

GETTING STARTED WITH MATHEMATICA

Loading Mathematica : If you are on any Loyola network computer, you should be able to load Mathematica by clicking on the start button (on the lower left of the computer screen), and searching for Mathematica. It might take a minute or two for Mathematica to load. You can also download a student copy of Mathematica onto your personal computer or laptop by following the directions posted on the link you can find on the course webpage.

Basic Calculations and Capabilities:

Mathematica has become one of the standard software platforms used by scientists in many disciplines. While we will only scratch the surface of what *Mathematica* can do, it is my goal that this semester will provide you with the foundation to expand upon your knowledge of *Mathematica* and use it not only for coursework, but in diverse research applications. Unlike many other software packages I have used, *Mathematica* has a very good online documentation center (click on the “help” tab at the top of each notebook).

Let's demonstrate a few of Mathematica's abilities. First, it acts as a calculator. If we want the value of the cos of 30 degrees we type :

In[1]:= **Cos[π / 6]**

Out[1]= $\frac{\sqrt{3}}{2}$

Notice that radians are the default measure for trig functions; the following command allows us to use degrees:

In[2]:= **Cos[30 Degree]**

Out[2]= $\frac{\sqrt{3}}{2}$

Once we input the command, we obtain output by simultaneously hitting the Shift and `ENTER` keys; if you have an extended keyboard, you can just hit the `ENTER` key on the extended keyboard.

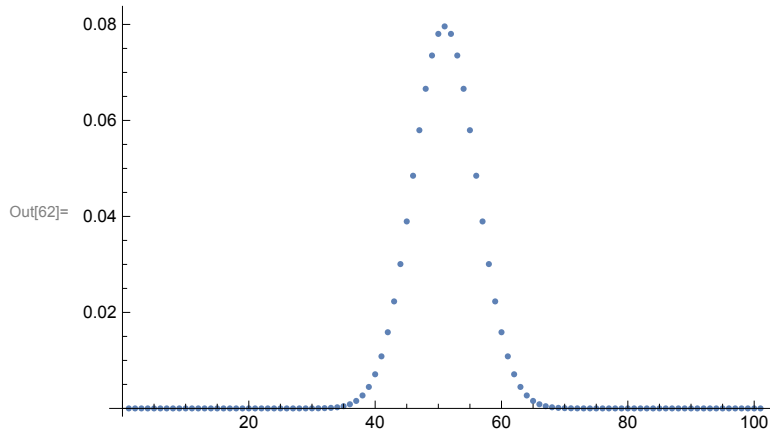
When you take thermodynamics, you will learn how to calculate probabilities; for instance, the probability of obtaining exactly 50 heads in 100 tosses of a fair coin is:

In[3]:= **(100! / (50! × 50!)) (0.5) ^ 100**

Out[3]= 0.0795892

Telling us that the probability of getting 50 heads is just under 8 % (why is this, the maximum probability, so low)? If you wanted to plot the total probability distribution, the following code will work :

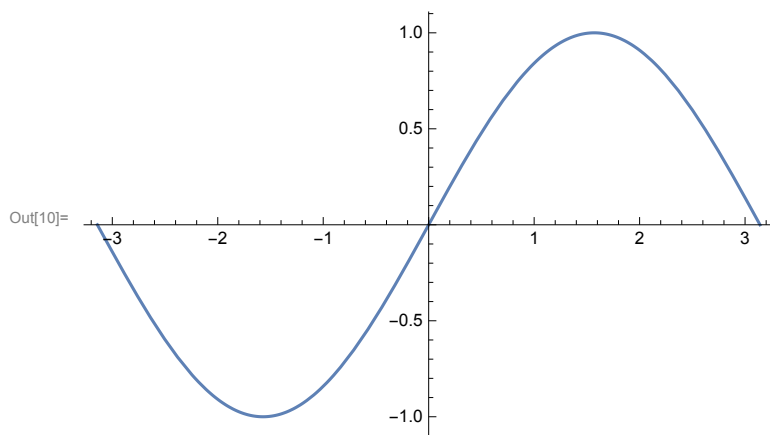
```
In[60]:= Clear[prob, n, ntotal, p, q]
prob[ntotal_,n_,p_,q_]:=ntotal!/((n!)(ntotal-n!)p^n q^(ntotal-n)
ListPlot[Table[prob[100,n,0.5,0.5],{n,0,100}],PlotRange->All]
```



And we produce a plot of the probability of flipping n heads out of 100 tosses. These three lines of code saved a lot of grinding and finding with a calculator.

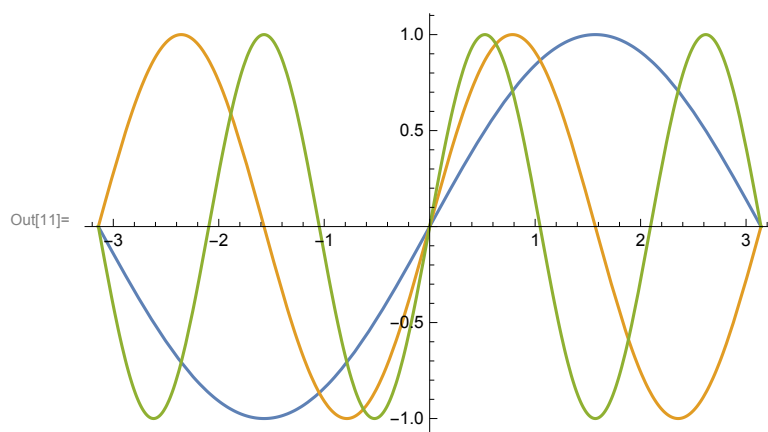
Graphing : Mathematica will allow you to produce a wide array of plots and graphs; these will be very helpful to us throughout the semester. First, a simple example, the graph of $\sin x$ from $-\pi$ to π :

```
In[10]:= Plot[Sin[x], {x, - $\pi$ ,  $\pi$ }]
```



Now, plots of $\sin x$, $\sin 2x$ and $\sin 3x$ on the same set of axes :

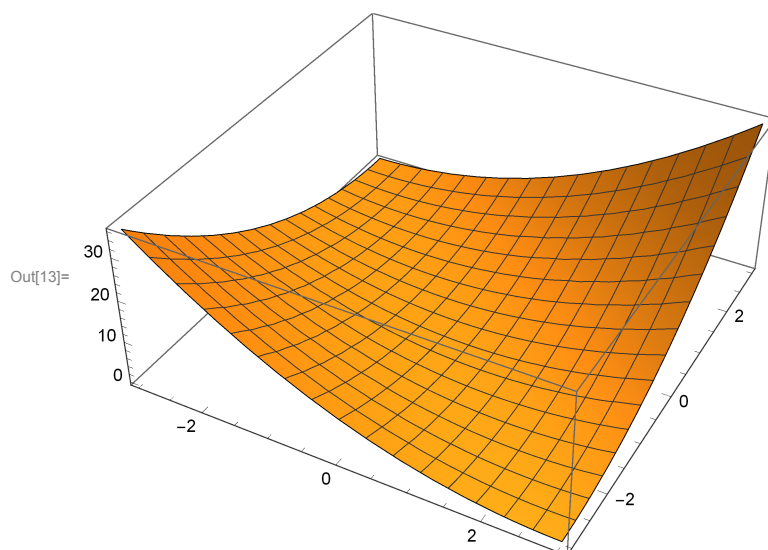
In[11]:= **Plot**[{Sin[x], Sin[2 x], Sin[3 x]}, {x, - π , π }]



If you study these examples, you will notice some patterns emerging. First, notice that all library functions in *Mathematica* (functions that already exist in *Mathematica*) start with capital letters. Then, notice that the argument of the function is always in square brackets. Braces, also known as curly brackets ({ }) are used for elements of a list (such as the list of functions to be plotted, or the list of parameters controlling the plot).

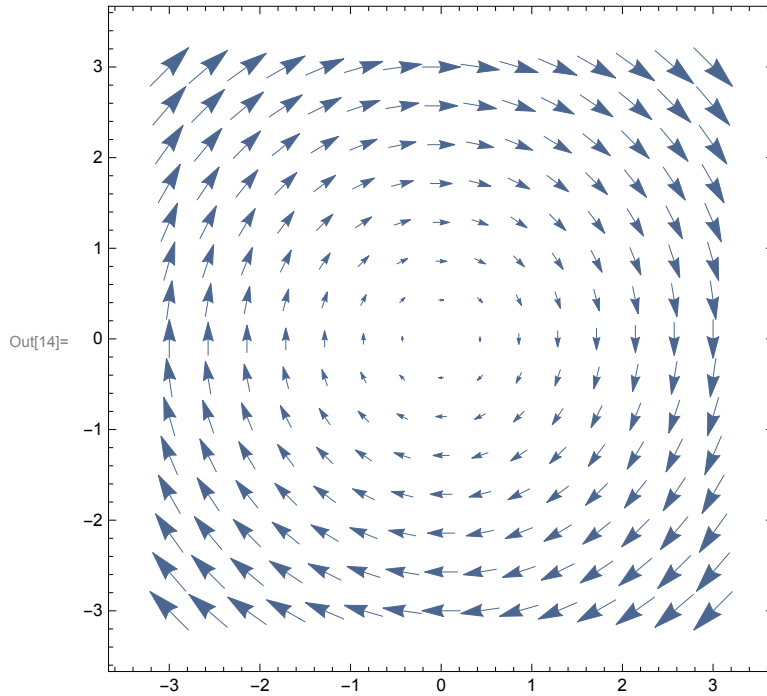
Mathematica can produce 3D plots:

In[13]:= **Plot3D**[$x^2 + 2xy + y^2$, {x, -3, 3}, {y, -3, 3}]



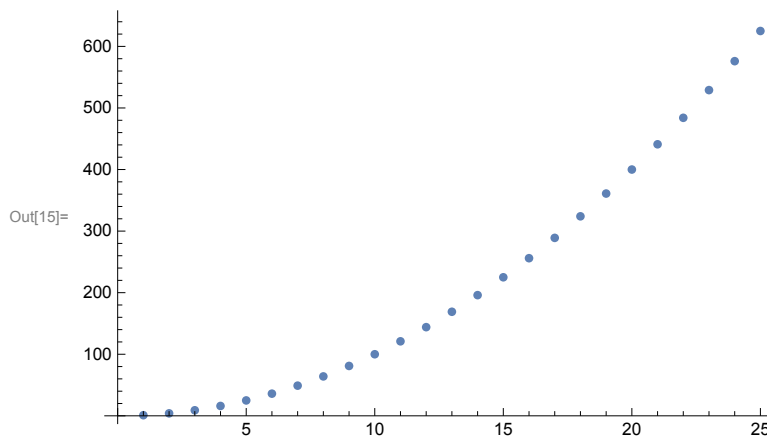
And plot vector fields:

In[14]:= **VectorPlot**[{y, -x}, {x, -3, 3}, {y, -3, 3}]



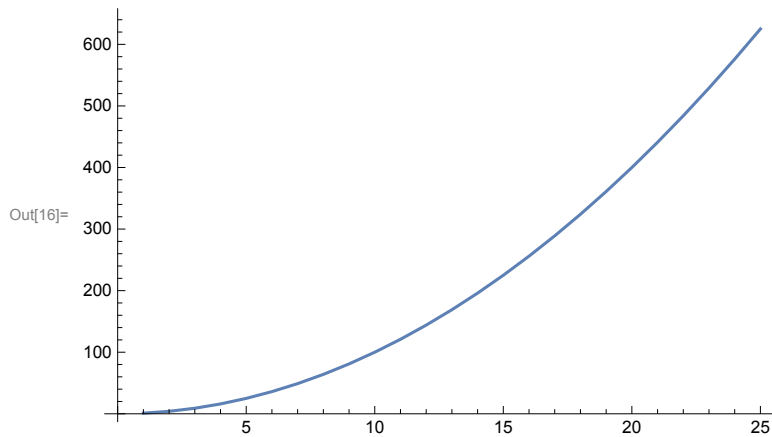
We saw above that “ListPlot” takes discrete points from a table and produces a graph. Here is a graph of the first 25 values of n^2 :

In[15]:= **ListPlot**[**Table**[n^2 , {n, 1, 25}]]



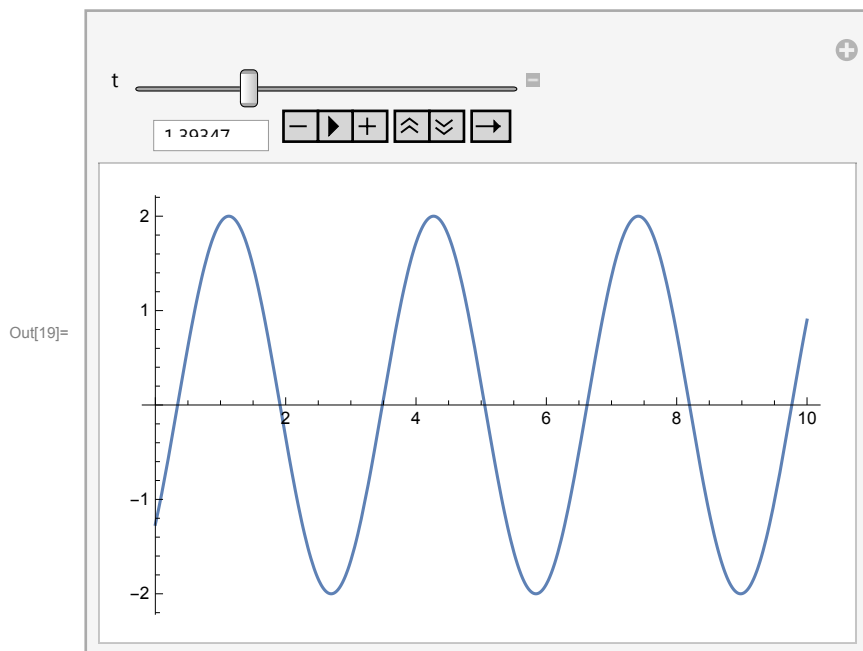
And to make this a continuous curve :

In[16]:= **ListLinePlot[Table[n ^ 2, {n, 1, 25}]]**



You can animate a graph using the Manipulate command. Before you type the code into your notebook, see if you can figure out what should happen. Now, type in the code and execute by hitting shift-**ENTER**:

```
Clear[x, y, amp, k,  $\omega$ , t]
y[amp_,k_,x_, $\omega$ _,t_]:= amp Sin[k x -  $\omega$  t]
Manipulate[Plot[y[2,2,x,5,t],{x,0,10}],{t,0,5}]
```

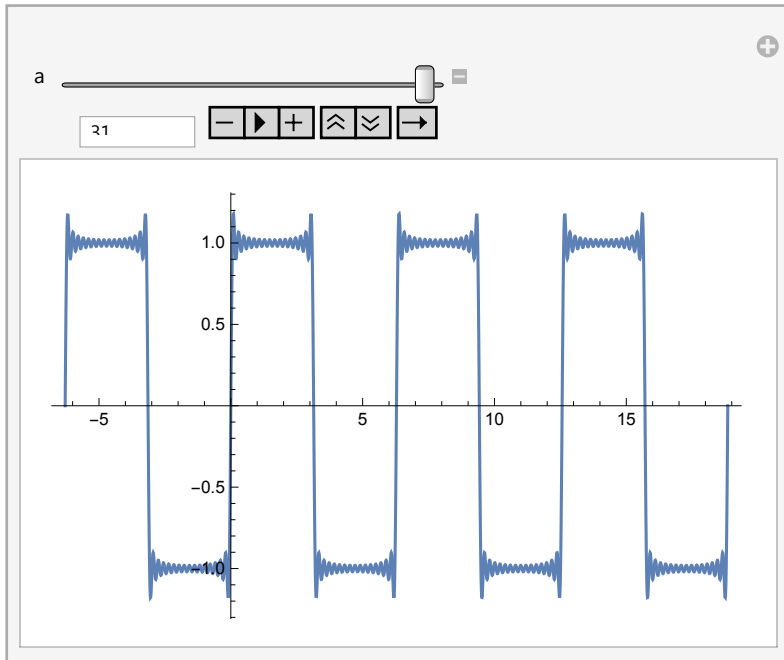


In a few weeks, we will study Fourier series in which we will learn how to express almost any periodic function as a series of sin waves. Let's see how a series of sin waves can produce a the square wave below :

In[20]:=

Clear[f,x,n]**Manipulate[Plot[(4/π)Sum[Sin[n x]/n,{n,1,a,2}],{x,-2π,6π}],{a,1,31}]**

Out[21]=



The free variable a represents the number of terms in the summation. If $a = 1$, we have just one sin wave and we obtain, of course, a pure sinusoidal wave. However, as we add additional sin waves, we can see that the sum converges to a square wave. Fourier series are a powerful way to analyze periodic phenomena.

Solving Equations : There are many routines in *Mathematica* that will allow you to solve all manner of problems. A simple quadratic can be solved via:

In[22]:= **Solve[3 x ^ 2 - 2 x + 6 == 0, x]**Out[22]= $\left\{ \left\{ x \rightarrow \frac{1}{3} \left(1 - i \sqrt{17} \right) \right\}, \left\{ x \rightarrow \frac{1}{3} \left(1 + i \sqrt{17} \right) \right\} \right\}$

And the output shows the two complex roots of this equation. We do not even need to use numbers; suppose we want to solve for the acceleration of the masses in an Atwood' s machine. We write Newton' s second law for the two masses (m and M) :

In[23]:= **Solve[{T - m g == m a, T - M g == - M a}, {a, T}]**Out[23]= $\left\{ \left\{ a \rightarrow -\frac{g m - g M}{m + M}, T \rightarrow \frac{2 g m M}{m + M} \right\} \right\}$

where T is the tension; the output yields analytic expressions for the acceleration of the system and the tension in the rope.

Differential equations can be analyzed via:

In[24]:= **DSolve**[y''[x] - 5 y'[x] + 6 y[x] == 0, y[x], x]

Out[24]= $\{\{y[x] \rightarrow e^{2x} C[1] + e^{3x} C[2]\}\}$

And you get the expected results for the equation $y'' - 5y' + 6y = 0$

And both definite and indefinite integrals can be evaluated:

In[25]:= **Integrate**[Tan[x], x]

Out[25]= $-\text{Log}[\text{Cos}[x]]$

In[27]:= **Integrate**[1 / (1 + x²)³, {x, 0, ∞}]

Out[27]= $\frac{3\pi}{16}$

Quirks and Cautions:

As with any software package, especially one this comprehensive, one can easily feel overwhelmed with all of the possible applications, utilities and opportunities for adding elegance and nuance to your work. I will do my best not to throw too much into any one classnote, and will allow you time to learn the software by using it--a few digestible bites at a time. *Mathematica* has a very good documentation center online (under the help tab), so I urge you to explore *Mathematica* as much as you can.

I want to mention a few points that you should keep in mind as you begin working with this program.

Using Functions in *Mathematica*:

Mathematica has hundreds if not thousands of library functions. We will use several of them, and the basic ones (like Sin, Cos, Log, Integrate, Plot and others) will become familiar to you.

.When you call a library function, you have to type it exactly as *Mathematica* expects. In particular, all *Mathematica* library functions becomes with a capital letter. Compare the output we get from these two statements:

In[28]:= **Cos**[π / 6]

Out[28]= $\frac{\sqrt{3}}{2}$

In[29]:= **cos**[π / 6]

Out[29]= $\text{cos}\left[\frac{\pi}{6}\right]$

In the first case, we obtain the value of $\cos 30^\circ$. In the second case, *Mathematica* does not recognize this as the library function for the cosine of an angle, since the statement did not start with a capital letter.

Delimiters : Brackets, Braces and Parentheses

In *Mathematica*, brackets, braces and parentheses all have very specific meanings. We have seen that you must use brackets whenever you call a library function.

Braces (curly brackets) are used when you are denoting lists; you encountered this when we plotted three sine functions on the same graph. In that case, we created a list of the three functions we wished to plot. We also used braces in solving two equations simultaneously (notice there were no braces when we solved just one equation); we use braces in setting up the range over which to plot a function : $\{x, -\pi, \pi\}$ is the *Mathematica* command meaning "plot over x from $-\pi$ to $+\pi$ ". Similarly, the braces used in the definite integral $\{x, -\pi, \pi\}$ mean "integrate over x , from $-\pi$ to $+\pi$ ".

Parentheses are used for grouping as they are in normal mathematical writing; however, in *Mathematica*, only parentheses are recognized as a means of grouping terms to clarify the order of operation

You can read more details about these in the online documentation by typing in "The Four Kinds of Bracketing."

Coefficients and Multiplication

Let's say you want to do a simple calculation and multiply 30 times 50. You can do this simply by typing in one number, leaving a space and then typing the next number :

```
In[30]:= 30 × 50
```

```
Out[30]= 1500
```

The "x" that appears was entered automatically by the program when I left a space; the output of 1500 was generated when I hit "Shift Enter"

In this version of *Mathematica*, the program will automatically put a space between a number and a variable. Try to reproduce these steps when you are trying out the program. First, I will set $x = 4$, and then evaluate $2x$:


```
In[35]:= x = 4  
2 x
```

```
Out[35]= 4
```

```
Out[36]= 8
```

Notice that we obtained two output lines; the first output line corresponds to the first input line and tells us

that we set $x = 4$. The second output line tells us that when I multiply x times 2, I get 8. (Yes, I know, horribly profound). If I only want the final output, I can suppress the first output by using a semicolon:

```
In[37]:= x = 5;  
2 x
```

```
Out[38]= 10
```

If you are inputting an equation using only symbols, say $F = m a$, you will need to leave a space between the two variables (the m , the a). Without this space, *Mathematica* will interpret “ ma ” as the new variable ma . See the two examples below; the first one with proper syntax:

```
In[57]:= m = 2; a = 5;  
f = m a;  
Print["The force is ",f]
```

```
The force is 10
```

Without proper syntax:

```
In[44]:= m = 2; a = 5;  
f = ma;  
Print["The force is ",f]
```

```
The force is ma
```

Equal Signs in *Mathematica*:

Mathematica has 3 different types of equal signs; it is important that we learn how to use each one in its proper context.

Immediate Assignment

In traditional mathematics, we use the “ $=$ ” sign for many different purposes. We make use of this

symbol when we want to assign a value to a variable ($x = 3$). We also use this sign when we establish a function ($f(x) = 2x + 2$) and also when we want to solve equations ($3x + 2y = 0$). While we use the same symbol for all of them, there is actually different logic involved in each operation.

To account for the different logical meanings of “equal”, there are different types of equal signs in *Mathematica*. You have already encountered two of them in this write up. The “=” you are familiar with (and the one used immediately above) is used when you want to make an immediate assignment of a value to a variable. In the examples above, each time we set x equal to a number that number was assigned to x immediately, and will remain assigned as the value of x until we either reassign x or `Clear[x]`. So what would happen if I just input “ x ” and hit shift-`ENTER`:

```
In[47]:= x
```

```
Out[47]= 5
```

Recall that I set $x = 5$ above. Since I had not cleared the value of x or assigned a new value to this variable, *Mathematica* will retain the assignment $x = 5$ until I clear or change it. If I now input the quadratic:

```
In[48]:= x^2 - 10x + 7
```

```
Out[48]= -18
```

Which is the value of this expression when $x = 5$. This is why it is always a good idea to Clear all variables before you execute any program.

Solving Equations and the Double Equal Sign

As we saw above, *Mathematica* is a very useful tool for solving various sorts of equations. When we solve equations, we make use of a double equal sign “==”. As shown in previous examples, we can solve single equations, systems of equations, and even solve equations symbolically. Let’s solve the general quadratic equation:

```
In[49]:= Solve[a x^2 + b x + c == 0, x]
```

```
Solve::ivar : 5 is not a valid variable. >>
```

```
Out[49]= Solve[125 + 5 b + c == 0, 5]
```

Well, now you know what *Mathematica* error statements look like. Why did we get this error? Remember we set $x = 5$; until we clear this value, *Mathematica* will equate x and 5 in all contexts.

Since we want to solve for x , *Mathematica* correctly tells us that 5 (which is still equivalent to x in *Mathematica* world) is not a variable. We correct this simply:

```
In[52]:= Clear[a,b,c,x]
Solve[a x^2 + b x + c ==0,x]
```

```
Out[53]= {{x ->  $\frac{-b - \sqrt{b^2 - 4 a c}}{2 a}$ }, {x ->  $\frac{-b + \sqrt{b^2 - 4 a c}}{2 a}$ }}
```

And we get the two roots of the quadratic equation. Note that "Clear[x]" starts with a capital "C", and the argument of the function is in brackets.

Creating functions and the colon-equal sign:

Suppose we want to create a function in *Mathematica*, say something as simple as $f(x) = x^2$. We proceed as:

```
In[54]:= Clear[f,x]
f[x_] := x^2
f[4.5]
```

```
Out[56]= 20.25
```

Note the two pieces of syntax here; we use an underscore after the x in the declaration of the function, and we use the $:=$ sign to indicate that x^2 will be substituted for x . Earlier, we saw how to create a multivariate function, when we defined the probability of a coin toss in terms of the total number of flips, the number of successes (n), and the probabilities of success (p) and failure (q).

This is just the barest of introductions to *Mathematica*. By the end of the semester, it is my goal that you will gain fluency in this very powerful programming language.