\pi(0.01)^2}} e^{-\frac{(x-0.05)^2}{2(0.01)^2}}$$

$$0.95 = \int_{0.05-k}^{0.05+k} \frac{1}{\sqrt{2\pi(0.01)^2}} e^{-\frac{(x-0.05)^2}{2(0.01)^2}} dx$$

$$0.95 = \frac{1}{2} \left[\operatorname{Erf}\left(\frac{0.05+k-0.05}{0.01\sqrt{2}}\right) - \operatorname{Erf}\left(\frac{0.05-k-0.05}{0.01\sqrt{2}}\right) \right]$$

$$k = 0.02$$

Therefore, 95% of healthy adult females have deoxygenated blood levels between 0.03 and 0.07.

b) This problem is solved much in the same way we solved part (a). However, in this case we are looking for the 95% confidence interval of the mean, and not the entire population. Therefore, the standard deviation must be converted to the standard error in the mean. Then, all the above calculations are repeated.

$$\sigma_{\mu} = \frac{\sigma}{\sqrt{n}} = \frac{0.01}{\sqrt{100}} = 0.001$$

$$P(\mu, \sigma_{\mu}) = \frac{1}{\sqrt{2\pi\sigma_{\mu}^2}} e^{-\frac{(x-\mu)^2}{2\sigma_{\mu}^2}}$$

$$P(\mu, \sigma_{\mu}) = \frac{1}{\sqrt{2\pi(0.001)^2}} e^{-\frac{(x-0.05)^2}{2(0.001)^2}}$$

$$0.95 = \int_{0.05-k}^{0.05+k} \frac{1}{\sqrt{2\pi(0.001)^2}} e^{-\frac{(x-0.05)^2}{2(0.001)^2}} dx$$

$$0.95 = \frac{1}{2} \left[\operatorname{Erf} \left(\frac{0.05 + k - 0.05}{0.001\sqrt{2}} \right) - \operatorname{Erf} \left(\frac{0.05 - k - 0.05}{0.001\sqrt{2}} \right) \right]$$

$$k = 0.002$$

Therefore, the 95% confidence interval of the mean is 0.05 ± 0.002 .

c) In order to compare the statistical significance of two different data sets, the concept of p-values must be used. Since we are interested comparing the means of these two data sets, standard deviation will be replaced by standard error in the mean. To find the probability (or p-value) that pregnancy results in higher levels of deoxygenated blood, we need to calculate the area under the Gaussian curve for healthy females that is 0.06 or more. Remember, we are evaluating the Gaussian function describing healthy females, so standard deviation data for the pregnant females is not needed.

$$\sigma_{\mu} = \frac{\sigma}{\sqrt{n}} = \frac{0.01}{\sqrt{100}} = 0.001$$

$$P(\mu, \sigma_{\mu}) = \frac{1}{\sqrt{2\pi\sigma_{\mu}^2}} e^{-\frac{(x-\mu)^2}{2\sigma_{\mu}^2}}$$

$$P(\mu, \sigma_{\mu}) = \frac{1}{\sqrt{2\pi(0.001)^2}} e^{-\frac{(x-0.05)^2}{2(0.001)^2}}$$

$$P(x \geq 0.06) = \int_{0.06}^{\infty} \frac{1}{\sqrt{2\pi(0.001)^2}} e^{-\frac{(x-0.05)^2}{2(0.001)^2}} dx$$

$$P(x \geq 0.06) = \frac{1}{2} \left[\text{Erf} \left(\frac{\infty - 0.05}{0.001\sqrt{2}} \right) - \text{Erf} \left(\frac{0.06 - 0.05}{0.001\sqrt{2}} \right) \right]$$

$$P(x \geq 0.06) = \frac{1}{2} \left[1 - \text{Erf} \left(\frac{0.06 - 0.05}{0.001\sqrt{2}} \right) \right]$$

$$P(x \geq 0.06) = 0$$

The p-value is equal to zero. By convention, p-values less than 0.05 are considered to be statistically significant. Therefore, we conclude that pregnancy statistically affects the level of deoxygenated blood in an adult women's body.

d) The size of the sample only has an affect on the standard error in the mean. To solve this problem, recalculate the standard error and repeat the calculations above.

$$\sigma_{\mu} = \frac{\sigma}{\sqrt{n}} = \frac{0.01}{\sqrt{10}} = 0.003$$

$$P(\mu, \sigma_{\mu}) = \frac{1}{\sqrt{2\pi\sigma_{\mu}^2}} e^{-\frac{(x-\mu)^2}{2\sigma_{\mu}^2}}$$

$$P(\mu, \sigma_{\mu}) = \frac{1}{\sqrt{2\pi(0.003)^2}} e^{-\frac{(x-0.05)^2}{2(0.003)^2}}$$

$$P(x \geq 0.06) = \int_{0.06}^{\infty} \frac{1}{\sqrt{2\pi(0.003)^2}} e^{-\frac{(x-0.05)^2}{2(0.003)^2}} dx$$

$$P(x \geq 0.06) = \frac{1}{2} \left[\text{Erf} \left(\frac{\infty - 0.05}{0.003\sqrt{2}} \right) - \text{Erf} \left(\frac{0.06 - 0.05}{0.003\sqrt{2}} \right) \right]$$

$$P(x \geq 0.06) = \frac{1}{2} \left[1 - \text{Erf} \left(\frac{0.06 - 0.05}{0.003\sqrt{2}} \right) \right]$$

$$P(x \geq 0.06) = 0.0004$$

In this case, the p-value is still less than 0.05, so we still arrive at the same conclusion. We also conclude that as sample size decreases, differences in sample means become less significant because the p-value has slightly increased.

14.6 Example 2: Comparison of Two Data Sets

This example is intended to demonstrate how increased sample size affects the comparison of two data sets.

Using a random number generator, four data sets (A,B,C,D) were generated. Each data set contains 100 total data points. For data sets A and B, two random numbers were averaged to attain each data point, while in C and D, five random numbers were averaged

for each point. This difference resulted in smaller standard deviations for data sets C and D. A summary of the four data sets created is shown in the following chart. M is the number of random samples averaged to obtain each data point. N is the total number of data points. The mean and standard deviation for each of the data sets is also given.

Data Set	m	n	Mean	St Dev
A	2	100	5	2.3
B	2	100	5.5	1.8
C	5	100	5	1.1
D	5	100	5.5	1.4

- Compare the means of data sets A and B by calculating the p-value
- Compare the means of data sets C and D by calculating the p-value
- Compare the p-values obtained for parts a) and b) above. Explain why the values make sense.
- What general effect does increasing sample size have on the comparison of two data sets?

14.6.1 Solution:

- The p-value comparing data sets A and B is computed as follows:

$$\sigma_{\mu} = \frac{\sigma}{\sqrt{n}} = \frac{2.3}{\sqrt{100}} = 0.23$$

$$P(\mu, \sigma_{\mu}) = \frac{1}{\sqrt{2\pi\sigma_{\mu}^2}} e^{-\frac{(x-\mu)^2}{2\sigma_{\mu}^2}}$$

$$P(\mu, \sigma_{\mu}) = \frac{1}{\sqrt{2\pi(0.23)^2}} e^{-\frac{(x-5)^2}{2(0.23)^2}}$$

$$P(x \geq 5.5) = \int_{5.5}^{\infty} \frac{1}{\sqrt{2\pi(0.23)^2}} e^{-\frac{(x-5)^2}{2(0.23)^2}} dx$$

$$P(x \geq 5.5) = \frac{1}{2} \left[\text{Erfc} \left(\frac{5.5 - 5}{0.23\sqrt{2}} \right) \right]$$

$$P(x \geq 5.5) = \frac{1}{2} \left[1 - \text{Erf} \left(\frac{5.5 - 5}{0.23\sqrt{2}} \right) \right]$$

$$P(x \geq 5.5) = 0.015$$

From this p-value, we can see that it is very unlikely that these two data sets are statistically the same. There is only a 1.5% chance of randomly getting a data set with a mean as high as 5.5! It is far more likely that these two data sets are actually statistically different.

b) The p-value comparing data sets C and D is computed as follows:

$$\sigma_{\mu} = \frac{\sigma}{\sqrt{n}} = \frac{1.1}{\sqrt{100}} = 0.11$$

$$P(\mu, \sigma_{\mu}) = \frac{1}{\sqrt{2\pi\sigma_{\mu}^2}} e^{-\frac{(x-\mu)^2}{2\sigma_{\mu}^2}}$$

$$P(\mu, \sigma_{\mu}) = \frac{1}{\sqrt{2\pi(0.11)^2}} e^{-\frac{(x-5)^2}{2(0.11)^2}}$$

$$P(x \geq 5.5) = \int_{5.5}^{\infty} \frac{1}{\sqrt{2\pi(0.11)^2}} e^{-\frac{(x-5)^2}{2(0.11)^2}} dx$$

$$P(x \geq 5.5) = \frac{1}{2} \left[\operatorname{Erfc} \left(\frac{5.5 - 5}{0.11\sqrt{2}} \right) \right]$$

$$P(x \geq 5.5) = \frac{1}{2} \left[1 - \operatorname{Erf} \left(\frac{5.5 - 5}{0.11\sqrt{2}} \right) \right]$$

$$P(x \geq 5.5) = 0$$

From this p-value, we can see that these two data sets are statistically different. There is an almost 0 percent chance of randomly getting a data set with a mean as high as 5.5!

c) Comparing the two p-values, we can see that the value for b) is smaller than a), indicating that we are more confident about a statistical difference between sets C and D than between A and B. Going back to the description of the problem, we can find a reason for this result. Because of the larger sampling of random numbers in data sets C and D (five numbers averaged for each data point, compared to just two), these data sets have smaller standard deviations. These smaller standard deviations mean that we have a higher level of confidence that the sample mean is the true mean. Because each data set is more likely to show the true mean, there is also an increased likelihood that one data set is statistically different from the other.

d) In a Gaussian distribution, as sample size increases, standard error decreases. This indicates that the sample mean is closer to the true mean, and two data sets are more likely to be statistically different from each other than if there are smaller sample sizes and higher standard deviations in the data sets.

14.7 Example 3

14.7.1 Control Charts

This section will provide a brief overview on control charts in order to complete example 3, in which our random number sampler is applied to a control chart situation. For a more detailed explanation on control charts, and the methodology behind them, please see this wiki page: [Control Charts](#)

Background

Controls charts are tools used to determine whether a particular part of a process is predictable or not. A process is predictable when it is in a state of statistical control and unpredictable when it is not in a state of statistical control. A state of statistical control simply means that we can accurately predict what the output of a process will be in the future based on past measurements; it does not mean that the product is on target or within any limits of consumer acceptability. The random number sampler is a useful tool that can be used to analyze control charts. As previously discussed, a data set is more Gaussian in nature as the amount of data points is increased. Therefore, one will expect that a large set of data generated with our random number sampler will always be in statistical control, but smaller sets may contain an element of unpredictability.

To create a control chart, we begin by looking at historical data measurements on the measurement (variable) of importance, e.g. acetic acid concentration. Once a reasonable amount of data has been gathered, it is used to calculate appropriate limits for the variable. If the historical data and future measurements fall within the range of the limits, it is safe to predict that future measurements will also continue to be within the range of the limits. Conversely, if the historical data does not fall within the range of the limits, it can be safely predicted that future measurements will not fall within the range of the limits.

Constructing Control Charts

The best way to illustrate how to create a control chart is to go through an example. This is done below. The initial assumption in developing a control chart is that the process is stable over period of time where a set of measurements can be made on a particular variable of the process. In the example below, this variable is acetic acid concentration.

Example

Chemical engineers often combine acetic anhydride and water to produce acetic acid in a moderately exothermic reaction. The reaction in this particular process is supposed to produce a product stream of acetic acid at 5.5 wt%. The composition of the product stream is measured four times every hour for ten hours. Each hour's measurements are viewed as a subgroup of data. Table 1 shows the data obtained from the 40 measurements. Table 1 also listed the average concentration and the range of concentrations for each subgroup of measurements.

Table 3. Sample Data - Acetic Acid Concentration

Subgroup	Concentration (wt%)				Average	Range
1	5.31	5.18	5.57	5.05	5.28	0.52
2	5.97	5.61	5.08	5.41	5.52	0.89
3	5.35	5.97	5.82	5.64	5.70	0.63
4	5.78	5.22	5.35	5.50	5.46	0.56
5	5.57	5.08	5.16	5.86	5.42	0.79
6	5.97	5.54	5.09	5.42	5.50	0.87
7	6.00	5.18	5.57	5.71	5.61	0.82
8	5.23	5.72	5.82	5.23	5.50	0.59
9	5.05	5.95	5.97	5.01	5.50	0.95
10	5.88	5.04	5.87	5.62	5.60	0.84

To create a control chart for this process, we must first compute the average concentration for each subset. Additionally, we must determine the range of data for each subset. These steps have already been completed and their values are listed in Table 3 in the last two columns on the right. Next the grand average concentration and average range should be computed by averaging the average concentrations of each subset and by taking the average of each subset's ranges. For the data in table 3, the grand average concentration is 5.51 wt% and the average range is 0.74 wt%. At this point, we are ready to determine our upper and lower control limits for our acetic acid concentration. To determine these limits we will need to use a table of constants that have been

mathematically derived for Gaussian distributions. These numbers can then be inserted into equations that find the upper and lower average control limits ($UCL_{\bar{x}}$ and $LCL_{\bar{x}}$) and the upper and lower range control limits (UCL_R and LCL_R). The following equations provide the control limits for the average concentrations and for their ranges.

$$UCL_{\bar{X}} = \bar{\bar{X}} + A_2 \bar{R}$$

$$LCL_{\bar{X}} = \bar{\bar{X}} - A_2 \bar{R}$$

$$UCL_R = D_4 \bar{R}$$

$$LCL_R = D_3 \bar{R}$$

Table 5. Constants for Average and Range Charts Based on the Average Range

Constants for Average Range Charts Based on the Average Range			
n	A ₂	D ₃	D ₄
2	1.88	0	3.268
3	1.023	0	2.574
4	0.739	0	2.282
5	0.577	0	2.114
6	0.483	0	2.004
7	0.419	0.076	1.924
8	0.373	0.136	1.864
9	0.337	0.184	1.816
10	0.308	0.223	1.777

For this example, our subgroup size, n, is 4, A₂ is 0.729, D₃ is 0 and D₄ is 2.282. When plugged into the above equations, they yield control limits of:

$$UCL_{\bar{X}} = 6.05$$

$$LCL_{\bar{X}} = 4.97$$

$$UCL_R = 1.70$$

$$LCL_R = 0$$

Graphically the control chart is represented by creating a plot of the average concentration values versus their subgroup number and creating a plot of each range value versus the subgroup number. Horizontal lines should be included on these plots which indicate the control limits. Control charts for this example are plotted in figures 3 and 4.

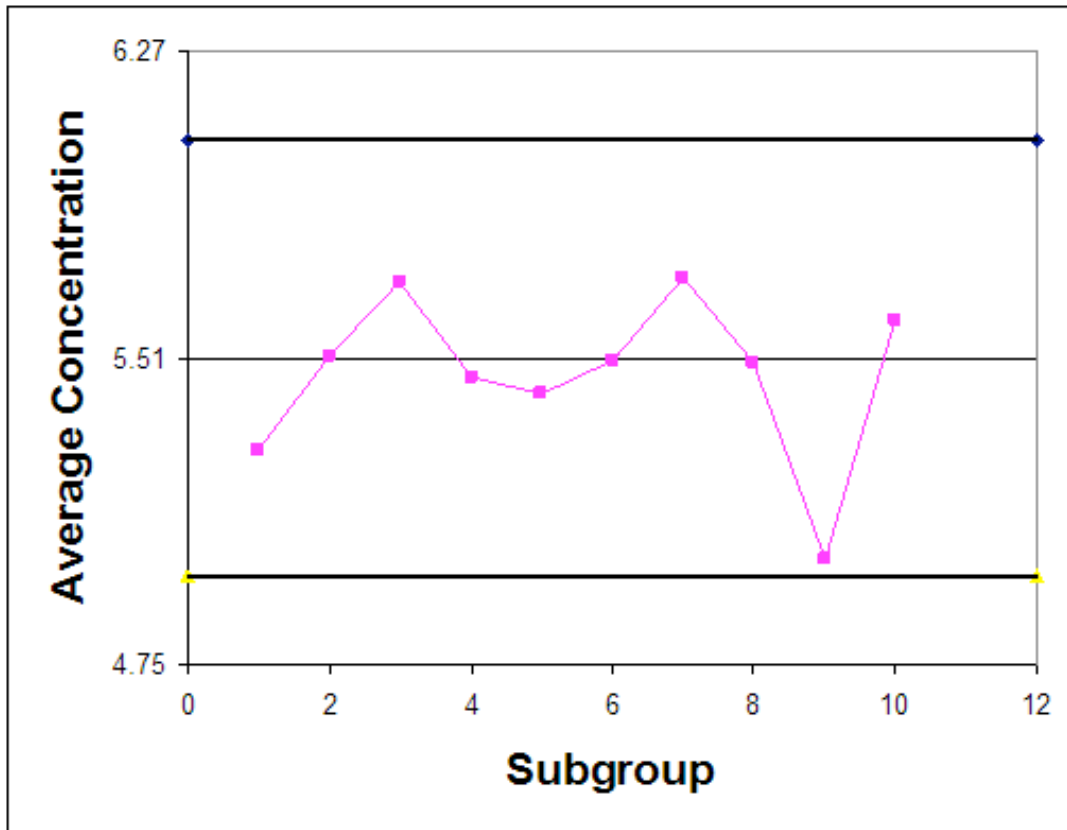


Figure 6. Control Chart for Average Acetic Acid Concentration

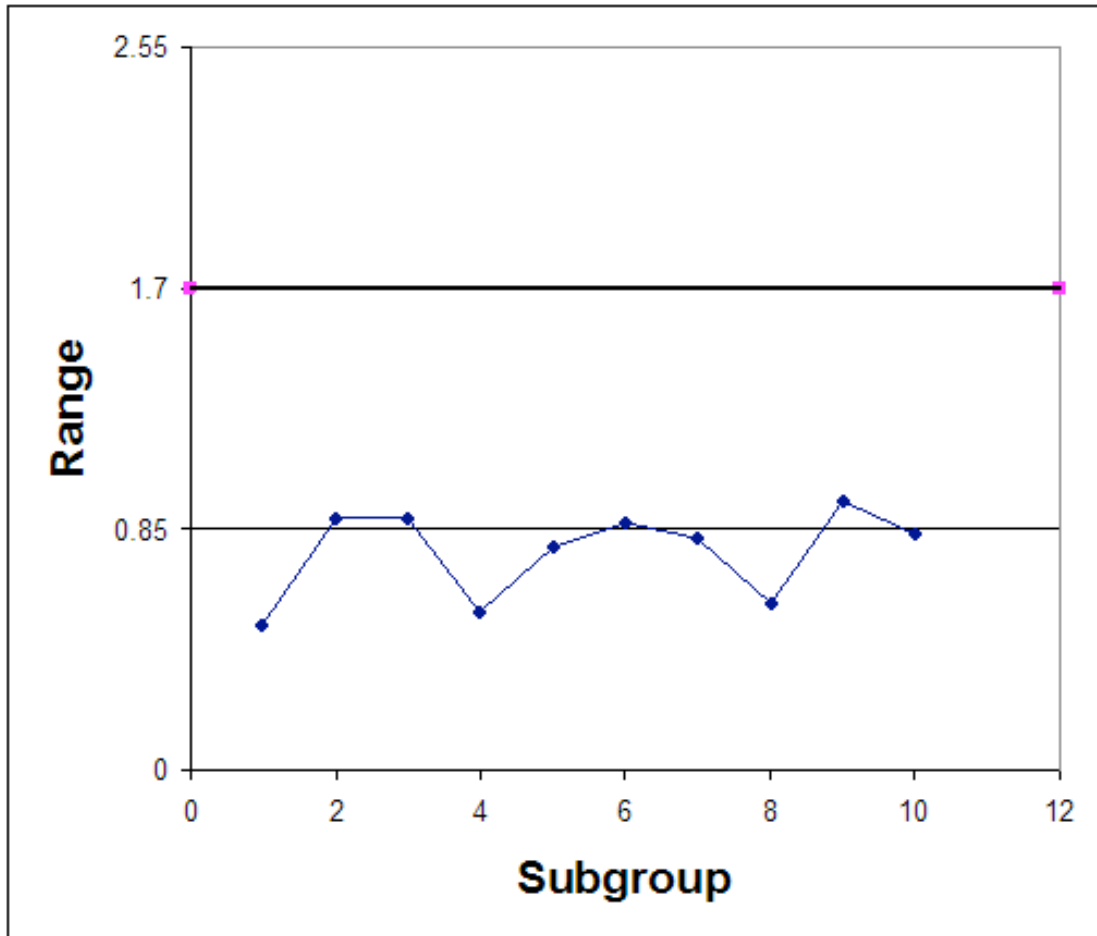


Figure 7. Control Chart for Ranges of Acetic Acid Concentration

Interpreting Control Charts

If any of the following rules hold true for the centering control chart, the process is not in statistical control.

1. One or more points fall outside the control limits.
2. Seven or more consecutive points fall on the same side of the centerline.
3. Ten of 11 consecutive points fall on the same side of the centerline.
4. Three or more consecutive points fall on the same side of the centerline and all are located closer to the control limit than the centerline.

Observe that in both the control chart for the average concentrations, the historical data never exceeds or goes below the control limits. Also, none of the other rules above hold

true for this chart. This suggests that the process is stable; however, to confirm this thought, future observations must be made. If the average acetic acid concentration and its range continues to stay within the control limits, the process is said to be stable.

In the event that the historical data did not stay within the control limits, the plots could have looked like figures 5 & 6.

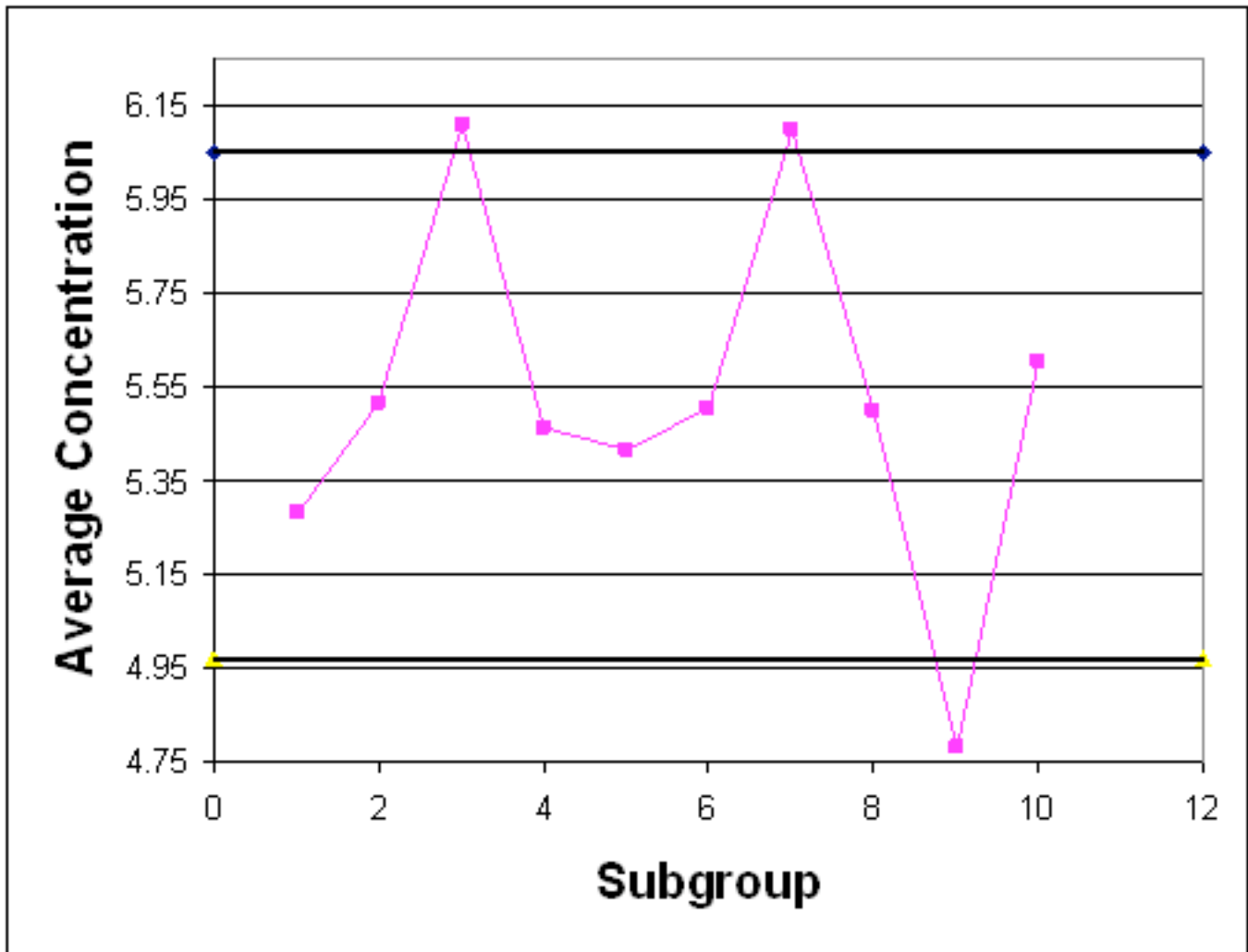


Figure 8. Control Chart for Average Acetic Acid Concentration (Unstable)

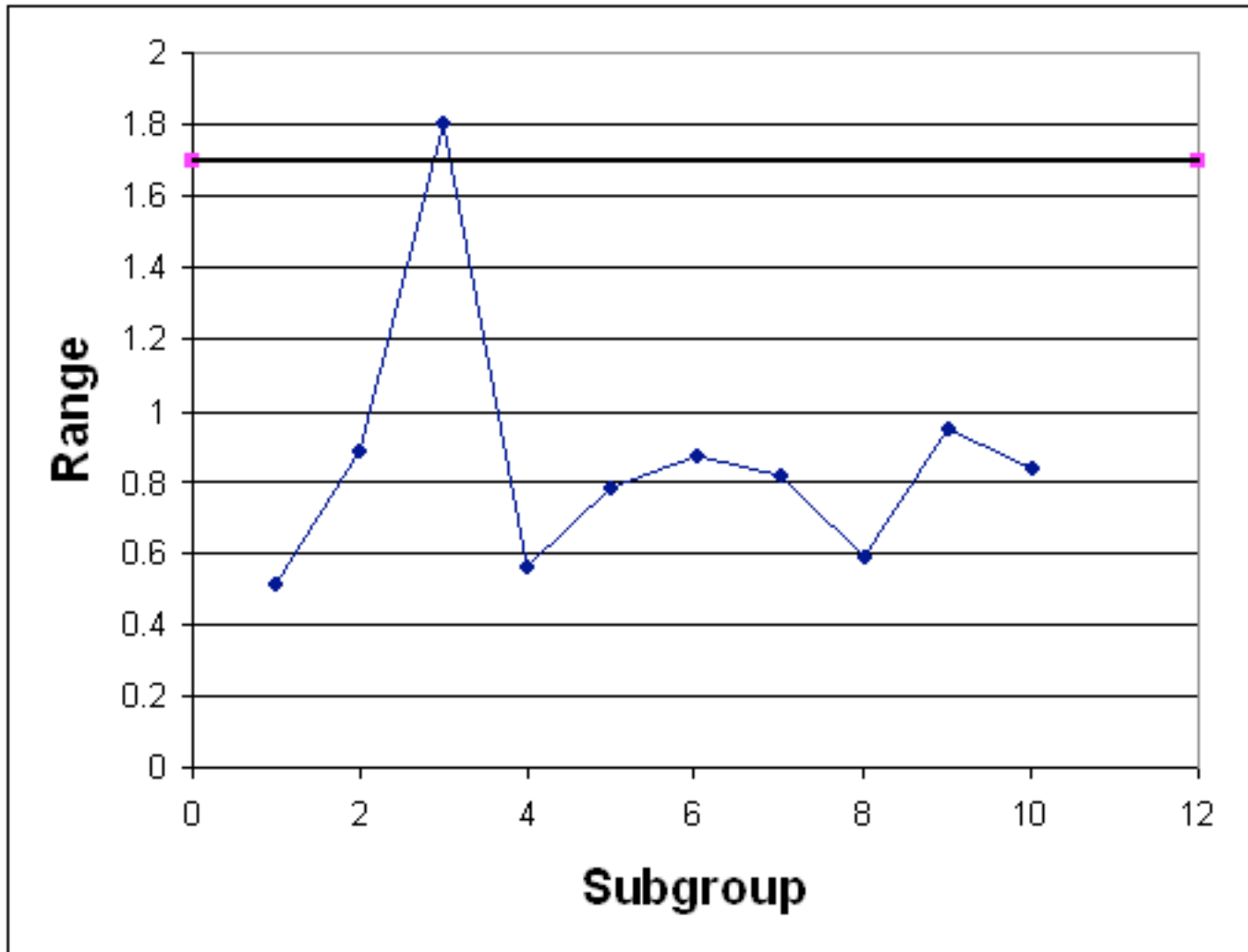


Figure 9. Control Chart for Ranges of Acetic Acid Concentration (Unstable)

Observe that in each of these control charts, the historical data does not stay within the control limits for the process. Based on this observation, it can be predicted that future data will also not stay within the control limits for the process and the process is not stable. In conclusion, control charts allow you to use samples of data to determine the control limits for a process and evaluate if the process is stable or not.

14.7.2 Random Sampling Problem

In an industrial bioengineering process, it is desired to obtain a 75% proline to 25% hydroxyproline ratio in a specialized enzyme. The relative compositions can be analyzed using a fluorescent dye, where a fluorescence of 10 corresponds to the correct ratio of these two amino acids. To monitor the stability of this process, five readings are taken every 30 minutes for the duration of the 10 hour production process. The results were

obtained using our random number sampler with a specified mean (10) and standard deviation (in this case 1.6). The results are in the table below

Time (hr)	Sample Flouresence				
	1	2	3	4	5
0.5	11.2	9.8	12.0	12.9	12.5
1	9.7	10.7	9.8	10.6	7.0
1.5	12.4	9.0	12.9	12.6	11.5
2	12.1	9.1	10.9	7.4	7.9
2.5	8.2	11.6	9.7	10.8	10.1
3	9.1	8.1	8.6	11.6	11.0
3.5	7.9	8.3	9.8	12.3	9.6
4	7.7	10.2	8.2	10.4	11.7
4.5	12.0	10.1	11.6	7.0	9.2
5	10.7	12.1	8.2	12.7	10.5
5.5	7.5	9.8	9.8	10.8	7.5
6	12.4	9.3	10.6	10.9	7.9
6.5	9.0	12.1	10.4	11.8	11.3
7	9.2	7.7	10.2	11.5	8.4
7.5	8.7	11.2	11.2	11.0	11.2
8	11.2	7.8	9.1	10.0	10.0
8.5	12.2	8.5	11.5	13.0	9.6
9	10.6	9.2	11.5	10.1	11.2
9.5	7.1	9.4	10.7	10.4	9.1
10	11.5	7.2	12.9	12.2	10.0

- a) Calculate the average and range for each data subgroup.
- b) Create an average and range chart for the entire time of production.
- c) Is this process in control?

14.7.3 Answer:

- a) The average and range can be calculated using the =AVERAGE() and =MAX()-MIN() functions of Microsoft excel.

Time (hr)	Sample Fluorescence					Avg	R
	1	2	3	4	5		
0.5	11.2	9.8	12.0	12.9	12.5	11.7	3.0
1	9.7	10.7	9.8	10.6	7.0	9.6	3.7
1.5	12.4	9.0	12.9	12.6	11.5	11.7	3.9
2	12.1	9.1	10.9	7.4	7.9	9.5	4.7
2.5	8.2	11.6	9.7	10.8	10.1	10.1	3.4
3	9.1	8.1	8.6	11.6	11.0	9.7	3.6
3.5	7.9	8.3	9.8	12.3	9.6	9.6	4.4
4	7.7	10.2	8.2	10.4	11.7	9.6	4.0
4.5	12.0	10.1	11.6	7.0	9.2	10.0	5.0
5	10.7	12.1	8.2	12.7	10.5	10.8	4.5
5.5	7.5	9.8	9.8	10.8	7.5	9.1	3.3
6	12.4	9.3	10.6	10.9	7.9	10.2	4.5
6.5	9.0	12.1	10.4	11.8	11.3	10.9	3.0
7	9.2	7.7	10.2	11.5	8.4	9.4	3.8
7.5	8.7	11.2	11.2	11.0	11.2	10.7	2.5
8	11.2	7.8	9.1	10.0	10.0	9.6	3.5
8.5	12.2	8.5	11.5	13.0	9.6	11.0	4.4
9	10.6	9.2	11.5	10.1	11.2	10.5	2.3
9.5	7.1	9.4	10.7	10.4	9.1	9.3	3.6
10	11.5	7.2	12.9	12.2	10.0	10.7	5.7

b) The grand average is 10.2 and the average range is 3.8. Using Table 2, $A_2 = 0.577$, $D_3 = 0$, and $D_4 = 2.114$. Therefore:

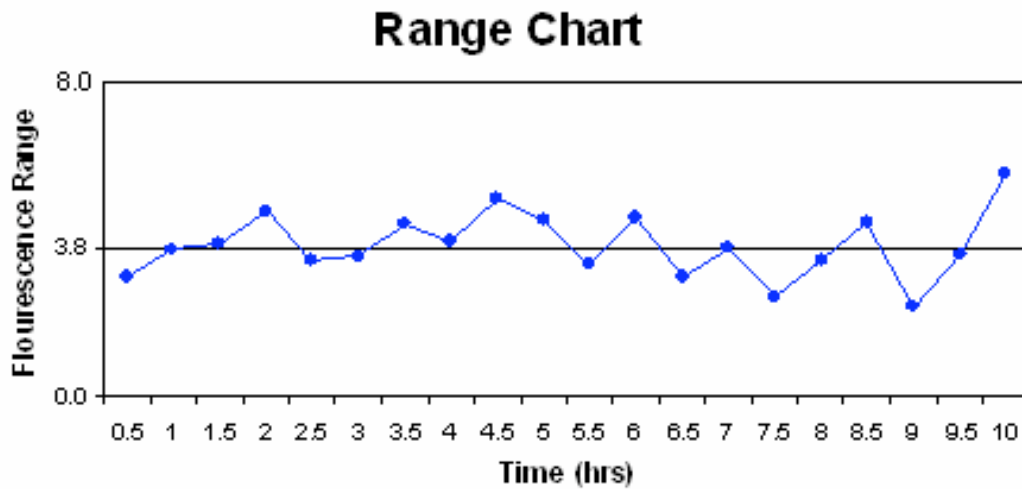
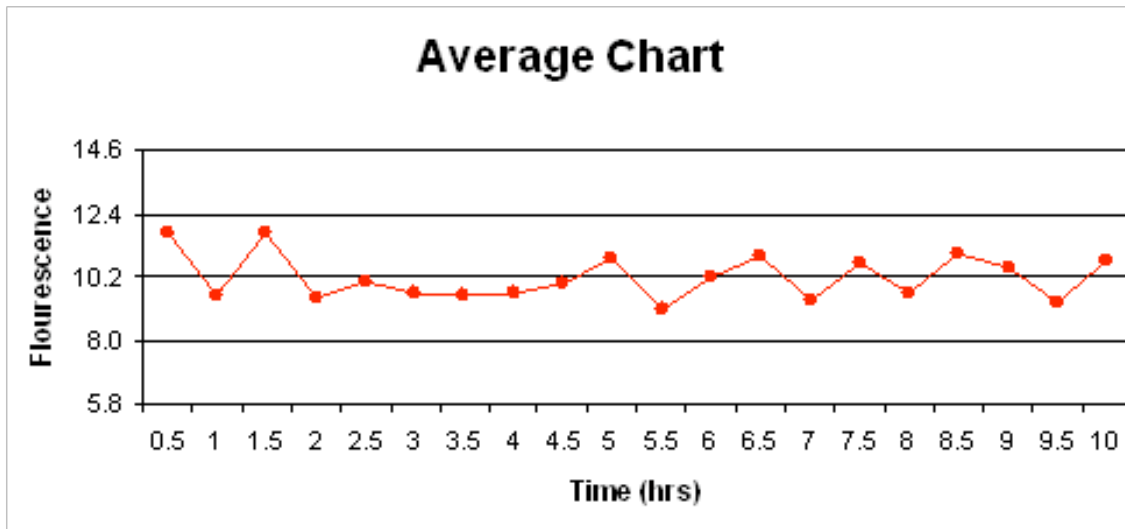
$$UCL_{\bar{X}} = \bar{\bar{X}} + A_2 \bar{R} = 10.2 + (0.577)(3.8) = 12.4$$

$$LCL_{\bar{X}} = \bar{\bar{X}} - A_2 \bar{R} = 10.2 - (0.577)(3.8) = 8.0$$

$$UCL_R = D_4 \bar{R} = (2.114)(3.8) = 8.0$$

$$LCL_R = D_3 \bar{R} = (0)(3.8) = 0$$

The charts are as follows:



c) The first rule is not violated as none of the points fall outside the upper and lower control limits. Seven or more points do not fall on one side of the centerline (the maximum was six), so rule two is not violated. Rule three was not violated, as 10 of 11 points did not fall on the same side of the centerline (in our case, eight was the mx). Finally, rule four was not violated as none of the points were closer to the control limits than the centerline. Therefore, this process is under statistic control since none of the rules were violated.

14.8 Multiple Choice Question 1

Our random number sampler was designed based on which key principle:

- a) Data points obtained by taking the average of several random numbers are more likely to fit a Gaussian distribution.
- b) The area under a Gaussian distribution is always between zero and one and equal to the 'y' value of the CDF.
- c) The distribution of data points in a Gaussian distribution is caused by random uncertainties.
- d) A process under Gaussian statistical control will not have a data sample exceed the upper or lower control limit

Answer: A

14.9 Multiple Choice Question 2

Which of the following would decrease the p-value if comparing two different data sets:

- a) Smaller sample size
- b) Smaller count of averaged random numbers
- c) Smaller standard deviation
- d) Smaller difference in mean values

Answer: C

14.10 Sage's Corner

<http://www.youtube.com/v/jVqZGoRVwLI>

[Rollin' the Dice slides without narration](#)


14.11 References

- Box, George E., William G. Hunter, and J S. Hunter. *Statistics for Experimenters: An Introduction to Design, Data Analysis, and Model Building*. New York: John Wiley & Sons. 43-45.
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Chapter 14. Design of Experiments

Section 1. Design of experiments via Taguchi methods: orthogonal arrays

Note:  [Video lecture](#) available for this section!

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Date Presented: 12/5/06; Revised: 11/27/07

- [First round reviews for this page](#)
- [Rebuttal for this page](#)

1.1 Introduction

The Taguchi method involves reducing the variation in a process through robust design of experiments. The overall objective of the method is to produce high quality product at low cost to the manufacturer. The Taguchi method was developed by Dr. Genichi Taguchi of Japan who maintained that variation. Taguchi developed a method for designing experiments to investigate how different parameters affect the mean and variance of a process performance characteristic that defines how well the process is functioning. The experimental design proposed by Taguchi involves using orthogonal arrays to organize the parameters affecting the process and the levels at which they should be varies. Instead of having to test all possible combinations like the factorial design, the Taguchi method tests pairs of combinations. This allows for the collection of the necessary data to determine which factors most affect product quality with a minimum amount of experimentation, thus saving time and resources. The Taguchi method is best used when there is an intermediate number of variables (3 to 50), few interactions between variables, and when only a few variables contribute significantly.

The Taguchi arrays can be derived or looked up. Small arrays can be drawn out manually; large arrays can be derived from deterministic algorithms. Generally, arrays can be found online. The arrays are selected by the number of parameters (variables) and the number of levels (states). This is further explained later in this article. Analysis of variance on the collected data from the Taguchi design of experiments can be used to select new parameter values to optimize the performance characteristic. The data from the arrays can be analyzed by plotting the data and performing a visual analysis, ANOVA, bin yield and Fisher's exact test, or Chi-squared test to test significance.

In this article, the specific steps involved in the application of the Taguchi method will be described and examples of using the Taguchi method to design experiments will be given.

1.2 Summary of Taguchi Method

1.2.1 Philosophy of the Taguchi Method

1. **Quality should be designed into a product, not inspected into it.** Quality is designed into a process through system design, parameter design, and tolerance design. Parameter design, which will be the focus of this article, is performed by determining what process parameters most affect the product and then designing them to give a specified target quality of product. Quality "inspected into" a product means that the product is produced at random quality levels and those too far from the mean are simply thrown out.

2. **Quality is best achieved by minimizing the deviation from a target. The product should be designed so that it is immune to uncontrollable environmental factors.** In other words, the signal (product quality) to noise (uncontrollable factors) ratio should be high.

3. **The cost of quality should be measured as a function of deviation from the standard and the losses should be measured system wide.** This is the concept of the loss function, or the overall loss incurred upon the customer and society from a product of poor quality. Because the producer is also a member of society and because customer dissatisfaction will discourage future patronage, this cost to customer and society will come back to the producer.

1.2.2 Taguchi Method Design of Experiments

The general steps involved in the Taguchi Method are as follows:

1. Define the process objective, or more specifically, a target value for a performance measure of the process. This may be a flow rate, temperature, etc. The target of a process may also be a minimum or maximum; for example, the goal may be to maximize the output flow rate. The deviation in the performance characteristic from the target value is used to define the loss function for the process.

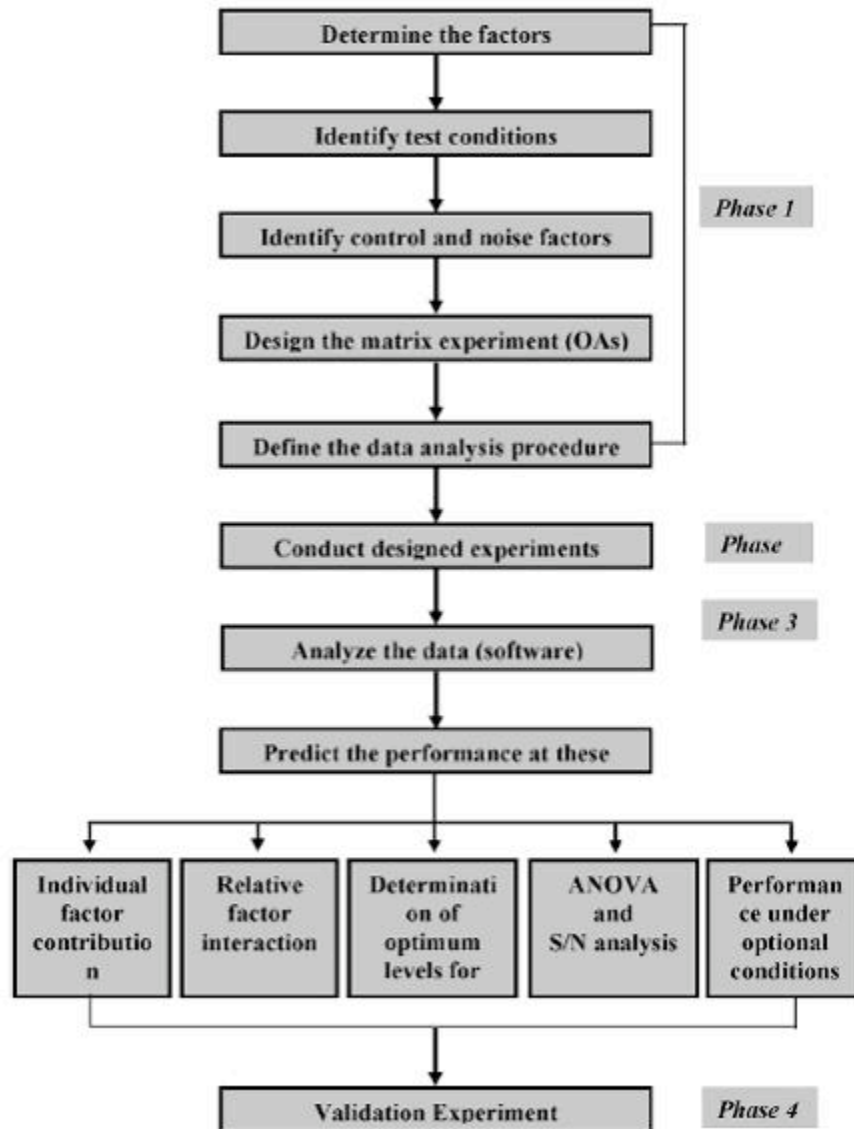
2. Determine the design parameters affecting the process. Parameters are variables within the process that affect the performance measure such as temperatures, pressures, etc. that can be easily controlled. The number of levels that the parameters should be varied at must be specified. For example, a temperature might be varied to a low and high value of 40 C and 80 C. Increasing the number of levels to vary a parameter at increases the number of experiments to be conducted.

3. Create orthogonal arrays for the parameter design indicating the number of and conditions for each experiment. The selection of orthogonal arrays is based on the number of parameters and the levels of variation for each parameter, and will be expounded below.

4. Conduct the experiments indicated in the completed array to collect data on the effect on the performance measure.

5. Complete data analysis to determine the effect of the different parameters on the performance measure.

See below for a pictorial depiction of these and additional possible steps, depending on the complexity of the analysis.



A detailed description of the execution of these steps will be discussed next.

1.3 Taguchi Loss Function

The goal of the Taguchi method is to reduce costs to the manufacturer and to society from variability in manufacturing processes. Taguchi defines the difference between the target value of the performance characteristic of a process, τ , and the measured value, y , as a loss function as shown below.

$$l(y) = k_c (y - \tau)^2$$

The constant, k_c , in the loss function can be determined by considering the specification limits or the acceptable interval, delta.

$$k_c = \frac{C}{\Delta^2}$$

The difficulty in determining k_c is that τ and C are sometimes difficult to define.

If the goal is for the performance characteristic value to be minimized, the loss function is defined as follows:

$$l(y) = k_c y^2 \quad \text{Where} \quad \tau = 0$$

If the goal is for the performance characteristic value to be maximized, the loss function is defined as follows:

$$l(y) = \frac{k_c}{y^2}$$

The loss functions described here are the loss to a customer from one product. By computing these loss functions, the overall loss to society can also be calculated.

1.4 Determining Parameter Design Orthogonal Array

The effect of many different parameters on the performance characteristic in a condensed set of experiments can be examined by using the orthogonal array experimental design proposed by Taguchi. Once the parameters affecting a process that can be controlled have been determined, the levels at which these parameters should be varied must be determined. Determining what levels of a variable to test requires an in-depth understanding of the process, including the minimum, maximum, and current value of the parameter. If the difference between the minimum and maximum value of a parameter is

large, the values being tested can be further apart or more values can be tested. If the range of a parameter is small, then less values can be tested or the values tested can be closer together. For example, if the temperature of a reactor jacket can be varied between 20 and 80 degrees C and it is known that the current operating jacket temperature is 50 degrees C, three levels might be chosen at 20, 50, and 80 degrees C. Also, the cost of conducting experiments must be considered when determining the number of levels of a parameter to include in the experimental design. In the previous example of jacket temperature, it would be cost prohibitive to do 60 levels at 1 degree intervals. Typically, the number of levels for all parameters in the experimental design is chosen to be the same to aid in the selection of the proper orthogonal array.

Knowing the number of parameters and the number of levels, the proper orthogonal array can be selected. Using the array selector table shown below, the name of the appropriate array can be found by looking at the column and row corresponding to the number of parameters and number of levels. Once the name has been determined (the subscript represents the number of experiments that must be completed), the predefined array can be looked up. Links are provided to many of the predefined arrays given in the array selector table. These arrays were created using an algorithm Taguchi developed, and allows for each variable and setting to be tested equally. For example, if we have three parameters (voltage, temperature, pressure) and two levels (high, low), it can be seen the proper array is L4. Clicking on the link L4 to view the L4 array, it can be seen four different experiments are given in the array. The levels designated as 1, 2, 3 etc. should be replaced in the array with the actual level values to be varied and P1, P2, P3 should be replaced with the actual parameters (i.e. voltage, temperature, etc.)

Array Selector

		Number of Parameters (P)																														
		2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	
Number of Levels	2	L4	L4	L8	L8	L8	L8	L12	L12	L12	L12	L16	L16	L16	L16	L32	L32	L32	L32	L32	L32	L32	L32	L32	L32	L32	L32	L32	L32	L32	L32	L32
	3	L9	L9	L9	L18	L18	L18	L18	L27	L27	L27	L27	L36	L36	L36	L36	L36	L36	L36	L36	L36	L36	L36	L36								
	4	L'16	L'16	L'16	L'16	L'32	L'32	L'32	L'32	L'32																						
	5	L25	L25	L25	L25	L25	L50	L50	L50	L50	L50	L50																				
	6																															

Links to Orthogonal Arrays

The following links are connected to images of the orthogonal array named in the link title:

[L4 Array](#)

[L8 Array](#)

[L9 Array](#)

[L12 Array](#)

[L16 Array](#)

[L'16 Array](#)

[L18 Array](#)

[L25 Array](#)

[L27 Array](#)

[L32 Array](#)

[L'32 Array](#)

[L36 Array](#)

[L50 Array](#)

1.4.1 Important Notes Regarding Selection + Use of Orthogonal Arrays

Note 1

The array selector assumes that each parameter has the same number of levels. Sometimes this is not the case. Generally, the highest value will be taken or the difference will be split.

The following examples offer insight on choosing and properly using an orthogonal array. Examples 1 and 2 focus on array choice, while Example 3 will demonstrate how to use an orthogonal array in one of these situations.

Example 1:

```
# parameter: A, B, C, D = 4    # levels:    3, 3, 3, 2 =  
~3    array: L9
```

Example 2:

```
# parameter: A, B, C, D, E, F = 6    # levels:    4, 5,  
3, 2, 2, 2 = ~3    array: modified L16
```

Example 3:

A reactor's behavior is dependent upon impeller model, mixer speed, the control algorithm employed, and the cooling water valve type. The possible values for each are as follows:

Impeller model: A, B, or C

Mixer speed: 300, 350, or 400 RPM

Control algorithm: PID, PI, or P

Valve type: butterfly or globe

There are 4 parameters, and each one has 3 levels with the exception of valve type. The highest number of levels is 3, so we will use a value of 3 when choosing our orthogonal array.

Using the array selector above, we find that the appropriate orthogonal array is L9:

Experiment	P1	P2	P3	P4
1	1	1	1	1
2	1	2	2	2
3	1	3	3	3
4	2	1	2	3
5	2	2	3	1
6	2	3	1	2
7	3	1	3	2
8	3	2	1	3
9	3	3	2	1

When we replace P1, P2, P3, and P4 with our parameters and begin filling in the parameter values, we find that the L9 array includes 3 levels for valve type, while our system only has 2. The appropriate strategy is to fill in the entries for P4=3 with 1 or 2 in a random, balanced way. For example:

Experiment	Impeller	Motor Speed	Control	Valve
1	A	300	PID	BF
2	A	350	PI	G
3	A	400	P	G
4	B	300	PI	BF
5	B	350	P	BF
6	B	400	PID	G
7	C	300	P	G
8	C	350	PID	BF
9	C	400	PI	BF

Here, the third value was chosen twice as butterfly and once as global.

Note 2

If the array selected based on the number of parameters and levels includes more parameters than are used in the experimental design, ignore the additional parameter columns. For example, if a process has 8 parameters with 2 levels each, the L12 array should be selected according to the array selector. As can be seen below, the L12 Array has columns for 11 parameters (P1-P11). The right 3 columns should be ignored.

Experiment	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	P11
1	1	1	1	1	1	1	1	1	1	1	1
2	1	1	1	1	1	2	2	2	2	2	2
3	1	1	2	2	2	1	1	1	2	2	2
4	1	2	1	2	2	1	2	2	1	1	2
5	1	2	2	1	2	2	1	2	1	2	1
6	1	2	2	1	2	2	1	2	1	1	1
7	1	2	2	2	1	2	2	1	2	1	1
8	2	1	2	1	2	2	2	1	1	1	2
9	2	1	1	2	2	2	1	2	2	1	1
10	2	2	2	1	1	1	1	2	2	1	2
11	2	2	1	2	1	2	1	1	1	2	2
12	2	2	1	1	2	1	2	1	2	2	1

1.5 Analyzing Experimental Data

Once the experimental design has been determined and the trials have been carried out, the measured performance characteristic from each trial can be used to analyze the relative effect of the different parameters. To demonstrate the data analysis procedure, the following L9 array will be used, but the principles can be transferred to any type of array.

In this array, it can be seen that any number of repeated observations (trials) may be used. $T_{i,j}$ represents the different trials with i = experiment number and j = trial number. It should be noted that the Taguchi method allows for the use of a noise matrix including external factors affecting the process outcome rather than repeated trials, but this is outside of the scope of this article.

Experiment Number	P1	P2	P3	P4	T1	T2	...	Tn
1	1	1	1	1	$T_{1,1}$	$T_{1,2}$...	$T_{1,N}$
2	1	2	2	2	$T_{2,1}$	$T_{2,2}$...	$T_{2,N}$
3	1	3	3	3	$T_{3,1}$	$T_{3,2}$...	$T_{3,N}$
4	2	1	2	3	$T_{4,1}$	$T_{4,2}$...	$T_{4,N}$
5	2	2	3	1	$T_{5,1}$	$T_{5,2}$...	$T_{5,N}$
6	2	3	1	2	$T_{6,1}$	$T_{6,2}$...	$T_{6,N}$
7	3	1	3	2	$T_{7,1}$	$T_{7,2}$...	$T_{7,N}$
8	3	2	1	3	$T_{8,1}$	$T_{8,2}$...	$T_{8,N}$
9	3	3	2	1	$T_{9,1}$	$T_{9,2}$...	$T_{9,N}$

To determine the effect each variable has on the output, the signal-to-noise ratio, or the SN number, needs to be calculated for each experiment conducted. The calculation of the SN for the first experiment in the array above is shown below for the case of a specific target value of the performance characteristic. In the equations below, \bar{y}_i is the mean value and s_i is the variance. y_i is the value of the performance characteristic for a given experiment.

$$SN_i = 10 \log \frac{\bar{y}_i^2}{s_i^2}$$

Where

$$\bar{y}_i = \frac{1}{N_i} \sum_{u=1}^{N_i} y_{i,u}$$

$$s_i^2 = \frac{1}{N_i - 1} \sum_{u=1}^{N_i} (y_{i,u} - \bar{y}_i)^2$$

$i = \text{Experiment number}$

$u = \text{Trial number}$

$N_i = \text{Number of trials for experiment } i$

For the case of minimizing the performance characteristic, the following definition of the SN ratio should be calculated:

$$SN_i = -10 \log \left(\sum_{u=1}^{N_i} \frac{y_u^2}{N_i} \right)$$

For the case of maximizing the performance characteristic, the following definition of the SN ratio should be calculated:

$$SN_i = -10 \log \left[\frac{1}{N_i} \sum_{u=1}^{N_i} \frac{1}{y_u^2} \right]$$

After calculating the SN ratio for each experiment, the average SN value is calculated for each factor and level. This is done as shown below for Parameter 3 (P3) in the array:

Experiment Number	P1	P2	P3	P4	S _{ii}
1	1	1	1	1	SN1
2	1	2	2	2	SN2
3	1	3	3	3	SN3
4	2	1	2	3	SN4
5	2	2	3	1	SN5
6	2	3	1	2	SN6
7	3	1	3	2	SN7
8	3	2	1	3	SN8
9	3	3	2	1	SN9

$$SN_{P3,1} = \frac{(S_{N1} + S_{N6} + S_{N8})}{3}$$

$$SN_{P3,2} = \frac{(S_{N2} + S_{N4} + S_{N9})}{3}$$

$$SN_{P3,3} = \frac{(S_{N3} + S_{N5} + S_{N7})}{3}$$

Once these SN ratio values are calculated for each factor and level, they are tabulated as shown below and the range R (R = high SN - low SN) of the SN for each parameter is calculated and entered into the table. The larger the R value for a parameter, the larger the effect the variable has on the process. This is because the same change in signal causes a larger effect on the output variable being measured.

Level	P1	P2	P3	P4
1	SNP1,1	SNP2,1	SNP3,1	SNP4,1
2	SNP1,2	SNP2,2	SNP3,2	SNP4,2
3	SNP1,3	SNP2,3	SNP3,3	SNP4,3
Δ	RP1	RP2	RP3	RP4
Rank

Please refer to the Worked Out Example for a numeric example of how the data analysis procedure described here is applied.

1.6 Advantages and Disadvantages

An advantage of the Taguchi method is that it emphasizes a mean performance characteristic value close to the target value rather than a value within certain specification limits, thus improving the product quality. Additionally, Taguchi's method for experimental design is straightforward and easy to apply to many engineering situations, making it a powerful yet simple tool. It can be used to quickly narrow down the scope of a research project or to identify problems in a manufacturing process from data already in existence. Also, the Taguchi method allows for the analysis of many different parameters without a prohibitively high amount of experimentation. For example, a process with 8 variables, each with 3 states, would require 6561 (3^8) experiments to test all variables. However using Taguchi's orthogonal arrays, only 18 experiments are necessary, or less than .3% of the original number of experiments. In this way, it allows for the identification of key parameters that have the most effect on the performance characteristic value so that further experimentation on these parameters can be performed and the parameters that have little effect can be ignored.

The main disadvantage of the Taguchi method is that the results obtained are only relative and do not exactly indicate what parameter has the highest effect on the performance characteristic value. Also, since orthogonal arrays do not test all variable combinations, this method should not be used with all relationships between all variables are needed. The Taguchi method has been criticized in the literature for difficulty in accounting for interactions between parameters. Another limitation is that the Taguchi methods are offline, and therefore inappropriate for a dynamically changing process such as a simulation study. Furthermore, since Taguchi methods deal with designing quality in rather than correcting for poor quality, they are applied most effectively at early stages of process development. After design variables are specified, use of experimental design may be less cost effective.

1.7 Other Methods of Experimental Design

Two other methods for determining experimental design are factorial design and random design. For scenarios with a small number of parameters and levels (1-3) and where each variable contributes significantly, [factorial design](#) can work well to determine the specific interactions between variables. However, factorial design gets increasingly complex with an increase in the number of variables. For large systems with many variables (50+) where there are few interactions between variables, random design can be used. Random design assigns each variable a state based on a uniform sample (ex: 3 states = 0.33 probability) for the selected number of experiments. When used properly (in a large system), random design usually produces an experimental design that is desired. However, random design works poorly for systems with a small number of variables.

To obtain a even better understanding of these three different methods, it's good to get a visual of these three methods. It will illustrate the degree of efficiency for each experimental design depending on the number of variables and the number of states for each variable. The following will have the three experimental designs for the same scenario.

Scenario. You have a CSTR that has four(4) variables and each variable has three or two states. You are to design an experiment to systematically test the effect of each of the variables in the current CSTR.

These variables can take the following values:

Impellers: model A, B, or C

Motor speed for mixer: 300, 350, or 400 RPM

Control algorithm: PID, PI, or P only

Cooling water valve type: butterfly or globe

Experimental Design #1: Factorial Design By looking at the # variables and # states, there should be a total of 54 experiments because (3impellers)(3speeds)(3controllers)(2valves)=54. Here's a list of these 54 experiments:

A, 300,PID, B A, 300,PI, B A, 300,P, B A, 300,PI, G A, 300,PID, G A, 300,P, G
 B, 300,PID, B B, 300,PI, B B, 300,P, B B, 300,PI, G B, 300,PID, G B, 300,P, G
 C, 300,PID, B C, 300,PI, B C, 300,P, B C, 300,PI, G C, 300,PID, G C, 300,P, G
 A, 350,PID, B A, 350,PI, B A, 350,P, B A, 350,PI, G A, 350,PID, G A, 350,P, G
 B, 350,PID, B B, 350,PI, B B, 350,P, B B, 350,PI, G B, 350,PID, G B, 350,P, G
 C, 350,PID, B C, 350,PI, B C, 350,P, B C, 350,PI, G C, 350,PID, G C, 350,P, G
 A, 400,PID, B A, 400,PI, B A, 400,P, B A, 400,PI, G A, 400,PID, G A, 400,P, G
 B, 400,PID, B B, 400,PI, B B, 400,P, B B, 400,PI, G B, 400,PID, G B, 400,P, G
 C, 400,PID, B C, 400,PI, B C, 400,P, B C, 400,PI, G C, 400,PID, G C, 400,P, G

Experimental Design #2: Taguchi Method Since you know the # of states and variables, you can refer to the table above in this wiki and obtain the correct Taguchi array. It turns out to be a L9 array.

L9

Experiment	P1	P2	P3	P4
1	1	1	1	1
2	1	2	2	2
3	1	3	3	3
4	2	1	2	3
5	2	2	3	1
6	2	3	1	2
7	3	1	3	2
8	3	2	1	3
9	3	3	2	1

With the actual variables and states, the L9 array should look like the following:

Experiment	Impeller	Moter Speed	Control	Valve
1	A	300	PID	BF
2	A	350	PI	G
3	A	400	P	G
4	B	300	PI	BF
5	B	350	P	BF
6	B	400	PID	G
7	C	300	P	G
8	C	350	PID	BF
9	C	400	PI	BF

Experimental Design #3: Random Design

Since we do not know the number of signal recoveries we want and we don't know the probabilities of each state to happen, it will be difficult to construct a random design table. It will mostly be used for extreme large experiments. Refer to the link below to help you obtain a better grasp on the random design concept.

http://groups.csail.mit.edu/drl/journal_club/papers/CS2-Candes-Romberg-05.pdf

1.8 Worked out Example

NOTE: *The data for the following example is not real, and details pertaining to microprocessor fabrication may not be completely accurate.*

A microprocessor company is having difficulty with its current yields. Silicon processors are made on a large die, cut into pieces, and each one is tested to match specifications. The company has requested that you run experiments to increase processor yield. The factors that affect processor yields are temperature, pressure, doping amount, and deposition rate.

a) Question: Determine the Taguchi experimental design orthogonal array. The operating conditions for each parameter and level are listed below:

- **A: Temperature**
 - A1 = 100°C
 - A2 = 150°C (current)
 - A3 = 200°C

- **B: Pressure**
 - B1 = 2 psi
 - B2 = 5 psi (current)
 - B3 = 8 psi

- **C: Doping Amount**
 - C1 = 4%
 - C2 = 6% (current)
 - C3 = 8%

- **D: Deposition Rate**
 - D1 = 0.1 mg/s
 - D2 = 0.2 mg/s (current)
 - D3 = 0.3 mg/s

a) Solution: The L9 orthogonal array should be used. The filled in orthogonal array should look like this:

Experiment Number	Temperature	Pressure	Doping Amount	Deposition Rate
1	100	2	4	0.1
2	100	5	6	0.2
3	100	8	8	0.3
4	150	2	6	0.3
5	150	5	8	0.1
6	150	8	4	0.2
7	200	2	8	0.2
8	200	5	4	0.3
9	200	8	6	0.1

This setup allows the testing of all four variables without having to run 81 [=3⁴=(3 Temperatures)(3 Pressures)(3 Doping Amounts)(3 Deposition rates)] separate trials.

b) Question: Conducting three trials for each experiment, the data below was collected. Compute the SN ratio for each experiment for the target value case, create a response chart, and determine the parameters that have the highest and lowest effect on the processor yield.

Experiment Number	Temperature	Pressure	Doping Amount	Deposition Rate	Trial 1	Trial 2	Trial 3	Mean
1	100	2	4	0.1	87.3	82.3	70.7	80.1
2	100	5	6	0.2	74.8	70.7	63.2	69.6
3	100	8	8	0.3	56.5	54.9	45.7	52.1
4	150	2	6	0.3	79.8	78.2	62.3	73.4
5	150	5	8	0.1	77.3	76.5	54.9	69.3
6	150	8	4	0.2	89	87.3	83.2	86.5
7	200	2	8	0.2	64.8	62.3	55.7	60.9
8	200	5	4	0.3	99	93.2	87.3	93.2
9	200	8	6	0.1	75.7	74	63.2	71

b) Solution: Shown below is the calculation and tabulation of the SN ratio.

$$S_{m1} = \frac{(87.3 + 82.3 + 70.7)^2}{3} = 19248.0$$

$$S_{T1} = 87.3^2 + 82.3^2 + 70.7^2 = 19393.1$$

$$S_{e1} = S_{T1} - S_{m1} = 19393.1 - 19248.0 = 145.0$$

$$V_{e1} = \frac{S_{e1}}{N - 1} = \frac{145.1}{2} = 72.5$$

$$SN_1 = 10 \log \frac{(1/N)(S_{m1} - V_{e1})}{V_{e1}} = 10 \log \frac{(1/3)(19248.0 - 145.1)}{145.1} = 19.5$$

Experiment Number	A (temp)	B (pres)	C (dop)	D (dep)	T1	T2	T3	SN
1	1	1	1	1	87.3	82.3	70.7	19.5
2	1	2	2	2	74.8	70.7	63.2	21.4
3	1	3	3	3	56.5	54.0	45.7	19.3
4	2	1	2	3	79.8	78.2	62.3	17.6
5	2	2	3	1	77.3	76.5	54.0	14.3
6	2	3	1	2	89.0	87.3	83.2	29.2
7	3	1	3	2	64.8	62.3	55.7	22.2
8	3	2	1	3	99.0	93.2	87.3	24.0
9	3	3	2	1	75.7	74.0	63.2	20.4

Shown below is the response table. This table was created by calculating an average SN value for each factor. A sample calculation is shown for Factor B (pressure):

Experiment Number	A (temp)	B (pres)	C (dop)	D (dep)	SN
1	1	1	1	1	19.5
2	1	2	2	2	21.4
3	1	3	3	3	19.3
4	2	1	2	3	17.6
5	2	2	3	1	14.3
6	2	3	1	2	29.2
7	3	1	3	2	22.2
8	3	2	1	3	24.0
9	3	3	2	1	20.4

$$SN_{B1} = \frac{(19.5 + 17.6 + 22.2)}{3} = 19.8$$

$$SN_{B2} = \frac{(21.4 + 14.3 + 24.0)}{3} = 19.9$$

$$SN_{B3} = \frac{(19.3 + 29.2 + 20.4)}{3} = 23.0$$

The effect of this factor is then calculated by determining the range:

$$\Delta = Max - Min = 23.0 - 19.8 = 3.2$$

Level	A (temp)	B (pres)	C (dop)	D (dep)
1	20.1	19.8	24.2	18.1
2	20.4	19.9	19.8	24.3
3	22.2	23.0	18.6	20.3
Δ	2.2	3.2	5.6	6.3
Rank	4	3	2	1

It can be seen that deposition rate has the largest effect on the processor yield and that temperature has the smallest effect on the processor yield.

1.9 Extreme Example: Sesame Seed Suffering

Problem: You have just produced one thousand 55 gallon drums of sesame oil for sale to your distributors. However, just before you are to ship oil, one of your employees remembers that one of the oil barrels was temporarily used to store insecticide and is almost surely contaminated. Unfortunately, all of the barrels look the same.

One barrel of sesame oil sells for \$1000, while each assay for insecticide in food oil costs \$1200 and takes 3 days. Tests for insecticide are extremely expensive. What do you do?

Solution: Extreme multiplexing. This is similar to using a Taguchi method but optimized for very sparse systems and specific cases. For example, instead of 1000 barrels, let us consider 8 barrels for now, one of which is contaminated. We could test each one, but that would be highly expensive. Another solution is to mix samples from each barrel and test the mixtures.

Mix barrels 1,2,3,4 ---> Sample A

Mix barrels 1,2,5,6 ---> Sample B

Mix barrels 1,3,5,7 ---> Sample C

We claim that from testing only these three mixtures, we can determine which of the 8 barrels was contaminated. Let us consider some possible results of these tests. We will use the following label scheme: +/-, +/-, +/- in order of A, B, C. Thus, +, -, + indicates A and C showed contamination but not B.

Possible Result 1: -, -, - The only barrel not mixed in was #8, so it is contaminated.

Possible Result 2: +,-,- Barrel #4 appears in A, but not in B and C. Since only A returned positive, barrel #4 was contaminated.

Possible Result 3: -,+,- Barrel #6 appears in B, but not in A and C. Since only B returned positive, barrel #6 was contaminated.

We can see that we have $2^3 = 8$ possible results, each of which corresponds to a particular barrel being contaminated. We leave the rest of the cases for the reader to figure out.

Solution with 1,000 barrels: Mix samples from each barrel and test mixtures. Each mixture will consist of samples from a unique combination of 500 barrels. Experiments required = $\log_2(1000) \approx 10$.

Solution with 1,000,000 barrels: Experiments required = $\log_2(1000000) \approx 20$.

Thus, by using extreme multiplexing, we can greatly reduce the # of experiments needed, since the # of experiments scales with $\log_2(\# \text{ of barrels})$ instead of # of barrels.

1.10 Multiple Choice Questions

1.10.1 Question 1

You are producing decaffeinated coffee using supercritical carbon dioxide as a solvent. To optimize the effectiveness of caffeine removal, you would like to test 2 different possible pressures of CO₂, 3 possible temperatures, 3 ratios of CO₂ to coffee beans, 3 residence times of supercritical CO₂ with beans, and 2 different procedures for preroasting the beans prior to caffeine extraction. What is the most appropriate method to design your optimization experiments?

- A. Factorial design
- B. Taguchi methods
- C. Random design
- D. None of the above. Coffee should never be decaffeinated

Solution: To perform a full factorial experiment, you'd need to account for: (2 pressures)(3 temperatures)(3 ratios)(3 times)(2 roasts) = 108 experiments! Thus, factorial design is not a practical choice: a good rule of thumb is 1-3 variables with few states for a manageable factorial analysis. However, selecting 3 for the number of levels and consulting the array selector, we see that an L18 array will suffice for a Taguchi analysis. 18 is a much more feasible number of experiments than 108. Finally, random design is only practical when >50 variables are involved and few will have significant impact on

the system, which is not the case here. Thus, although the author is of the opinion that choice 'D' has significant merit, the correct answer is 'B'.

1.10.2 Question 2

Which of the following is inconsistent with the Taguchi philosophy of quality control?

- A. Variation is the opposite of quality
- B. Interactions between parameters affecting product quality are unimportant and should never be considered
- C. Customer dissatisfaction is the most important measure for process variation, and should be minimized
- D. A high signal to noise ratio (SN) should be present in a process to make it robust against uncontrollable factors that would cause variation

Solution: Choice 'A' is another way of expressing point 3 of the Taguchi philosophy above. Similarly, choice 'C' is another way of expressing the cost function, and choice 'D' is consistent with philosophy 2. Although it is true that the Taguchi methods do not account well for interactions between variables, choice 'B' is incorrect for two reasons. 1) Pair-wise interactions between variables are accounted for in Taguchi orthogonal arrays. 2) Negligibility of interactions between parameters is not so much a central tenet of Taguchi philosophy as a necessary simplifying assumption. An analog is decoupling of MIMO systems. Since applying this assumption yields good results, it is consistent with Taguchi thinking to say that makes it valid.

1.11 Sage's Corner

Raising Tamagatchi using the Taguchi Method

<http://video.google.com/googleplayer.swf?docId=5615355814531160984>

Applying the Taguchi Method to a Heat Treatment Process for Steel


<http://video.google.com/googleplayer.swf?docId=-5748124283961697916>

[Powerpoint Slides with No Narration](#)

1.12 References

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Section 2. Design of experiments via factorial designs

Note:  [Video lecture](#) available for this section!

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- [First round reviews for this page](#)
- [Rebuttal for this page](#)

2.1 Introduction

Factorial design is an important method to determine the effects of multiple variables on a response. Traditionally, experiments are designed to determine the effect of ONE variable upon ONE response. R.A. Fisher showed that there are advantages by combining the study of multiple variables in the same factorial experiment. Factorial design can reduce the number of experiments one has to perform by studying multiple factors simultaneously. Additionally, it can be used to find both main effects (from each independent factor) and interaction effects (when both factors must be used to explain the outcome). However, factorial design can only give relative values, and to achieve actual numerical values the math becomes difficult, as regressions (which require minimizing a sum of values) need to be performed. Regardless, factorial design is a useful method to design experiments in both laboratory and industrial settings.

Factorial design tests all possible conditions. Because factorial design can lead to a large number of trials, which can become expensive and time-consuming, factorial design is best used for a small number of variables with few states (1 to 3). Factorial design works well when interactions between variables are strong and important and where every variable contributes significantly.

2.2 What is Factorial Design?

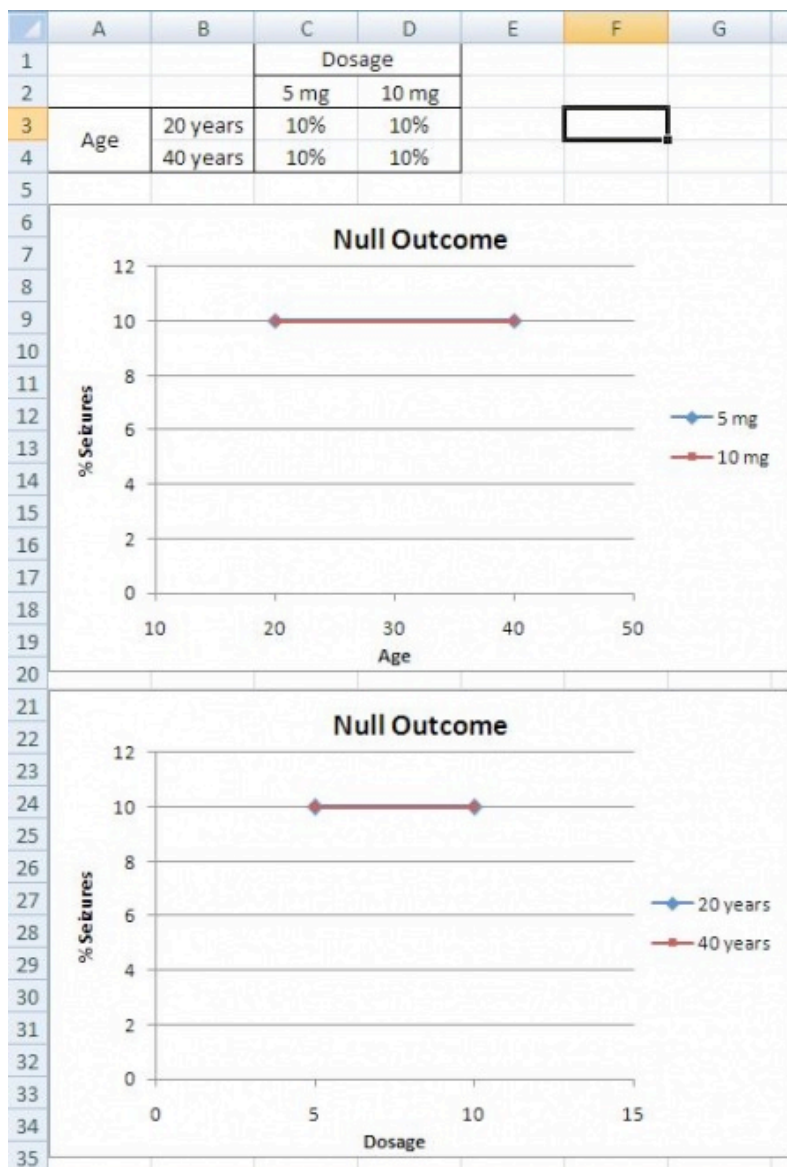
2.2.1 Factorial Design Example

The easiest way to understand how factorial design works is to read an example. Suppose that you, a scientist working for the FDA, would like to study and measure the probability of patients suffering from seizures after taking a new pharmaceutical drug called CureAll. CureAll is a novel drug on the market and can cure nearly any ailment of the body. You along with your co-workers at the FDA have decided to test two dosage levels: 5 mg and 10 mg. You are also interested in determining whether the drug side-effects differ between younger adults (age 20) and older adults (age 40). Based on the given information, you see that there are two factors: dosage and age. Factors are the main categories to explore when determining the cause of seizures in patients. Under each of these factors, there are different levels: 5 and 10 mg for the dosage; 20 and 40

years for age. A level is basically one of the subdivisions that make up a factor. From this information, we can see that we have a 2 x 2 factorial design, which means that we will have 2 * 2 = 4 groups. A group is set of conditions that will make up that particular experiment.

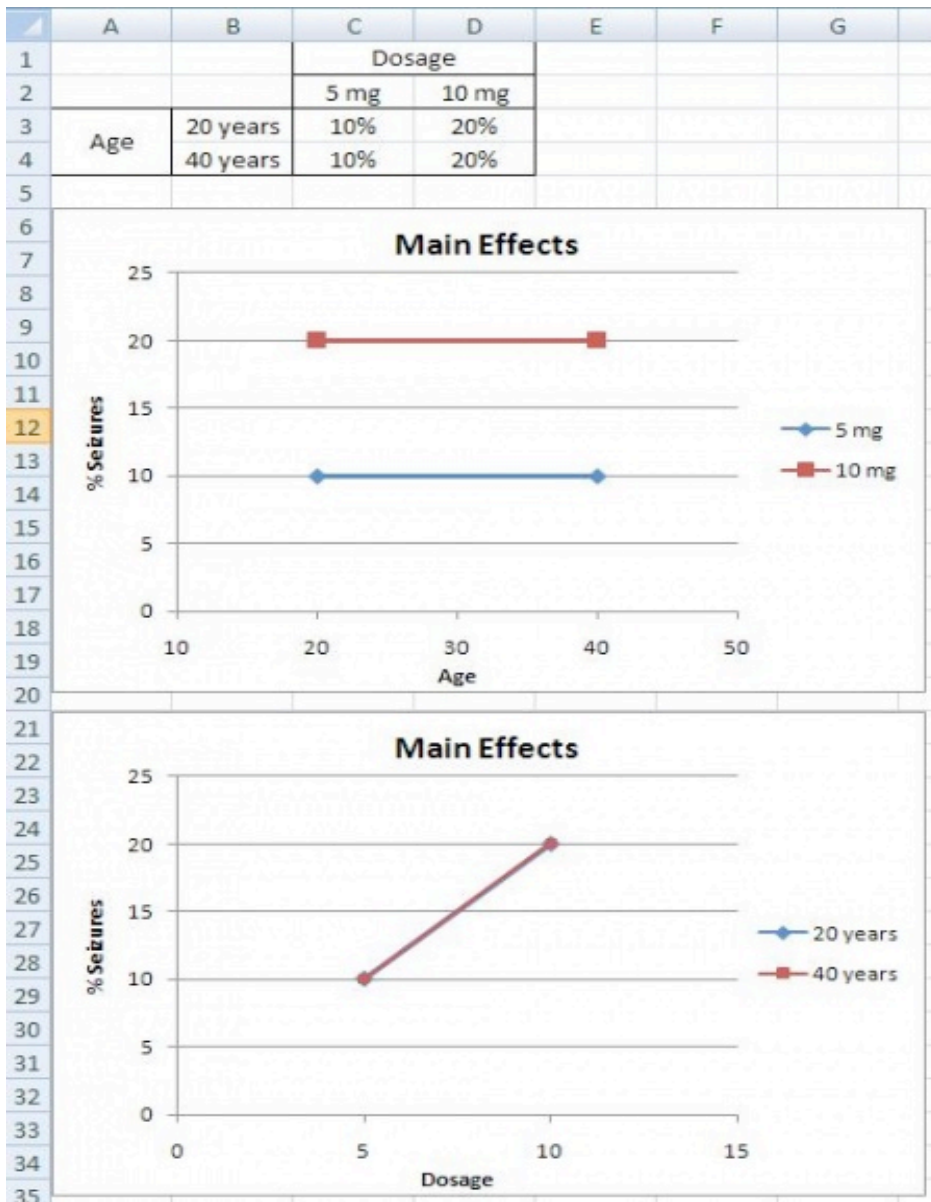
2.2.2 Null Outcome

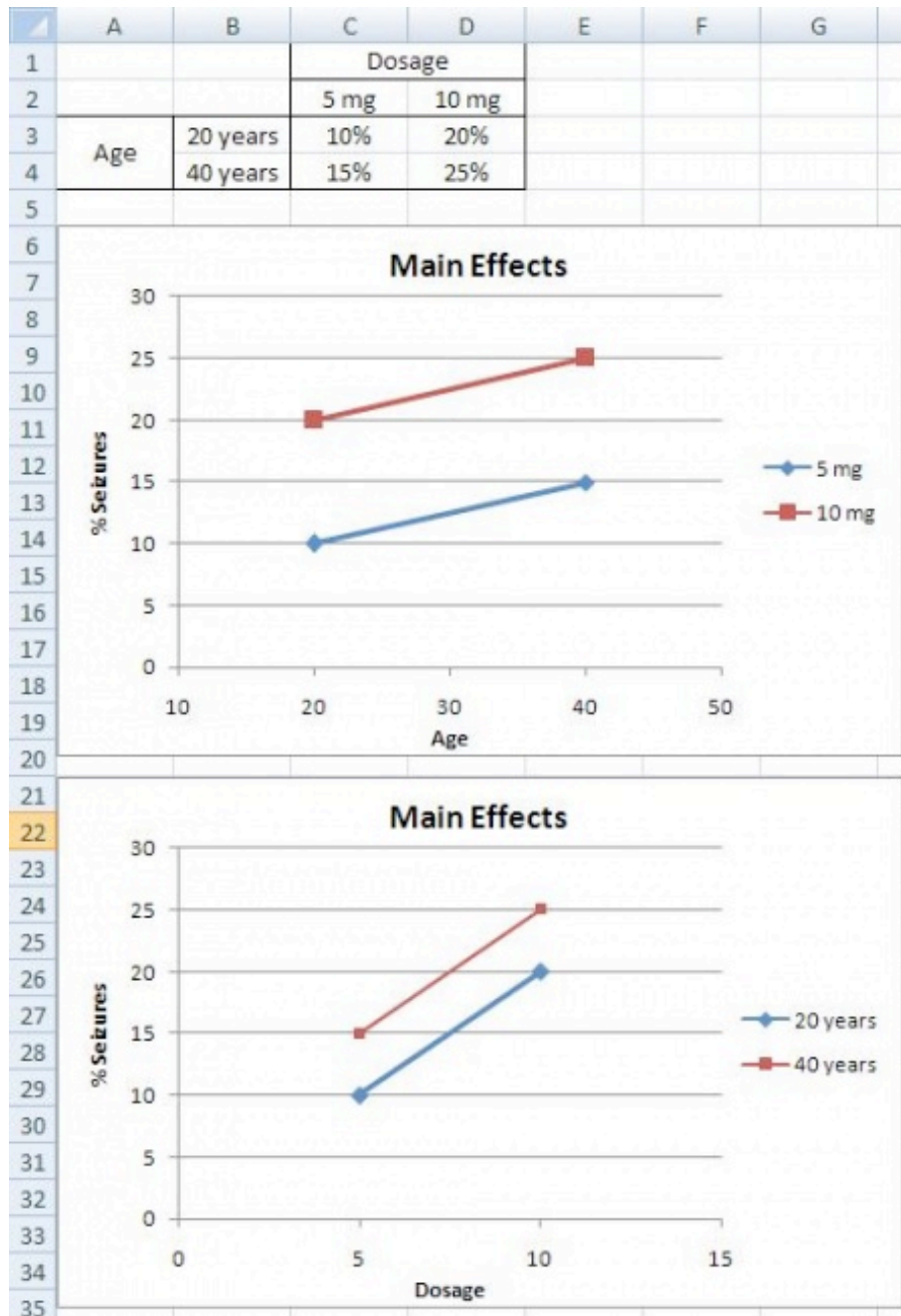
A null outcome situation is when the outcome of your experiment is the same regardless of how the levels within your experiment were combined. From the example above, a null outcome would exist if you received the same percentage of seizures occurring in patients with varying dose and age. The graphs below illustrate no change in the percentage of seizures for all factors, so you can conclude that the chance of suffering from a seizure is not affected by the dosage of the drug or the age of the patient.



2.2.3 Main Effects

A main effects situation is when there exists a consistent trend among the different levels of a factor. From the example above, suppose you find that as dosage increases, the percentage of people who suffer from seizures increases as well. You also notice that age does not play a role; both 20 and 40 year olds suffer the same percentage of seizures for a given amount of CureAll. From this information, you can conclude that the chance of a patient suffering a seizure is minimized at lower dosages of the drug (5 mg). The second graph illustrates that with increased drug dosage there is an increased percentage of seizures, while the first graph illustrates that with increased age there is no change in the percentage of seizures. Both of these graphs only contain one main effect, since only dose has an effect the percentage of seizures. Whereas, graphs three and four have two main effects, since dose and age both have an effect on the percentage of seizures.

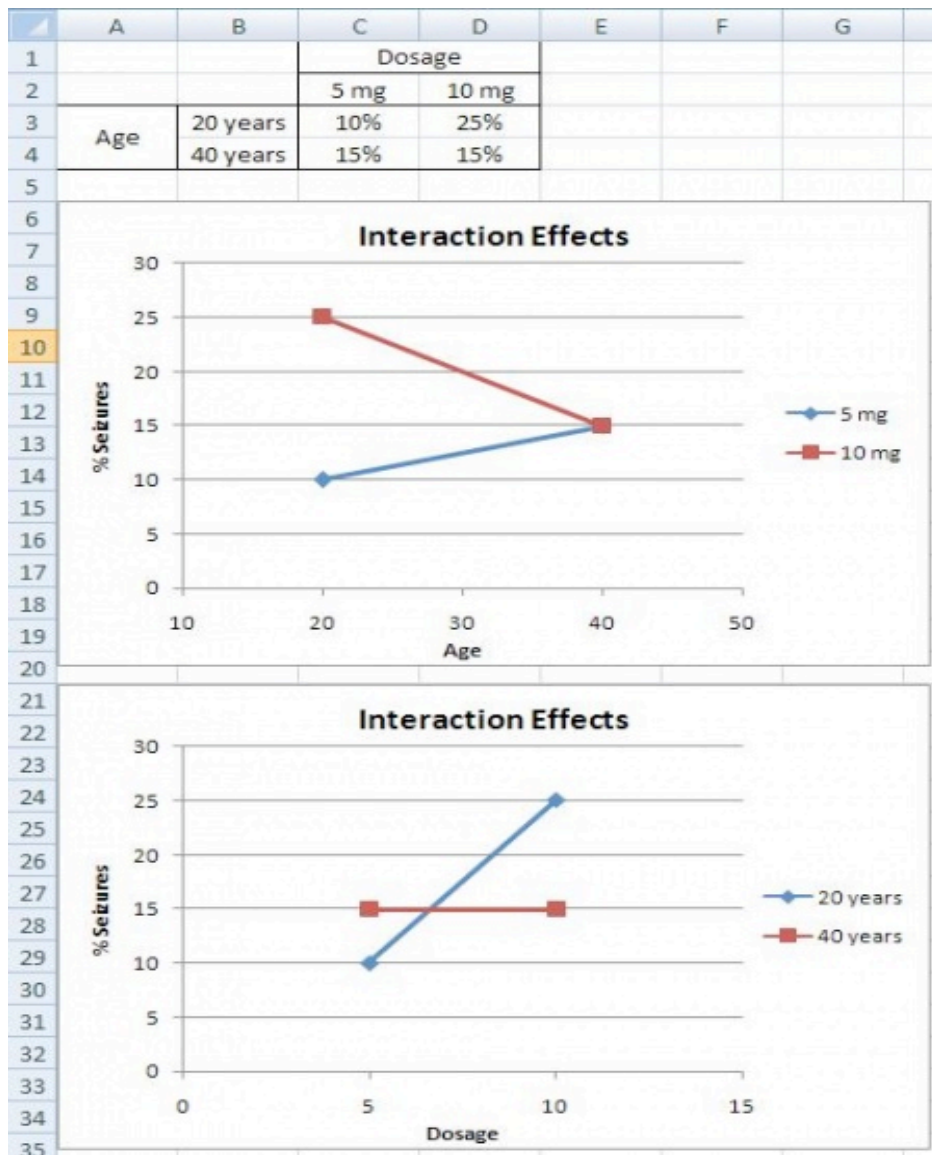




2.2.4 Interaction Effects

The interaction effects situation is the last outcome that can be detected using factorial design. From the example above, suppose you find that 20 year olds will suffer from seizures 10% of the time when given a 5 mg CureAll pill, while 20 year olds will suffer 25% of the time when given a 10 mg CureAll pill. When 40 year olds, however, are given

a 5 mg pill or a 10 mg pill, 15% suffer from seizures at both of these dosages. This correlation can be seen in the graphs below. There is an increasing chance of suffering from a seizure at higher doses for 20 year olds, but no difference in suffering from seizures for 40 year olds. Thus, there must be an interaction effect between the dosage of CureAll, and the age of the patient taking the drug. When you have an interaction effect it is impossible to describe your results accurately without mentioning both factors. You can always spot an interaction in the graphs because when there are lines that are not parallel an interaction is present. If you observe the main effect graphs above, you will notice that all of the lines within a graph are parallel. In contrast, for interaction effect graphs, you will see that the lines are not parallel.



2.3 Mathematical Analysis Approach

In the previous section, we looked at a qualitative approach to determining the effects of different factors using factorial design. Now we are going to shift gears and look at factorial design in a quantitative approach in order to determine how much influence the factors in an experiment have on the outcome.

2.3.1 How to Deal with a 2^n Factorial Design

Suppose you have two variables A and B and each have two levels a_1, a_2 and b_1, b_2 . You would measure combination effects of A and B ($a_1b_1, a_1b_2, a_2b_1, a_2b_2$). Since we have two factors, each of which has two levels, we say that we have a 2×2 or a 2^2 factorial design. Typically, when performing factorial design, there will be two levels, and n different factors. Thus, the general form of factorial design is 2^n .

In order to find the main effect of A, we use the following equation:

$$A = (a_2b_1 - a_1b_1) + (a_2b_2 - a_1b_2)$$

Similarly, the main effect of B is given by:

$$B = (b_2a_1 - b_1a_1) + (b_2a_2 - b_1a_2)$$

By the traditional experimentation, each experiment would have to be isolated separately to fully find the effect on B. This would have resulted in 8 different experiments being performed. Note that only four experiments were required in factorial designs to solve for the eight values in A and B. This shows how factorial design is a timesaver.

By taking the coefficients in A and B, the table below was created.

	Coefficient Effect			
	a_1b_1	a_2b_1	a_1b_2	a_2b_2
A	-1	+1	-1	+1
B	-1	-1	+1	+1
AB	+1	-1	-1	+1

AB is found by multiplying the coefficients of a_xb_x to get the new coefficient effect.

The additional complication is the fact that more than one trial/replication is required for accuracy, so this requires adding up each sub-effect (e.g adding up the three trials of a_1b_1). By adding up the coefficient effects with the sub-effects (multiply coefficient with sub-effect), a **total factorial effect** can be found. This value will determine if the factor

has a significant effect on the outcome. For larger numbers, the factor can be considered extremely important and for smaller numbers, the factor can be considered less important. The sign of the number also has a direct correlation to the effect being positive or negative.

To get a mean factorial effect, the totals needs to be divided by 2 times the number of **replicates**, where a replicate is a repeated experiment.

$$\text{mean factorial effect} = \text{total factorial effect} / 2r$$

By adding a third variable (C), the process of obtaining the coefficients becomes significantly complicated. The main factorial effect for A:

$$A = (a_2b_1c_1 - a_1b_1c_1) + (a_2b_2c_1 - a_1b_2c_1) + (a_2b_1c_2 - a_1b_1c_2) + (a_2b_2c_2 - a_1b_2c_2)$$

The table of coefficients is listed below

	Coefficient Effect							
	$a_1b_1c_1$	$a_2b_1c_1$	$a_1b_2c_1$	$a_2b_2c_1$	$a_1b_1c_2$	$a_2b_1c_2$	$a_1b_2c_2$	$a_2b_2c_2$
A	-1	+1	-1	+1	-1	+1	-1	+1
B	-1	-1	+1	+1	-1	-1	+1	+1
AB	+1	-1	-1	+1	+1	-1	-1	+1
C	-1	-1	-1	-1	+1	+1	+1	+1
AC	+1	-1	+1	-1	-1	+1	-1	+1
BC	+1	+1	-1	-1	-1	-1	+1	+1
ABC	-1	+1	+1	-1	+1	-1	-1	+1

It is clear that in order to find the total factorial effects, you would have to find the main effects of the variable and then the coefficients. Yates Algorithm can be used to simplify the process.

2.3.2 Yates Algorithm

[Frank Yates](#) created an algorithm to easily find the total factorial effects in a 2ⁿ factorial that is easily programmable in Excel. While this algorithm is fairly straightforward, it is also quite tedious and is limited to 2ⁿ factorial designs. Thus, modern technology has allowed for this analysis to be done using statistical software programs through regression.

Steps:

1. In the first column, list all the individual experimental combinations

According to the yates order, such as follows for a 2^3 factorial design

- - -
 + - -
 - + -
 + + -
 - - +
 + - +
 - + +
 + + +

2. In the second column, list all the totals for each combination
3. The 1st four entries in the third column (Stage 1) are obtained by adding pairs together from the "totals list" (previous column). The next four numbers are obtained by subtracting the top number from the bottom number of each pair.

Combination	Total		(1)
$a_1b_1c_1$	52	+	119.5
$a_2b_1c_1$	67.5	+	121
$a_1b_2c_1$	56	+	148
$a_2b_2c_1$	65	+	136
$a_1b_1c_2$	72		15.5
$a_2b_1c_2$	76		9
$a_1b_2c_2$	73		4
$a_2b_2c_2$	63		-10

Combination	Total	(1)
$a_1 b_1 c_1$	52	119.5
$a_2 b_1 c_1$	67.5	121
$a_1 b_2 c_1$	56	148
$a_2 b_2 c_1$	65	136
$a_1 b_1 c_2$	72	15.5
$a_2 b_1 c_2$	76	9
$a_1 b_2 c_2$	73	4
$a_2 b_2 c_2$	63	-10

4. The fourth column (Stage 2) is obtained in the same fashion, but this time adding and subtracting pairs from Stage 1.

Combination	Total	(1)	Stage (2)
$a_1 b_1 c_1$	52	119.5	240.5
$a_2 b_1 c_1$	67.5	121	284
$a_1 b_2 c_1$	56	148	24.5
$a_2 b_2 c_1$	65	136	-6
$a_1 b_1 c_2$	72	15.5	1.5
$a_2 b_1 c_2$	76	9	-12
$a_1 b_2 c_2$	73	4	-6.5
$a_2 b_2 c_2$	63	-10	-14

5. The fifth column (Stage 3) is obtained in the same fashion, but this time adding and subtracting pairs from Stage 2.

Combination	Total	Stage		
		(1)	(2)	(3)
$a_1b_1c_1$	52	119.5	240.5	524.5
$a_2b_1c_1$	67.5	121	284	18.5
$a_1b_2c_1$	56	148	24.5	-10.5
$a_2b_2c_1$	65	136	-6	-20.5
$a_1b_1c_2$	72	15.5	1.5	43.5
$a_2b_1c_2$	76	9	-12	-30.5
$a_1b_2c_2$	73	4	-6.5	-13.5
$a_2b_2c_2$	63	-10	-14	-7.5

Combination	Total	Stage		
		(1)	(2)	(3)
$a_1b_1c_1$	52	119.5	240.5	524.5
$a_2b_1c_1$	67.5	121	284	18.5
$a_1b_2c_1$	56	148	24.5	-10.5
$a_2b_2c_1$	65	136	-6	-20.5
$a_1b_1c_2$	72	15.5	1.5	43.5
$a_2b_1c_2$	76	9	-12	-30.5
$a_1b_2c_2$	73	4	-6.5	-13.5
$a_2b_2c_2$	63	-10	-14	-7.5

- Continue with Stages until reaching n , or the number of factors. This final column is the Effect Total. A positive value means a positive correlation, and a negative values means a negative correlation. These values are all relative, however, so there is no way to compare different effect totals from different experiments.

Ignoring the first row, look in the last stage and find the variable that has the largest relative number, then that row indicates the **MAIN TOTAL EFFECT**. The Main Total Effect can be related to input variables by moving along the row and looking at the first column. If the row in the first column is $a_2b_1c_1$ then the main total effect is A. The row for $a_1b_2c_1$ would be for B. The row for $a_2b_1c_2$ would be for AC.

This main total effect value for each variable or variable combination will be some value that signifies the relationship between the output and the variable. For instance, if your value is positive, then there is a positive relationship between the variable and the output (i.e. as you increase the variable, the output increases as well). A negative value would signify a negative relationship. Notice, however, that the values are all relative to one another. So while the largest main total effect value in one set of experiments may have a value of 128, another experiment may have its largest main total effect value be 43. There is no way to determine if a value of 128 in one experiment has more control over its output than a value of 43 does, but for the purposes of comparing variables within an

experiment, the main total effect does allow you to see the relative control the variables have on the output.

2.3.3 Factorial Design Example Revisited

Recall the example given in the previous section What is Factorial Design? In the example, there were two factors and two levels, which gave a 2^2 factorial design. The Yates Algorithm can be used in order to quantitatively determine which factor affects the percentage of seizures the most. For the use of the Yates algorithm, we will call age factor A with $a_1 = 20$ years, and $a_2 = 40$ years. Likewise, we will call dosage factor B, with $b_1 = 5$ mg, and $b_2 = 10$ mg. The data for the three outcomes is taken from the figures given in the example, assuming that the data given resulted from multiple trials.

Null Outcome

The following Yates algorithm table using the data for the null outcome was constructed. As seen in the table, the values of the main total factorial effect are 0 for A, B, and AB. This proves that neither dosage or age have any effect on percentage of seizures.

Combination	Total	Stage 1	Stage 2	Main Total Factorial Effect
a_1b_1	10	20	40	Doesn't Matter
a_2b_1	10	20	0	A
a_1b_2	10	0	0	B
a_2b_2	10	0	0	AB

Main Effect

The following Yates algorithm table using the data from the first two graphs of the main effects section was constructed. Besides the first row in the table, the row with the largest main total factorial effect is the B row, while the main total effect for A is 0. This means that dosage (factor B) affects the percentage of seizures, while age (factor A) has no effect, which is also what was seen graphically.

Combination	Total	Stage 1	Stage 2	Main Total Factorial Effect
a_1b_1	10	20	60	Doesn't Matter
a_2b_1	10	40	0	A
a_1b_2	20	0	20	B
a_2b_2	20	0	0	AB

The following Yates algorithm table using the data from second two graphs of the main effects section was constructed. Besides the first row in the table, the main total effect value was 10 for factor A and 20 for factor B. This means that both age and dosage affect percentage seizures. However, since the value for B is larger, dosage has a larger effect on percentage of seizures than age. This is what was seen graphically, since the graph with dosage on the horizontal axis has a slope with larger magnitude than the graph with age on the horizontal axis.

Combination	Total	Stage 1	Stage 2	Main Total Factorial Effect
a_1b_1	10	25	70	Doesn't Matter
a_2b_1	15	45	10	A
a_1b_2	20	5	20	B
a_2b_2	25	5	0	AB

Interaction Effect

The following Yates algorithm table was constructed using the data from the interaction effects section. Since the main total factorial effect for AB is non-zero, there are interaction effects. This means that it is impossible to correlate the results with either one factor or another; both factors must be taken into account.

Combination	Total	Stage 1	Stage 2	Main Total Factorial Effect
a_1b_1	10	25	65	Doesn't Matter
a_2b_1	15	40	-5	A
a_1b_2	25	5	15	B
a_2b_2	15	-10	-15	AB

2.4 Chemical Engineering Applications

It should be quite clear that factorial design can be easily integrated into a chemical engineering application. Many chemical engineers face problems at their jobs when dealing with how to determine the effects of various factors on their outputs. For example, suppose that you have a reactor and want to study the effect of temperature, concentration and pressure on multiple outputs. In order to minimize the number of experiments that you would have to perform, you can utilize factorial design. This will allow you to determine the effects of temperature and pressure while saving money on performing unnecessary experiments.

A 2007 study on converting wheat straw to fuel utilized factorial design to study the effect of four factors on the composition and susceptibility to enzyme hydrolysis of the

final product. (Perez, et.al.). The table below shows the full factorial design for the study. The four factors that were studied all had only two levels and dealt with pretreatment parameters. They were: Water temperature, residence time, solid fraction and overpressure in the reactor. It is not necessary to understand what each of these are to understand the experimental design. As seen in the table below, there were sixteen trials, or 2^4 experiments.

Table 1. Full factorial design conditions for Liquid Hot Water pretreatment of wheat straw

Full factorial design				
Run	A: Temp (°C)	B: Time (min)	C: Overpressure (bar)	D: Subs.loading (% w/w)
1	170	0	0	5
2	200	0	0	5
3	170	40	0	5
4	200	40	0	5
5	170	0	30	5
6	200	0	30	5
7	170	40	30	5
8	200	40	30	5
9	170	0	0	10
10	200	0	0	10
11	170	40	0	10
12	200	40	0	10
13	170	0	30	10
14	200	0	30	10
15	170	40	30	10
16	200	40	30	10

Source: Perez, et. al.

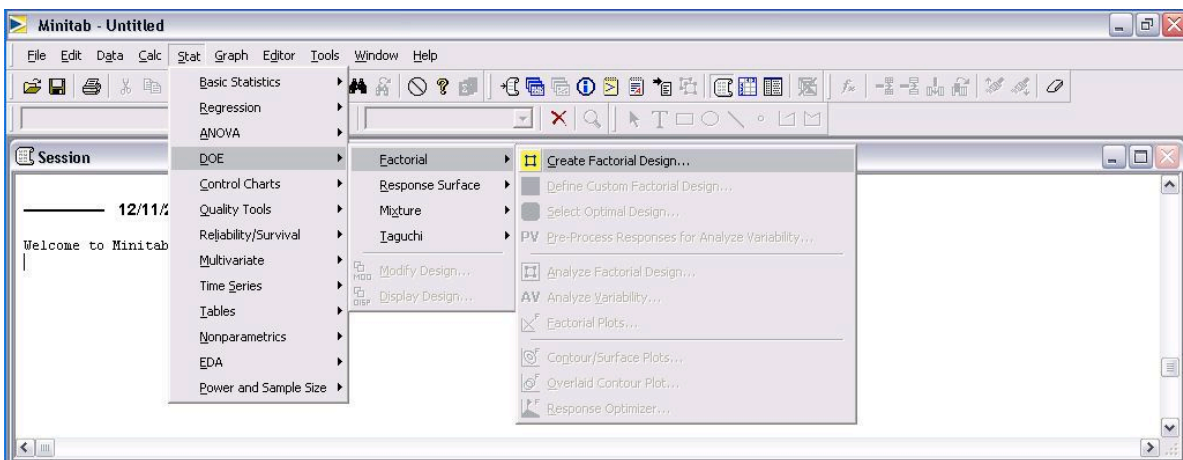
2.5 Minitab DOE Example

Minitab 15 Statistical Software is a powerful statistics program capable of performing regressions, ANOVA, control charts, DOE, and much more. Minitab is especially useful for creating and analyzing the results for DOE studies. It is possible to create factorial, response surface, mixture, and taguchi method DOEs in Minitab. The general method for creating factorial DOEs is discussed below.

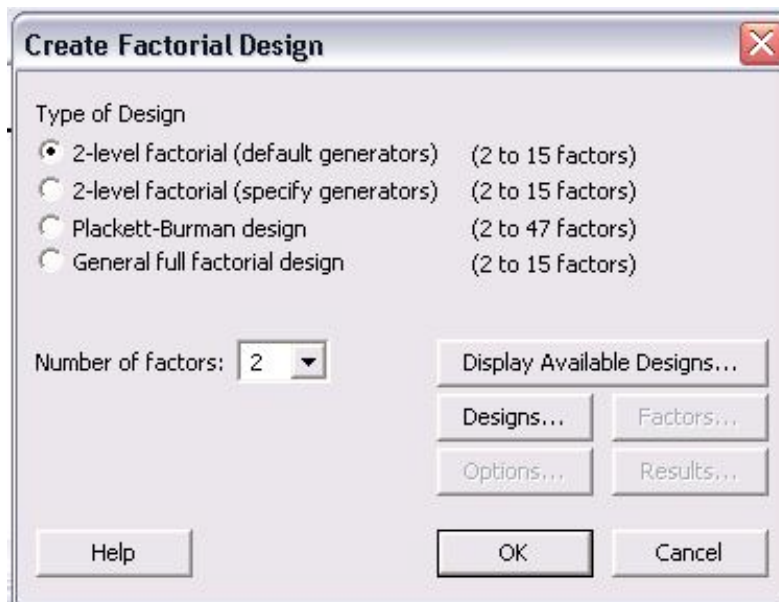
2.5.1 Creating Factorial DOE

Minitab provides a simple and user-friendly method to design a table of experiments. Additionally, analysis of multiple responses (results obtained from experimentation) to determine which parameters significantly affect the responses is easy to do with Minitab. Minitab 15 Statistical Software can be used via Virtual CAEN Labs by going to Start>All Programs>Math and Numerical Methods>Minitab Solutions>Minitab 15 Statistical Software.

The first step is creating the DOE by specifying the number of levels (typically 2) and number of responses. To do this, go to Stat>DOE>Factorial>Create Factorial Design as shown in the image below.

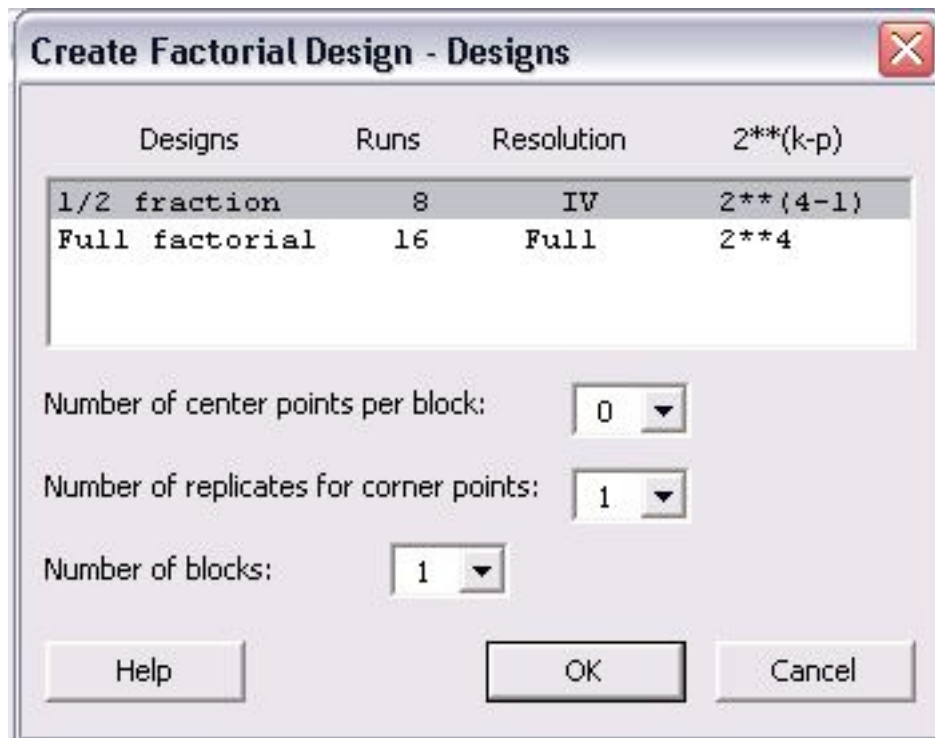


The next image is the "Create Factorial Design" options menu.



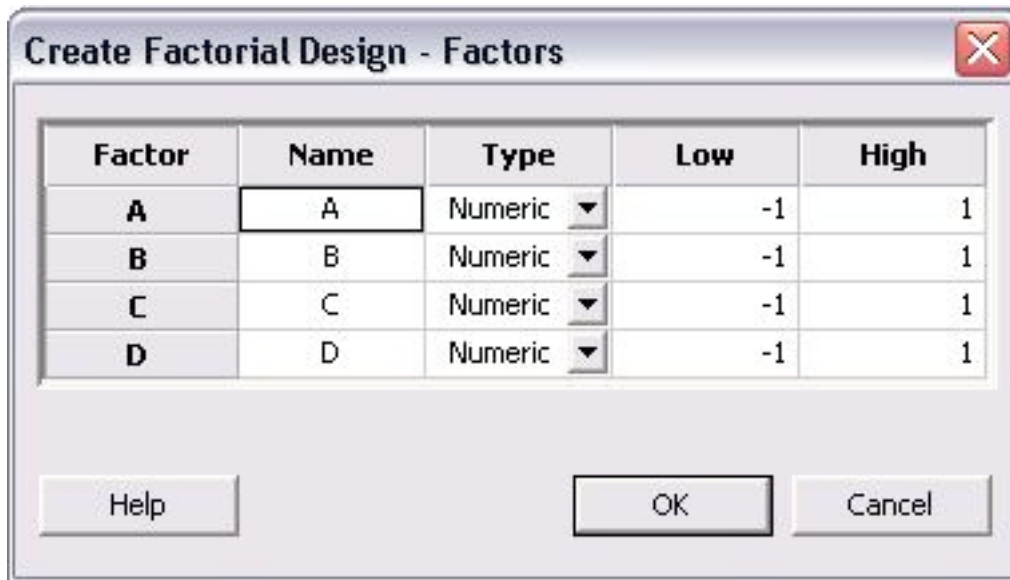
For a 2 level design, click the "2-level factorial (default generators)" radio button. Then specify the number of factors between 2 and 15. Other designs such as Plackett-Burman or a General full factorial design can be chosen. For information about these designs, please refer to the "Help" menu.

After the number of factors is chosen, click on the "Designs..." option to see the following menu.



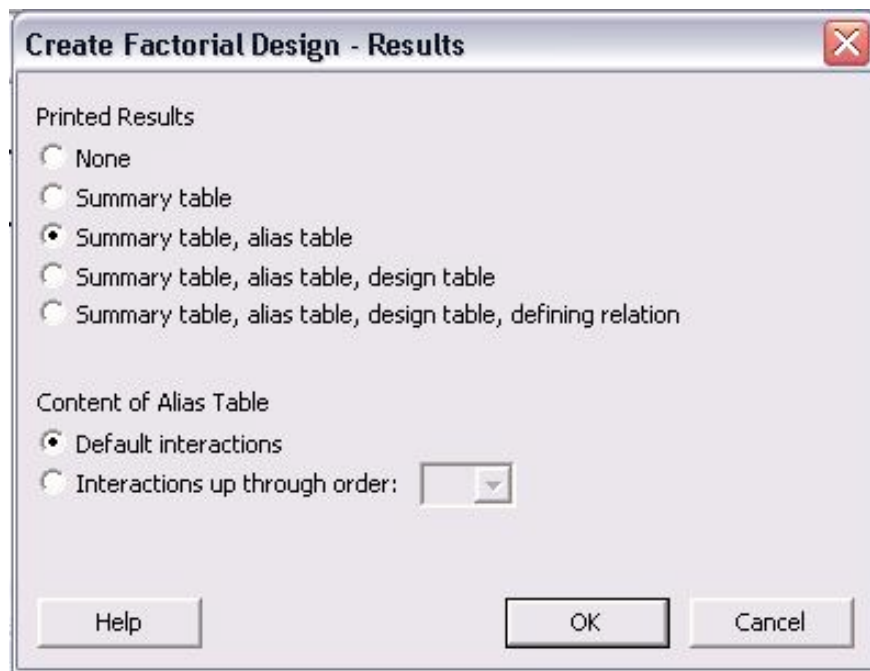
In this menu, a 1/2 fraction or full factorial design can be chosen. Although the full factorial provides better resolution and is a more complete analysis, the 1/2 fraction requires half the number of runs as the full factorial design. In lack of time or to get a general idea of the relationships, the 1/2 fraction design is a good choice. Additionally, the number of center points per block, number of replicates for corner points, and number of blocks can be chosen in this menu. Consult the "Help" menu for details about these options. Click "Ok" once the type of design has been chosen.

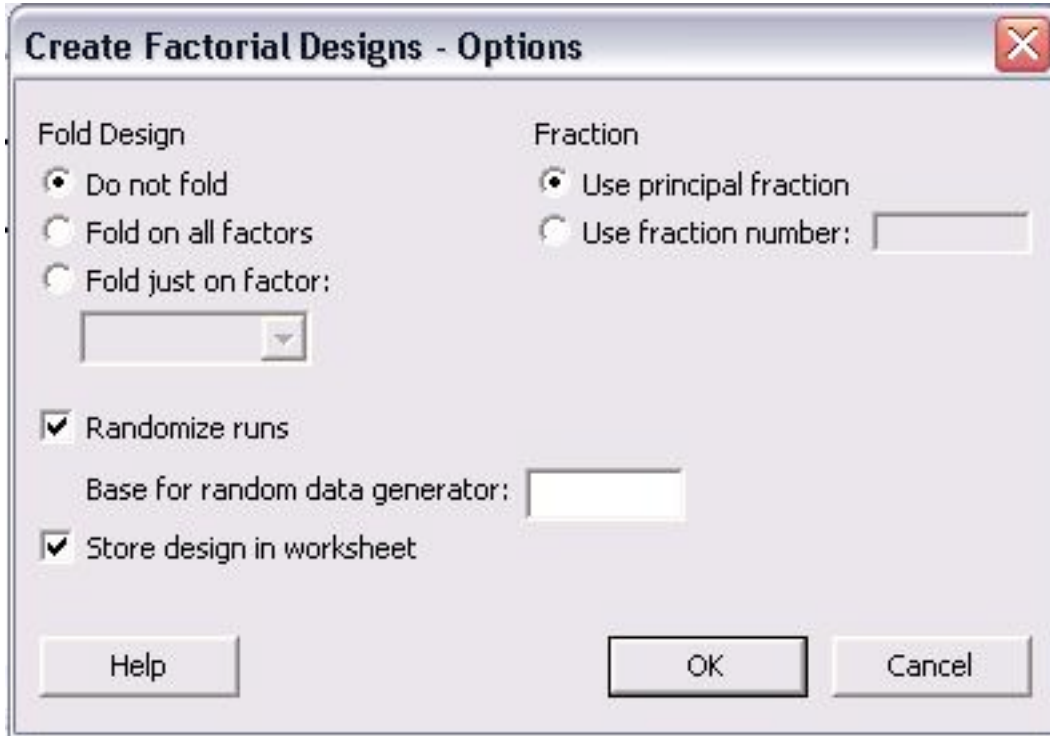
Once the design has been chosen, the "Factors...", "Options..." and "Results..." buttons become active in the "Create Factorial Designs" option menu. Click on "Factors..." button to see the following menu.



The above image is for a 4 factor design. Factors A - D can be renamed to represent the actual factors of the system. The factors can be numeric or text. Additionally, a low and high value are initially listed as -1 and 1, where -1 is the low and 1 is the high value. The low and high levels for each factor can be changed to their actual values in this menu. Click "OK" once this is completed.

The necessary steps for creating the DOE are complete, but other options for "Results..." and "Options..." can be specified. The menus for "Results..." and "Options..." are shown below.





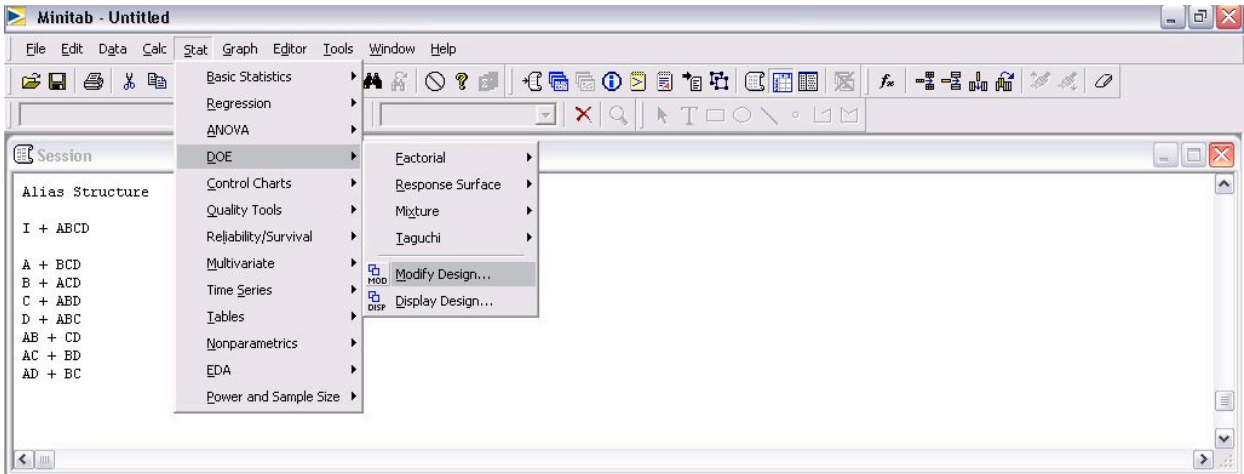
In the main "Create Factorial Design" menu, click "OK" once all specifications are complete. The following table is obtained for a 2-level, 4 factor, full factorial design. None of the levels were specified as they appear as -1 and 1 for low and high levels, respectively.

	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10
	StdOrder	RunOrder	CenterPt	Blocks	A	B	C	D		
1	11	1	1	1	-1	1	-1	1		
2	6	2	1	1	1	-1	1	-1		
3	2	3	1	1	1	-1	-1	-1		
4	16	4	1	1	1	1	1	1		
5	5	5	1	1	-1	-1	1	-1		
6	4	6	1	1	1	1	-1	-1		
7	1	7	1	1	-1	-1	-1	-1		
8	13	8	1	1	-1	-1	1	1		
9	15	9	1	1	-1	1	1	1		
10	12	10	1	1	1	1	-1	1		
11	3	11	1	1	-1	1	-1	-1		
12	7	12	1	1	-1	1	1	-1		
13	14	13	1	1	1	-1	1	1		
14	10	14	1	1	1	-1	-1	1		
15	8	15	1	1	1	1	1	-1		
16	9	16	1	1	-1	-1	-1	1		
17										

The above table contains all the conditions required for a full factorial DOE. Minitab displays the standard order and randomized run order in columns C1 and C2, respectively. Columns A-D are the factors. The first run (as specified by the random run order) should be performed at the low levels of A and C and the high levels of B and D. A total of 16 runs are required to complete the DOE.

2.5.2 Modifying DOE Table

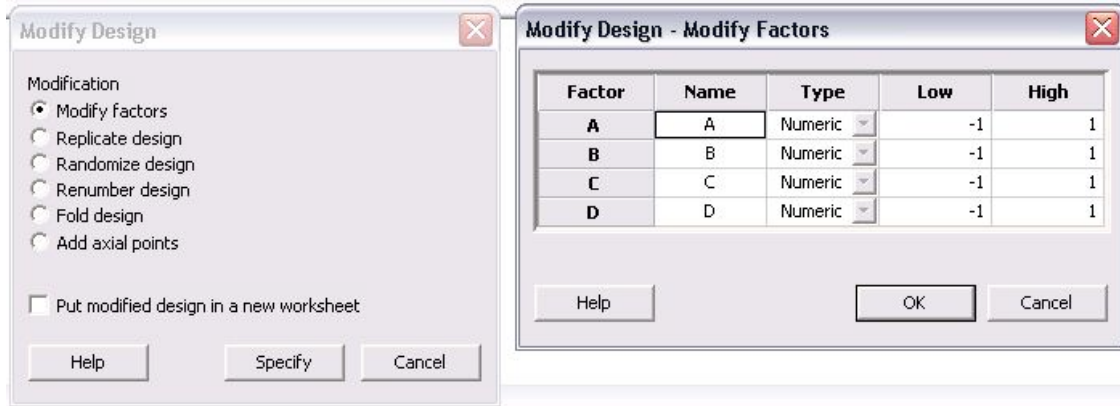
Once a table of trials for the DOE has been created, additional modifications can be made as needed. Some typical modifications include modifying the name of each factors, specifying the high and low level of each factor, and adding replicates to the design. To being modifications of a current design, go to Stat>DOE>Modify Design... as seen in the figure below.



The following menu is displayed for modifying the design.

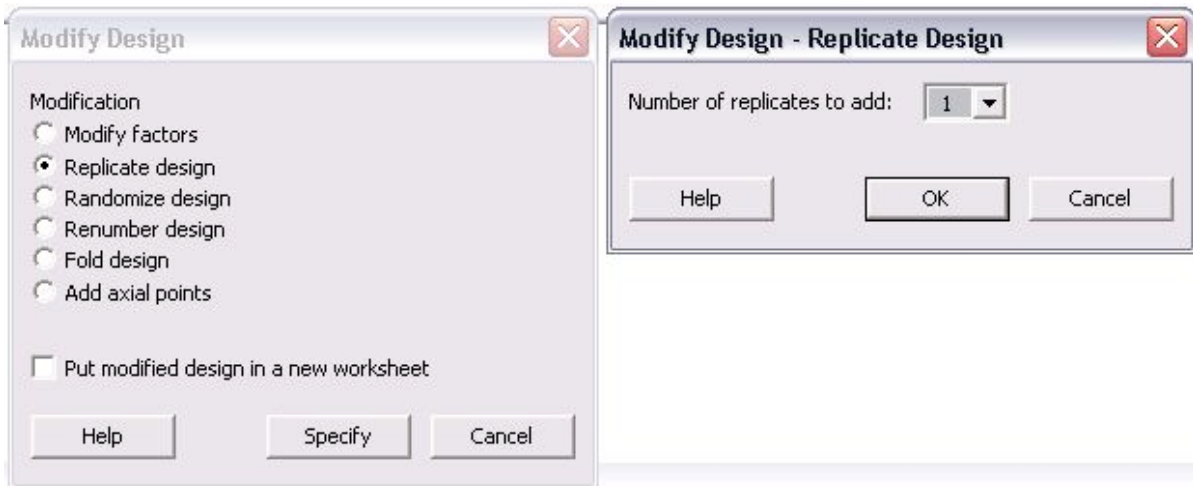


In the "Modify Design" menu, users can modify factors, replicate design, randomize design, renumber design, fold design, and add axial points. Additionally, any changes made can be put into a new worksheet. To change the factors, click the "Modify factors" radio button and then "Specify" to see the following options menu.



The default factors are named "A", "B", "C", and "D" and have respective high and low levels of 1 and -1. The name of the factors can be changed by simply clicking in the box and typing a new name. Additionally, the low and high levels for each factor can be modified in this menu. Since the high and low levels for each factor may not be known when the design is first created, it is convenient to be able to define them later. Click "OK" after modifications are complete.

Another typical modification is adding replicates to a design. Replicates are repeats of each trial that help determine the reproducibility of the design, thus increasing the number of trials and accuracy of the DOE. To add replicates, click the "Replicate design" radio button in the "Modify Design" menu. The following menu will be displayed.



The only option in this menu is the number of replicates to add. The number ranges between 1 and 10. To have a total of 3 trials of each, the user should add 2 replicates in this menu. If 4 replicates are added, there will be a total of 5 trials of each. Typically, if the same experimentation will occur for 3 lab periods, 2 replicates will be added.

Additional modifications to the design include randomizing and renumbering the design. These are very straightforward modifications which affect the ordering of the trials. For information about the "Fold design" and "Add axial points", consult the "Help" menu.

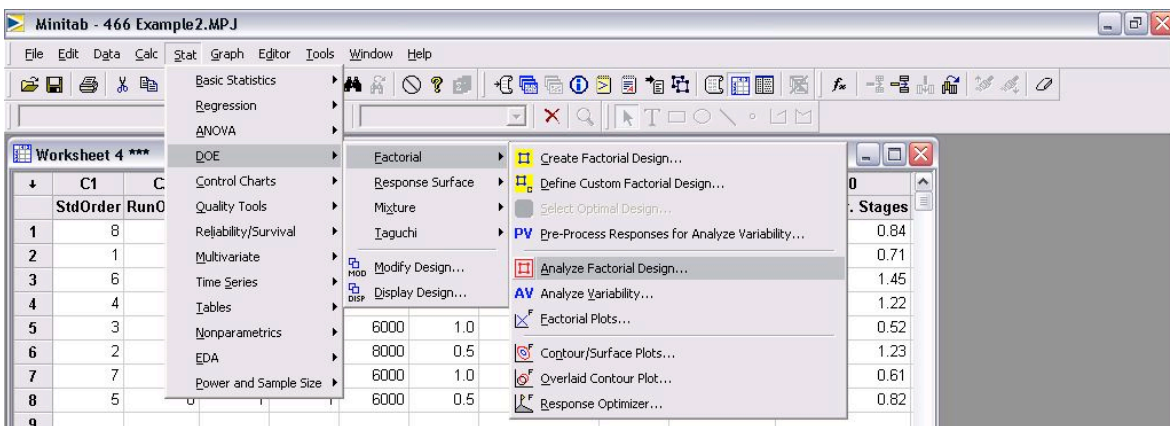
2.5.3 Analyzing DOE Results

After the complete DOE study has been performed, Minitab can be used to analyze the effect of experimental results (referred to as responses) on the factors specified in the design. The first step in analyzing the results is entering the responses into the DOE table. This is done much like adding data into an Excel data sheet. In the columns to the right of the last factor, enter each response as seen in the figure below.

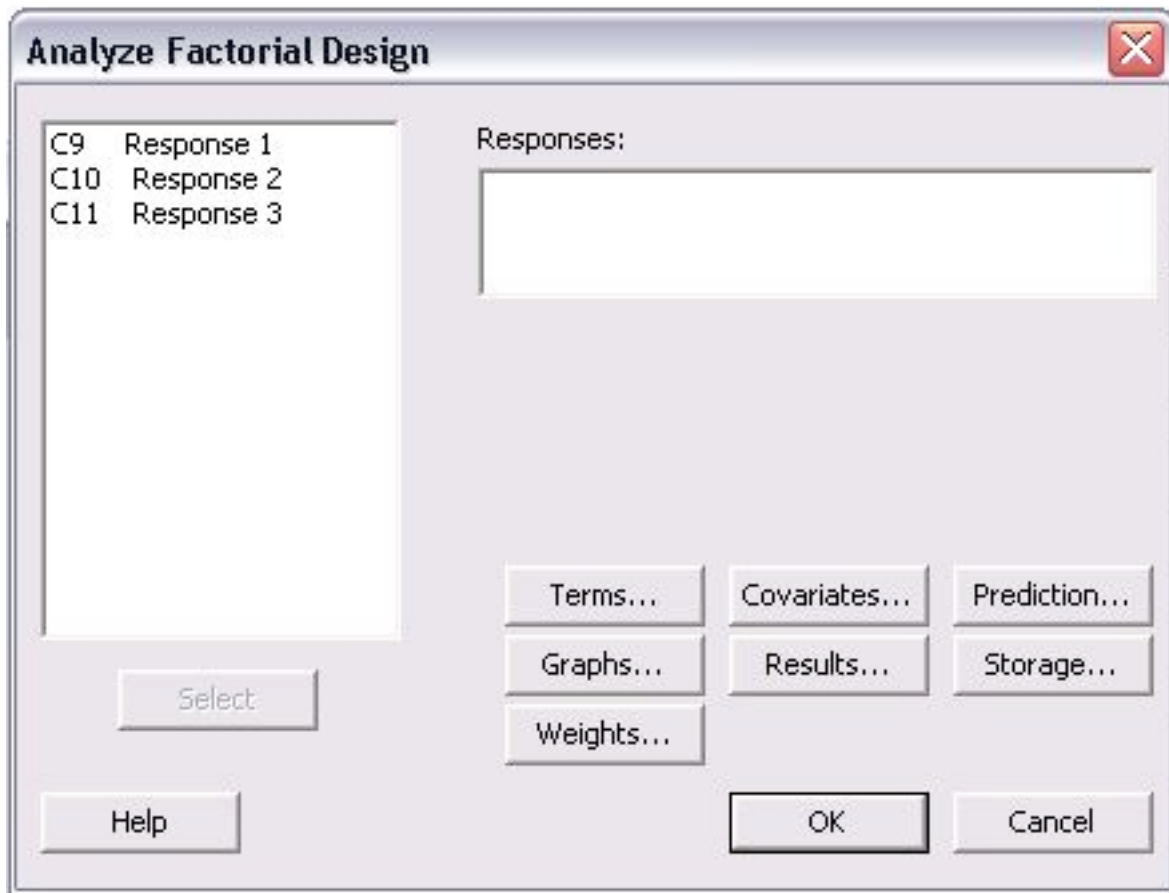
	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15
	StdOrder	RunOrder	CenterPt	Blocks	A	B	C	D	Response 1	Response 2	Response 3				
1	6	1	1	1	1	-1	1	-1							
2	13	2	1	1	-1	-1	1	1							
3	1	3	1	1	-1	-1	-1	-1							
4	5	4	1	1	-1	-1	1	1							
5	9	5	1	1	-1	-1	-1	-1							
6	14	6	1	1	1	-1	1	-1							
7	7	7	1	1	-1	1	1	1							
8	10	8	1	1	1	-1	-1	1							
9	2	9	1	1	1	-1	-1	1							
10	4	10	1	1	1	1	-1	-1							
11	8	11	1	1	1	1	1	1							
12	16	12	1	1	1	1	1	1							
13	3	13	1	1	-1	1	-1	1							
14	11	14	1	1	-1	1	-1	1							
15	15	15	1	1	-1	1	1	1							
16	12	16	1	1	1	1	-1	-1							

The above figure contains three response columns. The names of each response can be changed by clicking on the column name and entering the desired name. In the figure, the area selected in black is where the responses will be inputted. For instance, if the purity, yield, and residual amount of catalyst was measured in the DOE study, the values of these for each trial would be entered in the columns.

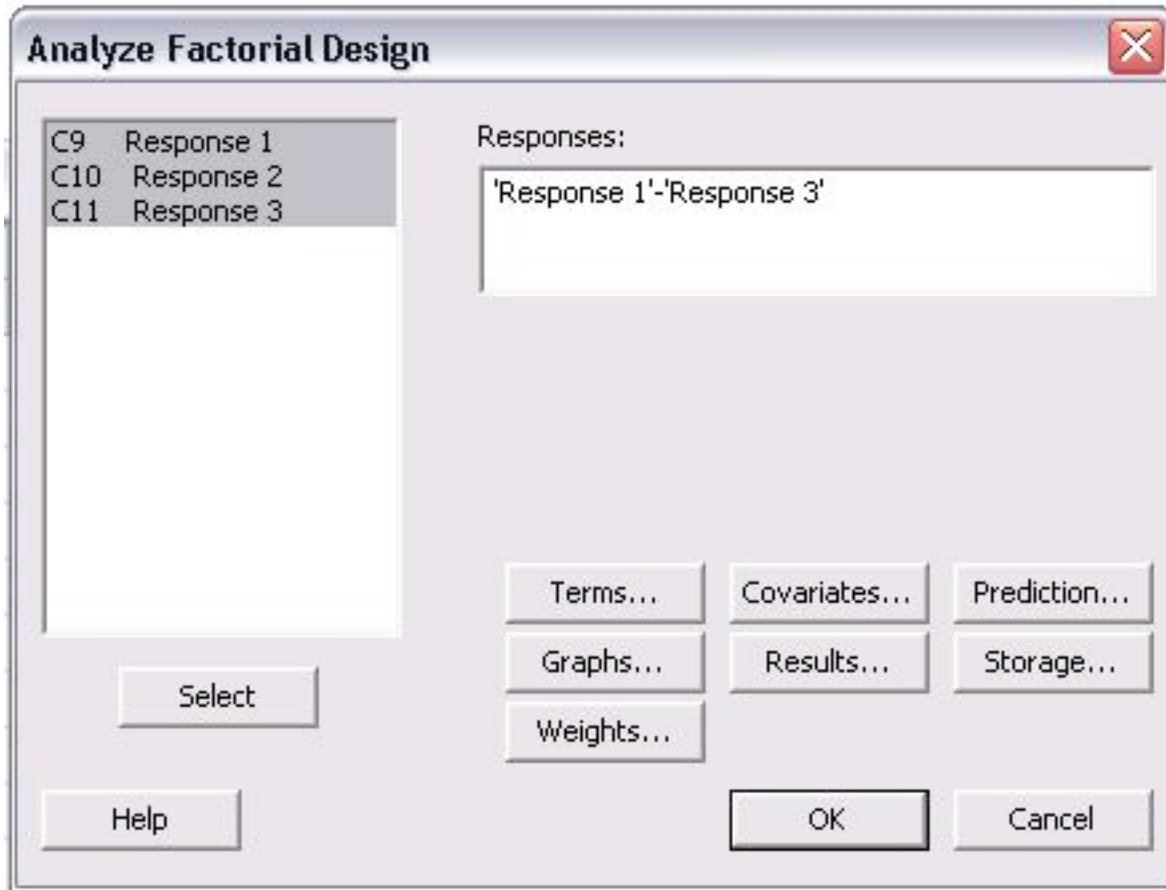
Once the responses are entered, statistical analysis on the data can be performed. Go to Stat>DOE>Factorial>Analyze Factorial Design... as seen in the following image.



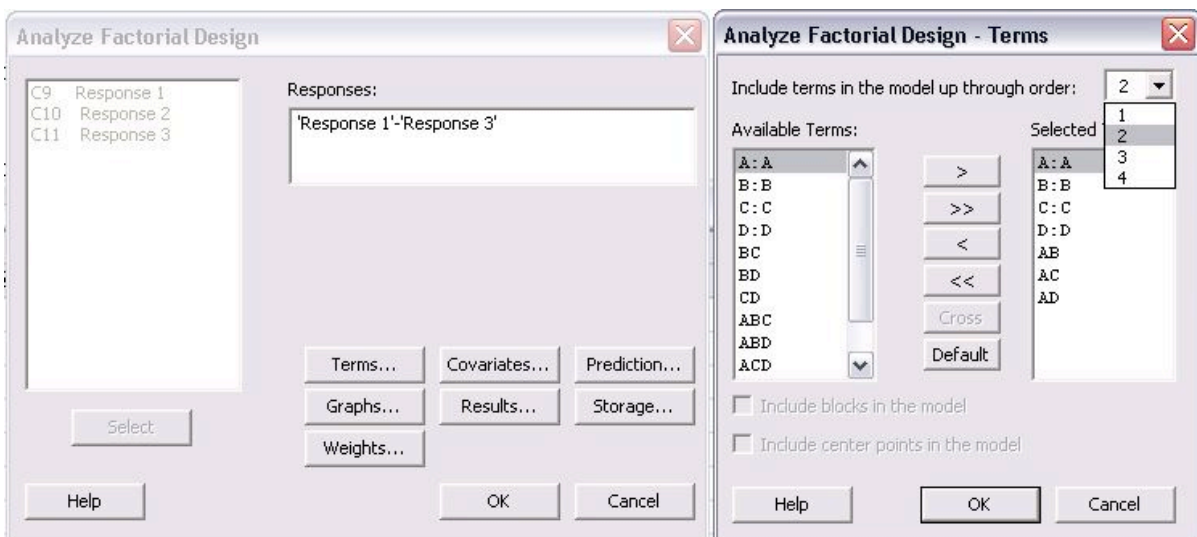
The menu that appears for analyzing factorial design is shown below.



In the "Analyze Factorial Design" menu, the responses are shown on the left of the screen. The first step is to choose the responses to be analyzed. All of the responses can be chosen at once or individually. To choose them, click (or click and drag to select many) and then click "Select" to add them into the "Responses:" section as seen below.



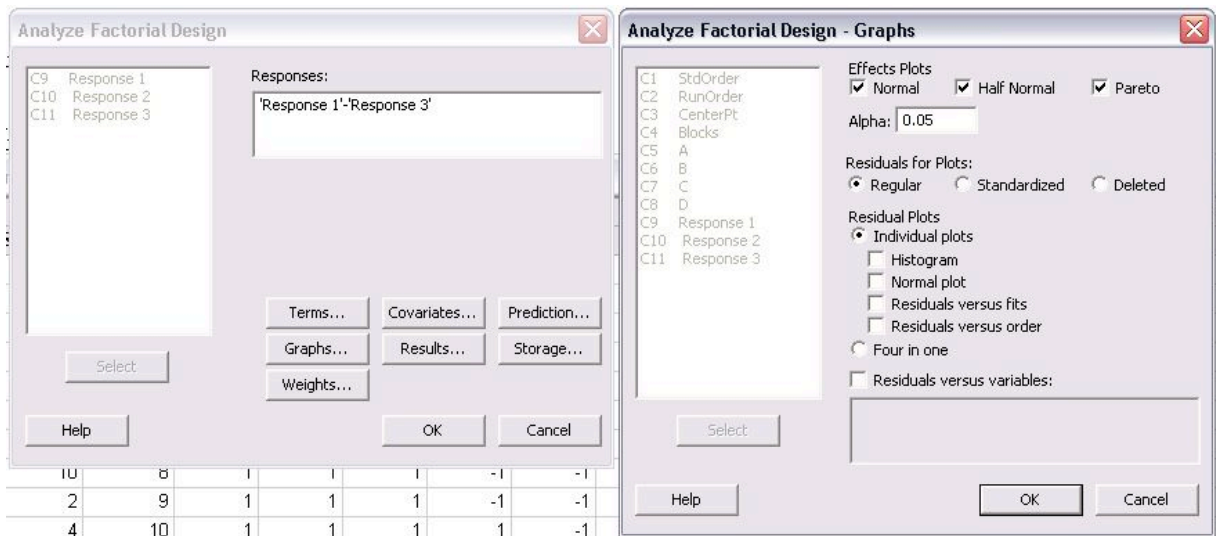
The next step is selecting which terms will be analyzed for the responses. To do this, click on "Terms..." and the following menu will appear.



The types of interactions between factors are chosen in this menu. For a first order model which excludes all factor-to-factor interactions, "1" should be chosen from the drop-down

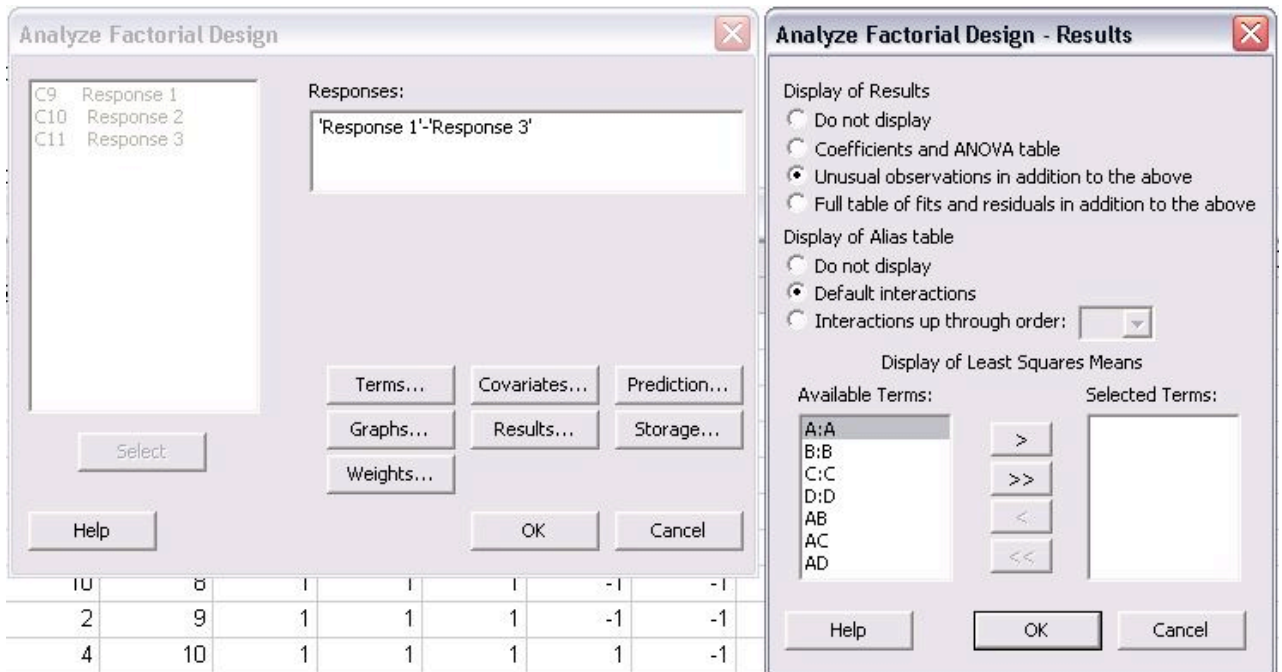
menu for "Include terms in the model up through order:". To include higher order terms and account for factor interactions, choose 2, 3, or 4 from the drop-down menu. Unless significant factor-to-factor interactions are expected, it is recommended to use a first order model which is a linear approximation.

Once the terms have been chosen, the next step is determining which graphs should be created. The types of graphs can be selected by clicking on "Graphs..." in the main "Analyze Factorial Design" menu.



In the Graphs menu shown above, the three effects plots for "Normal", "Half Normal", and "Pareto" were selected. These plots are different ways to present the statistical results of the analysis. Examples of these plots can be found in the Minitab Example for Centrifugal Contactor Analysis. The alpha value, which determines the limit of statistical significance, can be chosen in this menu also. Typically, the alpha value is 0.05. The last type of plots that can be chosen is residual plots. A common one to select is "Residuals versus fits" which shows how the variance between the predicted values from the model and the actual values.

The final option that must be specified is results. Click "Results..." from the "Analyze Factorial Design" menu to see the following screen.



In this menu, select all of the "Available Terms" and click the ">>" button to move them to the "Selected Terms". This will ensure that all the terms will be included in the analysis. Another feature that can be selected from this menu is to display the "Coefficients and ANOVA table" for the DOE study.

Other options can be selected from the "Analyze Factorial Design" menu such as "Covariates...", "Prediction...", "Storage...", and "Weights...". Consult the "Help" menu for descriptions of the other options. Once all desired changes have been made, click "OK" to perform the analysis. All of the plots will pop-up on the screen and a text file of the results will be generated in the session file.

2.5.4 Minitab Example for Centrifugal Contactor Analysis

Centrifugal Contactors, also known as Podbielniak (POD) centrifugal contactors, are used to purify a contaminated stream by counter-current, liquid-liquid extraction. Two immiscible fluids with different specific gravities are contacted counter-currently and the solute from the dirty stream is extracted by the clean stream. A common use for PODs methanol removal from biodiesel by contacting the stream with water. The amount of methanol remaining in the biodiesel (wt% MeOH) after the purification and the number of theoretical stages (No. Theor. Stages) obtained depend on the operating conditions of the POD. The four main operating parameters of the POD are rotational speed (RPM), ratio of biodiesel to water (Ratio), total flow rate of biodiesel and water (Flow Rate), and pressure (Pressure). A DOE study has been performed to determine the effect of the four operating conditions on the responses of wt% MeOH in biodiesel and number of theoretical stages achieved. (NOTE: The actual data for this example was made-up)

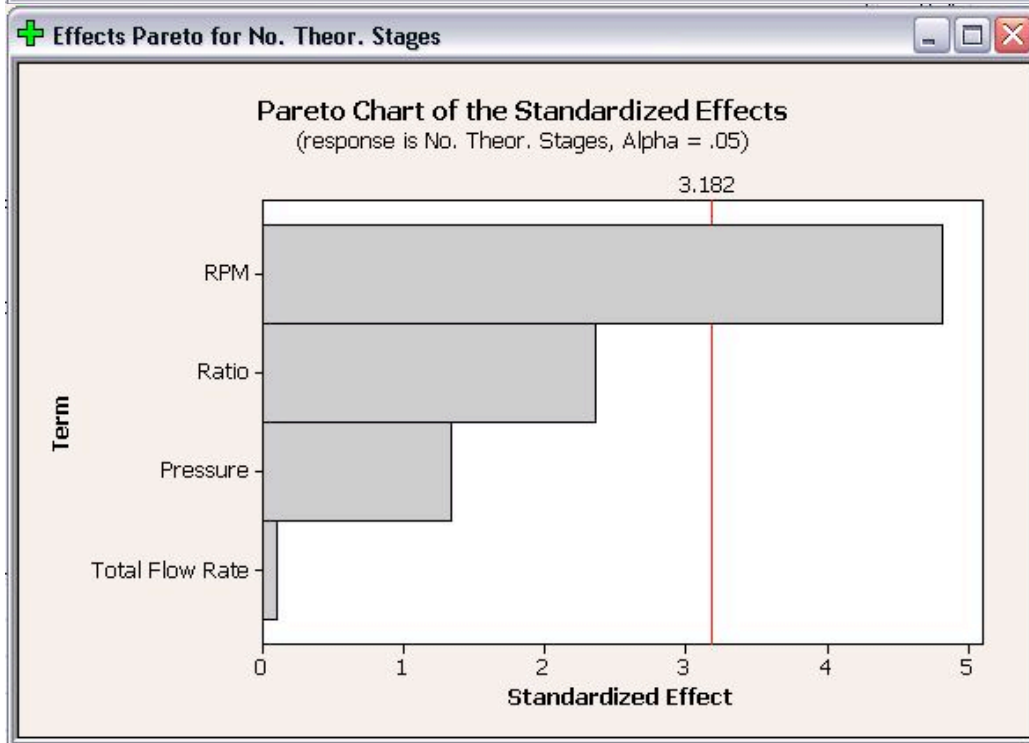
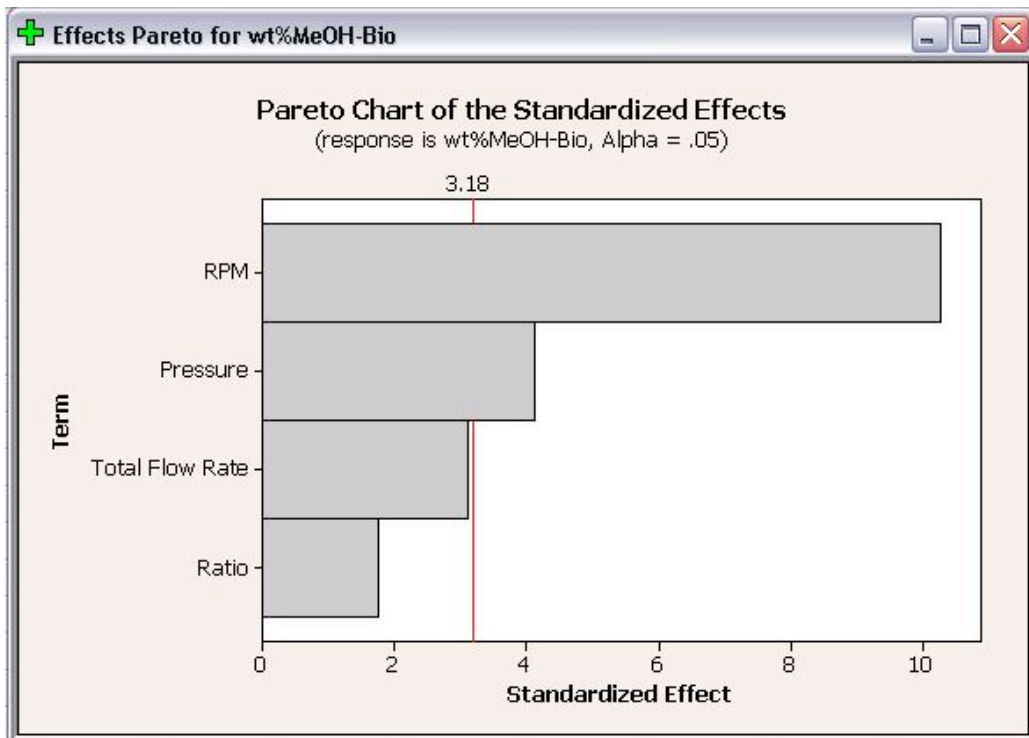
A 4-factor, 2-level DOE study was created using Minitab. Because experiments from the POD are time consuming, a half fraction design of 8 trial was used. The figure below contains the table of trials for the DOE.

	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16
	StdOrder	RunOrder	CenterPt	Blocks	RPM	Ratio	Pressure	Flow Rate								
1	1	1	1	1	6000	0.5	15	400								
2	5	2	1	1	6000	0.5	25	800								
3	3	3	1	1	6000	1.0	15	800								
4	7	4	1	1	6000	1.0	25	400								
5	2	5	1	1	8000	0.5	15	800								
6	4	6	1	1	8000	1.0	15	400								
7	6	7	1	1	8000	0.5	25	400								
8	8	8	1	1	8000	1.0	25	800								

After all the trials were performed, the wt% methanol remaining in the biodiesel and number of theoretical stages achieved were calculated. The figure below contains the DOE table of trials including the two responses.

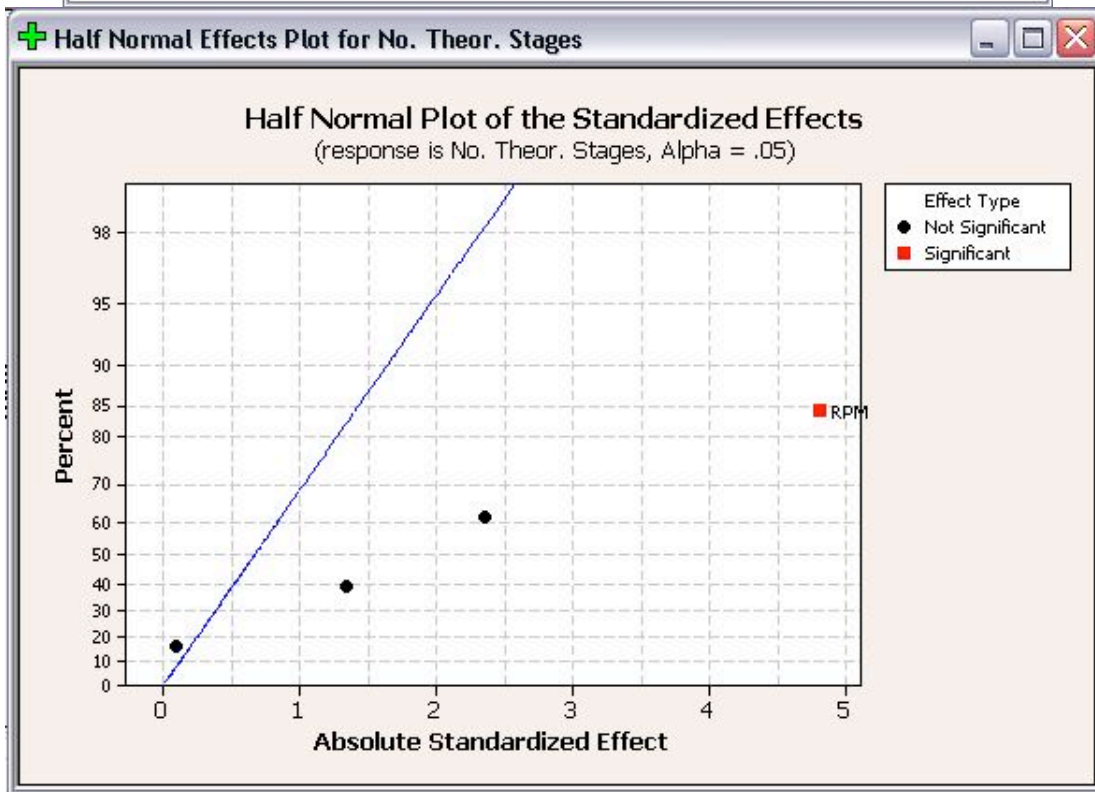
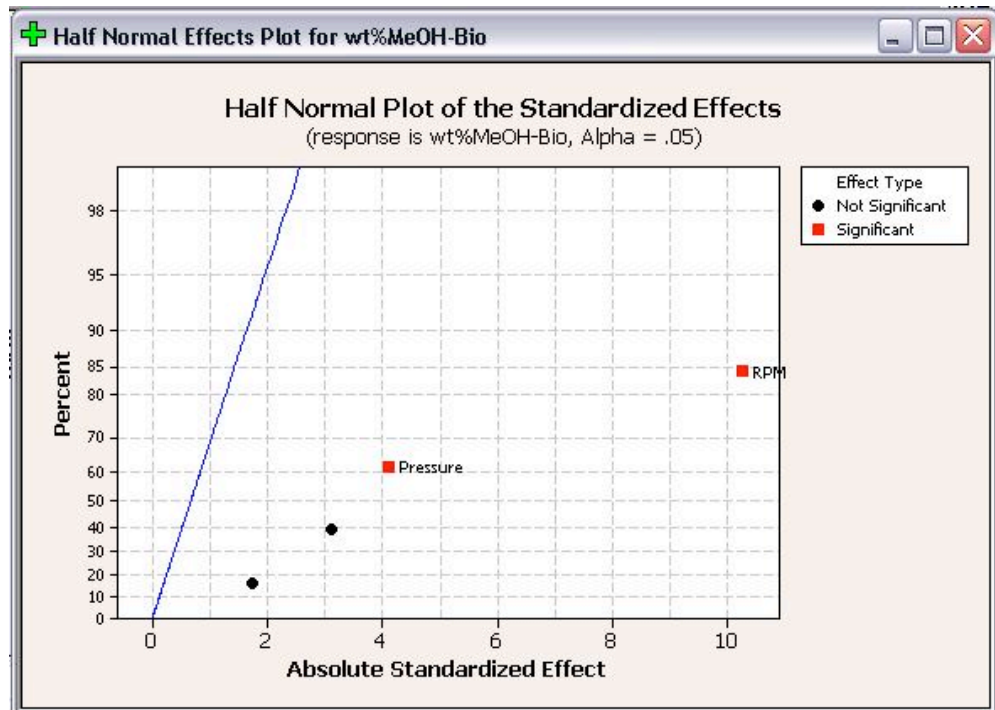
	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10
	StdOrder	RunOrder	CenterPt	Blocks	RPM	Ratio	Total Flow Rate	Pressure	wt%MeOH-Bio	No. Theor. Stages
1	8	1	1	1	8000	1.0	800	25	0.34	0.84
2	1	2	1	1	6000	0.5	400	15	0.44	0.71
3	6	3	1	1	8000	0.5	800	15	0.26	1.45
4	4	4	1	1	8000	1.0	400	15	0.20	1.22
5	3	5	1	1	6000	1.0	400	25	0.47	0.52
6	2	6	1	1	8000	0.5	400	25	0.28	1.23
7	7	7	1	1	6000	1.0	800	15	0.44	0.61
8	5	8	1	1	6000	0.5	800	25	0.61	0.82

Analysis was performed on the DOE study to determine the effects of each factor on the responses. Only first order terms were included in the analysis to create a linear model. Pareto charts for both wt% MeOH in biodiesel and number of theoretical stages are shown below.



The Pareto charts show which factors have statistically significant effects on the responses. As seen in the above plots, RPM has significant effects for both responses and pressure has a statistically significant effect on wt% methanol in biodiesel. Neither flow rate or ratio have statistically significant effects on either response. The Pareto charts are bar charts which allow users to easily see which factors have significant effects.

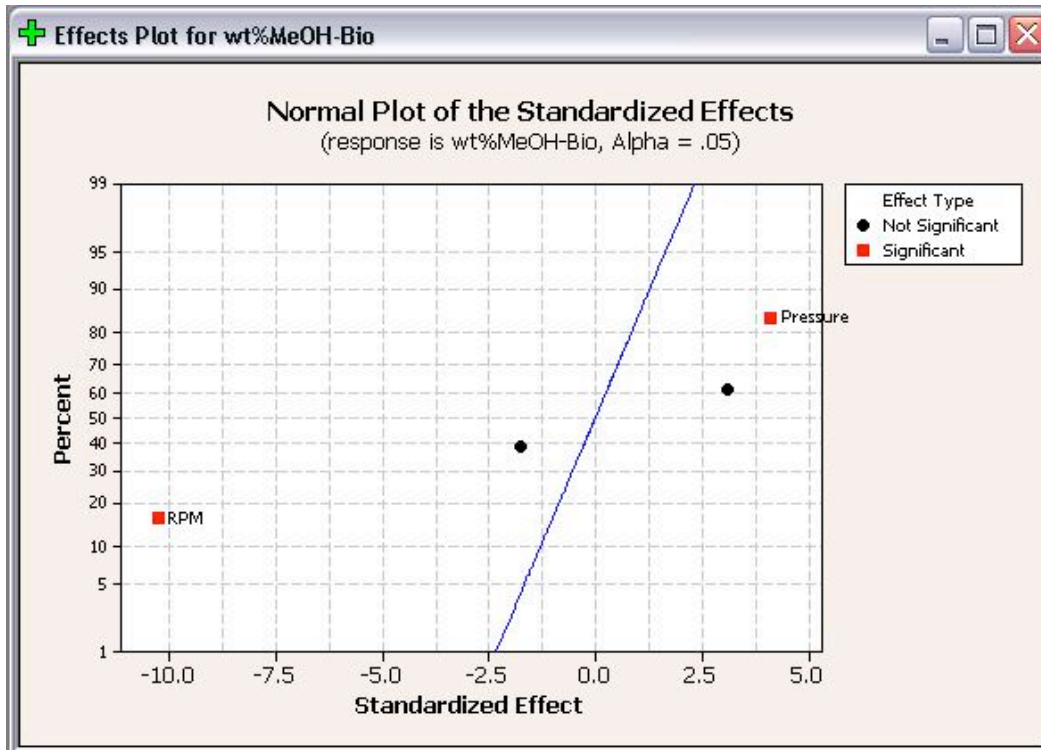
Half Normal Plots for wt% methanol in biodiesel and number of theoretical stages are shown below.

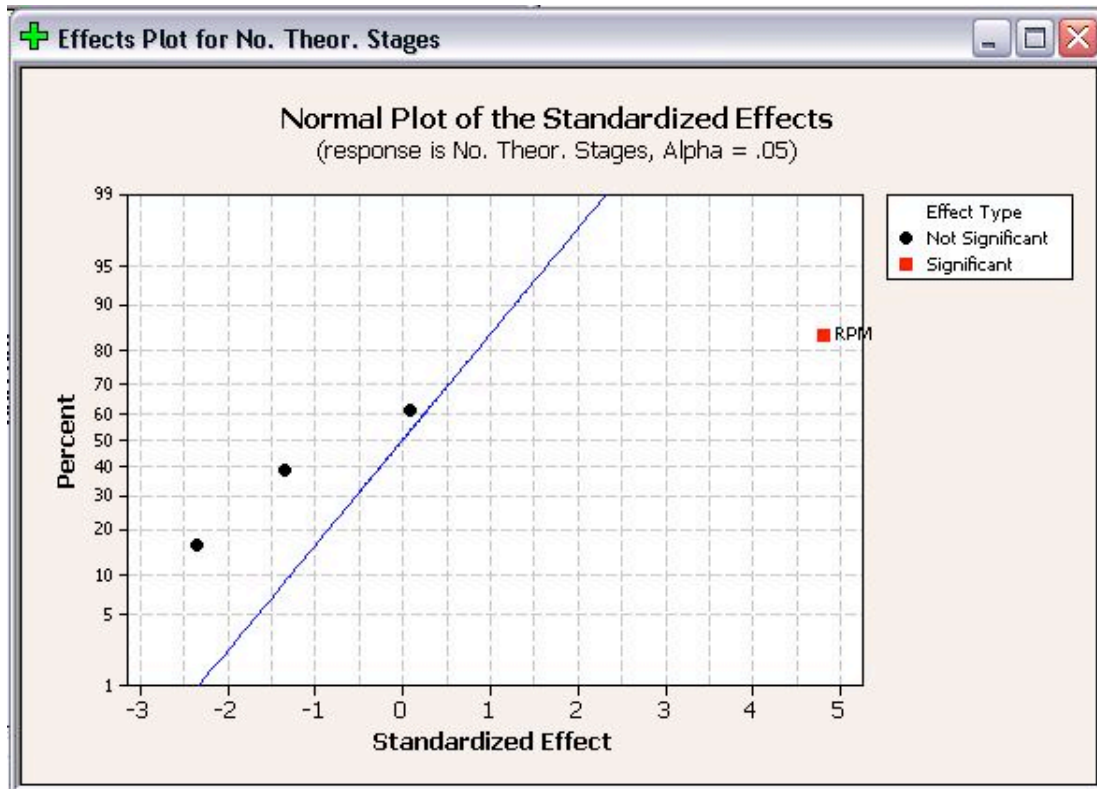


Like Pareto plots, Half Normal plots show which factors have significant effects on the responses. The factors that have significant effects are shown in red and the ones without

significant effects are shown in black. The further a factor is from the blue line, the more significant effect it has on the corresponding response. For wt% methanol in biodiesel, RPM is further from the blue line than pressure, which indicates that RPM has a more significant effect on wt% methanol in biodiesel than pressure does.

The final plot created is the Normal Effect Plot. The Normal Plot is similar to the Half Normal plot in design. However, the Normal Plot displays whether the effect of the factor is positive or negative on the response. The Normal Plots for the responses are shown below.





As seen above, RPM is shown with a positive effect for number of theoretical stages, but a negative effect for wt% methanol in biodiesel. A positive effect means that as RPM increases, the number of theoretical stages increases. Whereas a negative effect indicates that as RPM increases, the wt% methanol in biodiesel decreases. Fortunately for operation with the POD, these are desired results. When choosing operating conditions for the POD, RPM should be maximized to minimize the residual methanol in biodiesel and maximize the number of theoretical stages achieved.

In addition to the above effects plots, Minitab calculates the coefficients and constants for response equations. The response equations can be used as models for predicting responses at different operating conditions (factors). The coefficients and constants for wt% methanol in biodiesel and number of theoretical stages are shown below.

Estimated Coefficients for wt%MeOH-Bio using data in uncoded units

Term	Coef
Constant	0.926833
RPM	-1.09592E-04
Ratio	-0.0748768
Total Flow Rate	0.000165648
Pressure	0.00879626

Estimated Coefficients for No. Theor. Stages using data in uncoded units

Term	Coef
Constant	-0.239346
RPM	0.000260115
Ratio	-0.509538
Total Flow Rate	0.000025577
Pressure	-0.0144769

Since this is a first order, linear model, the coefficients can be combined with the operating parameters to determine equations. The equations from this model are shown below.

$$wt\%MeOH = 0.927 - 1.096 \cdot 10^{-4}(RPM) - 0.075(Ratio) + 1.656 \cdot 10^{-4}(FlowRate) + 8.796 \cdot 10^{-3}(Pressure)$$

$$NoStages = -0.239 + 2.601 \cdot 10^{-4}(RPM) - 0.510(Ratio) + 2.558 \cdot 10^{-5}(FlowRate) - 0.014(Pressure)$$

These equations can be used as a predictive model to determine wt% methanol in biodiesel and number of theoretical stages achieved at different operating conditions without actually performing the experiments. However, the limits of the model should be tested before the model is used to predict responses at many different operating conditions.

2.6 Worked out Example 1

You have been employed by SuperGym, a local personal training gym, who want an engineer's perspective on how to offer the best plans to their clients. SuperGym currently catagorizes her clients into 4 body types to help plan for the best possible program.

- Type 1 - Very healthy
- Type 2 - Needs tone
- Type 3 - Needs strength
- Type 4 - Needs tone and strength

In addition, SuperGym offers 4 different workout plans, A through D, none of which are directly catered to any of the different types. Create an experimental factorial design that could be used to test the effects of the different workout plans on the different types of people at the gym.

2.6.1 Solution to Example 1

In order to solve this problem, we need to determine how many different experiments would need to be performed. In order to solve this, we can see that we have two different factors, body type and workout plan. For each factor, there exist four different levels. Thus, we have a 4^2 factorial design, which gives us 16 different experimental groups. Creating a table of all of the different groups, we arrive at the following factorial design:

Solution			
A1	B1	C1	D1
A2	B2	C2	D2
A3	B3	C3	D3
A4	B4	C4	D4

Where A-D is the workout plan and 1-4 is the types

2.7 Worked out Example 2

Suppose that you are looking to study the effects of hours slept (A), hours spent with significant other (B), and hours spent studying (C) on a students exam scores. You are given the following table that relates the combination of these factors and the students scores over the course of a semester. Use the Yates method in order to determine the effect each variable on the students performance in the course.

Given Information								
Trials	a₁b₁c₁	a₂b₁c₁	a₁b₂c₁	a₂b₂c₁	a₁b₁c₂	a₂b₁c₂	a₁b₂c₂	a₂b₂c₂
1	17	24	19	21	22	28	25	24
2	18.5	21	20	19	26	22	27	19
3	16.5	22.5	22	25	24	26	21	20
Total	52	67.5	61	65	72	76	73	63

2.7.1 Solution to Example 2

Using the approach introduced earlier in this article, we arrive at the following Yates solution.

Solution					
			Stage		Main Total
Combination	Total	1	2	3	Factorial Effect
a₁b₁c₁	52	119.5	245.5	529.9	Doesn't matter

a₂b₁c₁	67.5	126	284	13.5	A
a₁b₂c₁	61	148	19.5	-5.5	B
a₂b₂c₁	65	136	-6	-25.5	AB
a₁b₁c₂	72	15.5	6.5	38.5	C
a₂b₁c₂	76	4	-12	-25.5	AC
a₁b₂c₂	73	4	-11.5	-18.5	BC
a₂b₂c₂	63	-10	-14	-2.5	ABC

From this table, we can see that there is positive correlation for factors A and C, meaning that more sleep and more studying leads to a better test grade in the class. Factor B, however, has a negative effect, which means that spending time with your significant other leads to a worse test score. The lesson here, therefore, is to spend more time sleeping and studying, and less time with your boyfriend or girlfriend.

2.8 Worked out Example 3

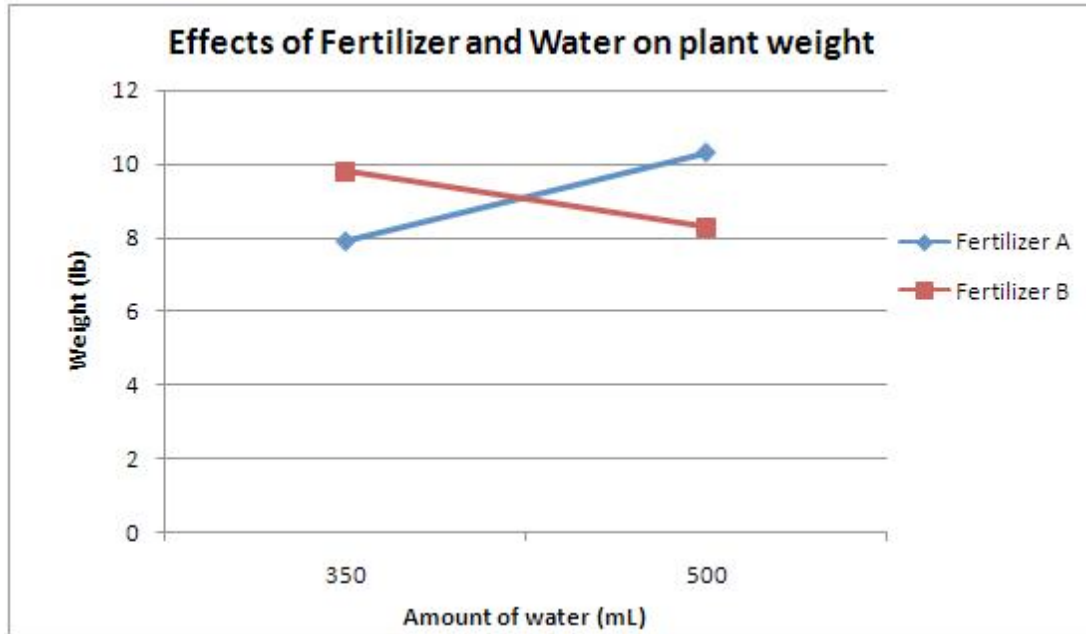
Your mom is growing a garden for the state fair and has done some experiments to find the ideal growing condition for her vegetables. She asks you for help interpreting the results and shows you the following data:

Plant No.	Fertilizer Type	Amount of water (mL)	Weight (lb)
1	A	350	7.9
2	B	350	9.8
3	A	500	10.3
4	B	500	8.3

Make plots to determine the main or interaction effects of each factor.

2.8.1 Solution to Example 3

Here is the plot you should have gotten for the given data.



From this one can see that there is an interaction effect since the lines cross. One cannot discuss the results without speaking about both the type of fertilizer and the amount of water used. Using fertilizer A and 500 mL of water resulted in the largest plant, while fertilizer A and 350 mL gave the smallest plant. Fertilizer B and 350 mL gave the second largest plant, and fertilizer B and 500 mL gave the second smallest plant. There is clearly an interaction due to the amount of water used and the fertilizer present. Perhaps each fertilizer is most effective with a certain amount of water. In any case, your mom has to consider both the fertilizer type and amount of water provided to the plants when determining the proper growing conditions.

2.9 Multiple Choice Question 1

Which of the following is not an advantage of the use of factorial design over one factor design?

- A. More time efficient
- B. Provides how each factor effects the response
- C. Does not require explicit testing
- D. Does not require regression

2.10 Multiple Choice Question 2

In a 2^2 factorial design experiment, a total main effect value of -5 is obtained. This means that

- A. there is a relative positive correlation between the two factors
- B. there is no correlation between the two factors
- C. there is a relative negative correlation between the two factors
- D. there is either a positive or negative relative correlation between the two factors

2.11 Sage's Corner

Factorial design, a method to prove OSU stupidity:

<http://video.google.com/googleplayer.swf?docId=5869605763016344026>
(we are currently working on fixing the 1 slide which is missing narration)

A copy of the slides without narration can be found here:

[File:Yates proves OSU stupidity test.ppt](#)

2.12 References

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Section 3. Design of experiments via random design

3.1 Introduction

Random design is an approach to designing experiments. As the name implies, random experimental design involves randomly assigning experimental conditions. However, numbers should not be picked without any thought. This type of experimental design is surprisingly powerful and often results in a high probability to create a near optimal design.

The simplified steps for random design include the following:

1. Choose a number of experiments to run (NOTE: This may be tricky to pick a number because it is dependent upon the amount of signal recovery you want.)
2. Assign to each variable a state based on a uniform sample. For instance, if there are 5 states, each state has a probability of 20%.

Random designs typically work well for large systems with many variables, 50 or more. There should be few interactions between variables and very few variables that contribute significantly. Random design does not work very well with relatively smaller systems. Generally speaking, Taguchi and random designs often perform better than factorial designs depending on size and assumptions. When choosing the design for an experiment, it is important to determine an efficient design that helps optimize the process and determines factors that influence variability.

There is more than one type of random design, randomized block design and completely randomized design. Randomized block design involves blocking, which is arranging experimental units into groups so they have a common similarity. The blocking factor is usually not a primary source of variability. An example of a blocking factor may include eye color of a patient, so if this variability source is controlled, greater precision is achieved. Completely randomized design is where the groups are chosen at random.

In various technological fields, it is important to design experiments where a limited number of experiments is required. Random design is practical for many design applications. Extensive mathematical theory has been used to explore random experimental design. Examples of random design include areas of data compression and medical imaging. The research conducted to support the practical application of random design can be found at <http://groups.csail.mit.edu/drl/journal_club/papers/CS2-Candes-Romberg-05.pdf>.

Other research has been conducted recently on random design, and more information can be found at: http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=1614066

More information on randomized block design can be found at:
http://en.wikipedia.org/wiki/Randomized_block_design

3.2 Completely Randomized Design (CRD)

3.2.1 Description of Design

Completely randomized design (CRD) is the simplest type of design to use. The most important requirement for use of this design is homogeneity of experimental units.

3.2.2 Procedure for Randomization

- 1) Assign treatments to experimental units completely at random.
- 2) Verify that every experimental unit has the same probability of receiving any treatment.
- 3) Perform randomization by using a random number table, computer, program, etc.

3.2.3 Example of CRD

If you have 4 treatments (I, II, III, IV) and 5 replicates, how many experimental units do you have?

{I} {IV} {III} {II} {II} {III} {III} {II} {I} {III} {I} {IV} {III} {IV} {I} {IV} {II} {I}
{II} {IV}

=20 randomized experimental units

3.3 Randomized Block Design (RBD)

3.3.1 Description of Design

Randomized block design (RBD) takes advantage of grouping similar experimental units into blocks or replicates. One requirement of RBD is that the blocks of experimental units be as uniform as possible. The reason for grouping experimental units is so that the observed differences between treatments will be largely due to “true” differences between treatments and not random occurrences or chance.

3.3.2 Procedure for Randomization

- 1) Randomize each replicate separately.
- 2) Verify that each treatment has the same probability of being assigned to a given experimental unit within a replicate.

3) Have each treatment appear at least once per replicate.

3.3.3 Advantages of RBD

1) Generally more precise than the CRD.

2) Some treatments may be replicated more times than others.

3) Missing plots are easily estimated.

4) Whole treatments or entire replicates may be deleted from the analysis.