Best Fit Line

today we are going to write our own code for fitting a line and then compare it to differnt functions in python. We are going to take our math form Daniel C. Harris, Quantitative Chemical Analysis pages 66 and 67. Python can fit a line for you. But it is good to do a few of these functions by hand to see how they work.

To begin we are going to cheat and make our lives easier and use the numpy package. This package lets us do some array operations really easily and we won't have to do for loops. I was thinking of being mean and using all for loops. But lets take advantage of python. First lets import numpy and see what we can do.

In [1]:
```
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
from scipy import stats
```

In [33]:
```
x=np.array([1.,3,4,6])
print (x)
type(x)
```

```
[1. 3. 4. 6.]
```

Out[33]:
```
numpy.ndarray
```

So we could enter a list but instead of calling it a list we call it a numpy array. This is like a supercharged list.

Now we can make the y

In [34]:
```
y=np.array([2,3,4,5])
```

Now this is where numpy gets really cool. you can multiply and add your lists. This is different than array math if you have taken linear algebra. But we will be able to do that also.

In [6]:
```
print (x*y)
```

```
[ 2.  9. 16. 30.]
```

do you see what it just did? It multiplied elementwise!

In [7]:
```
print (x+y)
```

```
[ 3.  6.  8. 11.]
```

In [8]:
```
print (x-y)
```

```
[-1.  0.  0.  1.]
```

In [9]:
```
print (x/y)
```

```
[0.5 1.  1.  1.2]
```

In [10]:
```
print (x%y)
```

```
[1. 0. 0. 1.]
```

If you are doing linear algebra there are methods to do true matrix multiplication. For example the dot product.

In [11]:
```
print (np.dot(x,y))
```

```
57.0
```

In [12]:
```
print (np.sum(x))
```

```
14.0
```

In [13]:
```
print (len(x))
```

```
4
```

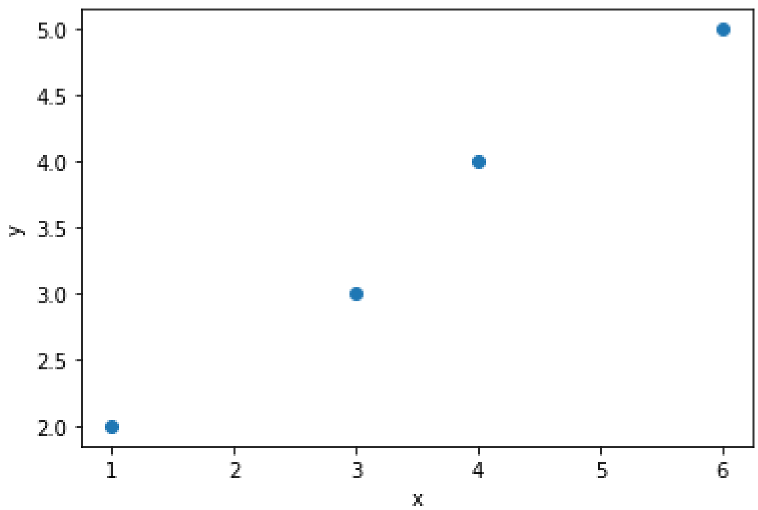
remember that tab is your friend. if you type np. and hit tab you will see a ton of functions we can call

In [ ]:
```
np.
```

What does our data look like?

In [5]:
```
fig,ax=plt.subplots()
ax.scatter(x,y)
ax.set_xlabel('x')
ax.set_ylabel('y')
```

Out[5]: `Text(0, 0.5, 'y')`



It is not a perfect line. So we need to fit a best fit line!

Now we can fit a line!!!!

I have now given you all the tools you need to figure out the best fit equation of a line. Remember the best fit equation of the line is y=mx+b where m is the slope and b is the intercept. We fit 2 points last time which define a line. When you have many points you have to find the best fit. We can do that! To do the fit when you have multiple points you get the equations

$$m = \frac{(n\Sigma x_i y_i - \Sigma x_i \Sigma y_i)}{(n\Sigma(x_i^2) - (\Sigma x_i)^2)}$$

$$b = \frac{\Sigma(x_i^2)\Sigma y_i - (\Sigma x_i y_i)\Sigma x_i)}{n\Sigma(x_i^2) - (\Sigma x_i)^2}$$

remember x_i means for each element in the list of x.

so in our case $x_0 = 1, x_1 = 3, x_2 = 4, x_3 = 6$

if we sum up all of one list that is $\Sigma x_i = 1 + 3 + 4 + 6 = 14$

n is the length of our list

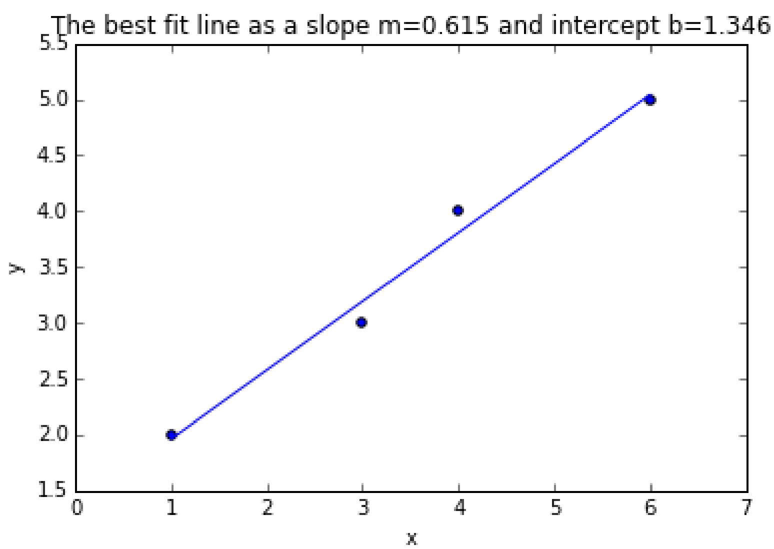
So lets plot our x and y data, look at it and then fit it.

So go ahead and figure out your m and b and then plot the line on the graph.

In [33]:

```
```

Out[33]: <matplotlib.text.Text at 0x10bff9290>



Now lets use Python to fit the line.

Two functions

1. linregress

2. Polyfit (not critical for now)

Linregress (short for linear regression)

I like linregress from scipy for my basic line fitting. the strength it has over polyfit is that it returns a p-value and an r which you can convert into r^2 along with the slope and intercept. Lets learn about it!

In [12]:
```
?stats.linregress
```

The key is we give it an x and y and then it returns:

slope : float slope of the regression line

intercept : float intercept of the regression line

r-value : float correlation coefficient

p-value : float two-sided p-value for a hypothesis test whose null hypothesis is that the slope is zero.

stderr : float Standard error of the estimate

We have talked about this some. But I want to say more explicitly here. In python when you call a function it can return many things. It doesn't have to return one number. It can return an array or multiple values. For linregress it returns 5 values. We can names these or put them in an array (I use array and list semi-interchangeably, I apologize and I will try to fix this). **HOW PYTHON CAN RETURN MANY THINGS ON THE LEFT SIDE OF AN EQUAL SIGN IS WEIRD**. Get used to it!

In [7]:
```
stats.linregress(x,y)
```

Out[7]:
```
LinregressResult(slope=0.6153846153846154, intercept=1.3461538461538458, rvalue=
0.9922778767136677, pvalue=0.007722123286332257, stderr=0.05439282932204183)
```

Why do I like stats.linregress? Becuase it gives us the r-value (square it and you have the r-squared) and the p-value. How do these results compare against yours that you calculated?

But if you want to use your stats results set it equal to something, it will make a list and then you can access it. Or you can set each item. so the two ways are.

First way. Set results equal to a list

In [8]:
```
stats_out=stats.linregress(x,y)
```

In [9]:
```
stats_out[0]
```

Out[9]:
```
0.6153846153846154
```

In [10]:
```
stats_out
```

Out[10]:
```
LinregressResult(slope=0.6153846153846154, intercept=1.3461538461538458, rvalue=
0.9922778767136677, pvalue=0.007722123286332257, stderr=0.05439282932204183)
```

We can give the output meaningful names!

In [38]:
```
slope, intercept, r_value,p_value,stderr= stats.linregress(x,y)
```

In [39]:
```
slope
```

Out[39]:
```
0.6153846153846154
```

In [40]:
```
intercept
```

Out[40]:
```
1.3461538461538458
```

We can give the output nonsensical names. Remember we control the computer and we are naming them!

In [41]:
```
phineas, ferb, perry,candace,isabelle= stats.linregress(x,y)
```

In [42]:
```
print (ferb)
```

```
1.3461538461538458
```

so it is up to you on how you want to get to the data from a function like stats.linregress()

I just learned a cool trick that I like. You can also use dot notation with your linregress output! This is nice!

In [43]:
```
stats_out=stats.linregress(x,y)
print (stats_out)
```

```
LinregressResult(slope=0.6153846153846154, intercept=1.3461538461538458, rvalue=
0.9922778767136677, pvalue=0.007722123286332257, stderr=0.05439282932204183)
```

But now you can use the names to get the results.

In [44]:
```
print (stats_out.slope)
```

```
0.6153846153846154
```

In [45]:
```
print (stats_out.intercept)
```

```
1.3461538461538458
```

I think this might be easier than using the array number or the names!

One thing I have problems with is long lines I want on multiple lines. For example sometimes I like to define a long string and then use that string as a title. To have it go over multiple lines you can use brackets. here is an example of a long string I made for a title. You can see me accessing the results both ways. Plus I added a \n to break lines and python let me break up the code on multiple lines since I was in a parantheses. Sometimes you can also add a \ to break the lines to get a line continuation. see https://stackoverflow.com/questions/4172448/is-it-possible-to-break-a-long-line-to-multiple-lines-in-python

In [46]:
```
title=('The best fit line as a slope m={:.3f} and intercept b={:.3f}'\
       .format(stats_out[0],stats_out[1])+
       '\nbest fit line linregress slope m={:.3f} and intercept b={:.3f} '\
       .format(slope,intercept))
print (title)
```

```
The best fit line as a slope m=0.615 and intercept b=1.346
best fit line linregress slope m=0.615 and intercept b=1.346
```

Now lets fix up our graph!

We can put the title back on.

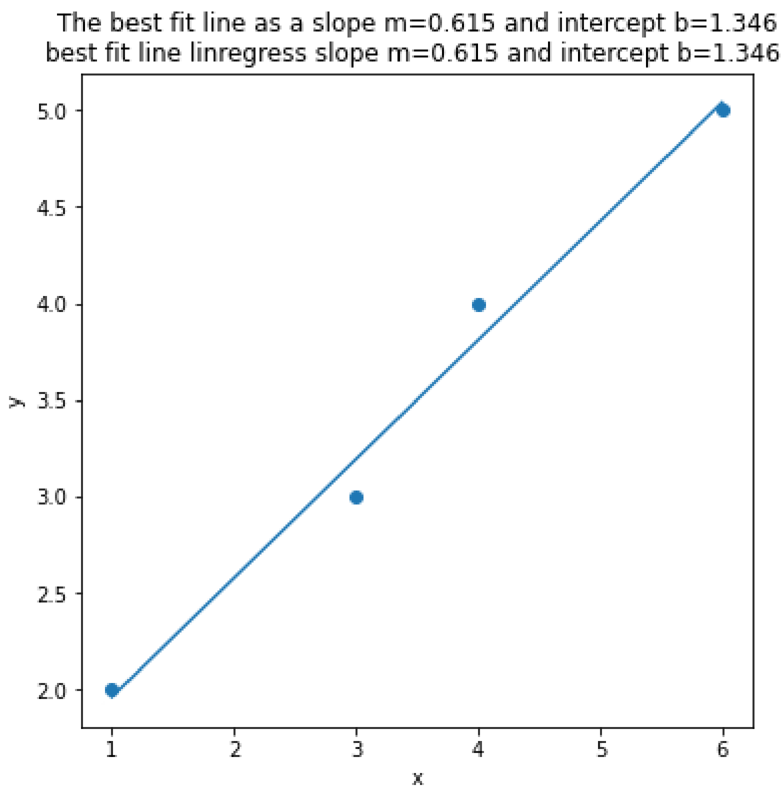
In [47]:
```
fig,ax=plt.subplots()
fig.set_size_inches(6,6)  # I made a square graph
ax.scatter(x,y)

#find the stats

#plot the best fit line
x_fit=np.linspace(np.min(x),np.max(x))
ax.plot(x_fit,x_fit*stats_out[0]+stats_out[1])

ax.set_xlabel('x')
ax.set_ylabel('y')
title=('The best fit line as a slope m={:.3f} and intercept b={:.3f}'\
       .format(stats_out[0],stats_out[1])+
       '\nbest fit line linregress slope m={:.3f} and intercept b={:.3f} '\
       .format(slope,intercept))
ax.set_title(title)
```

Out[47]:
```
Text(0.5, 1.0, 'The best fit line as a slope m=0.615 and intercept b=1.346\nbest
fit line linregress slope m=0.615 and intercept b=1.346 ')
```



But I think adding a textbox to the graph makes it look more professional

Sometimes when making a graph, instead of putting in a title it looks better to put in a text box with just the details. It is a three step process to make a nice box. Scroll down this link and you can see where I got the recipe from. http://matplotlib.org/users/recipes.html It is at the bottom

1. First you define the box by making a dictionary of the box properties. We ususally call it props for the properties of the box.

2. Then you make the text string you want in the box. for a linear equation you usually want slope, interecept, r^2, and p-value

3. You then say where you want the information. This is within the ax properties since we will put it into the graph. You tell it the relative location, Then you give it the text, somemore information, and then the props

4. Also add the linregress to this cell to do everything in one place to make it clean

In [49]:
```
fig,ax=plt.subplots()
fig.set_size_inches(6,6)  # I made a square graph
ax.scatter(x,y)

#Stats on the data
slope, intercept, r_value,p_value,stderr= stats.linregress(x,y)

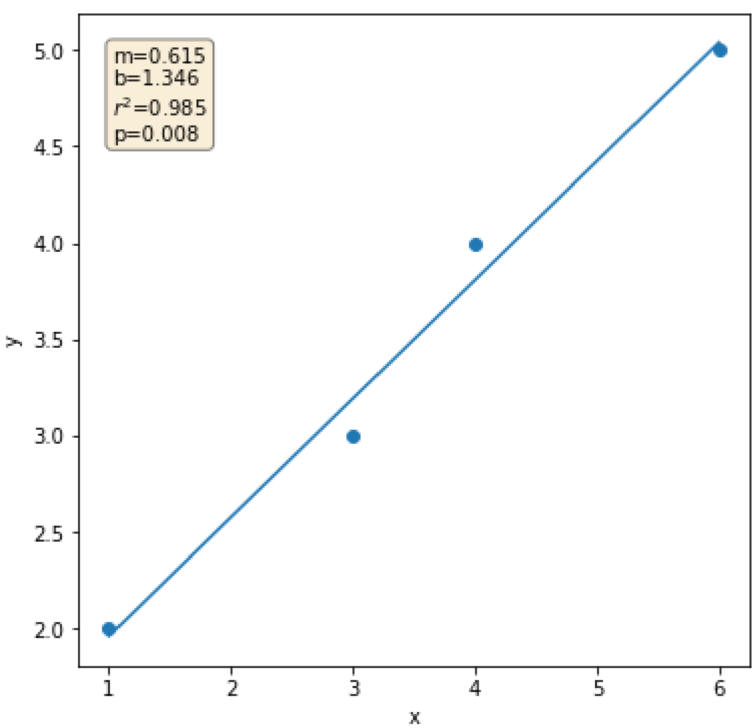
#plot the best fit line
x_fit=np.linspace(np.min(x),np.max(x))
ax.plot(x_fit,x_fit*stats_out[0]+stats_out[1])

ax.set_xlabel('x')
ax.set_ylabel('y')

# This is the code I added to get the box below with the normal graphing
props=dict(boxstyle='round',facecolor='wheat',alpha=0.5)

textstr='m={:.3f}\nb={:.3f}\n$r^2$={:.3f}\np={:.3f}'\
        .format(slope,intercept,r_value**2, p_value)
ax.text(0.05,0.95,textstr,transform=ax.transAxes\
        ,fontsize=10,verticalalignment='top',bbox=props)
```

Out[49]:
```
Text(0.05, 0.95, 'm=0.615\nb=1.346\n$r^2$=0.985\np=0.008')
```



In [ ]:

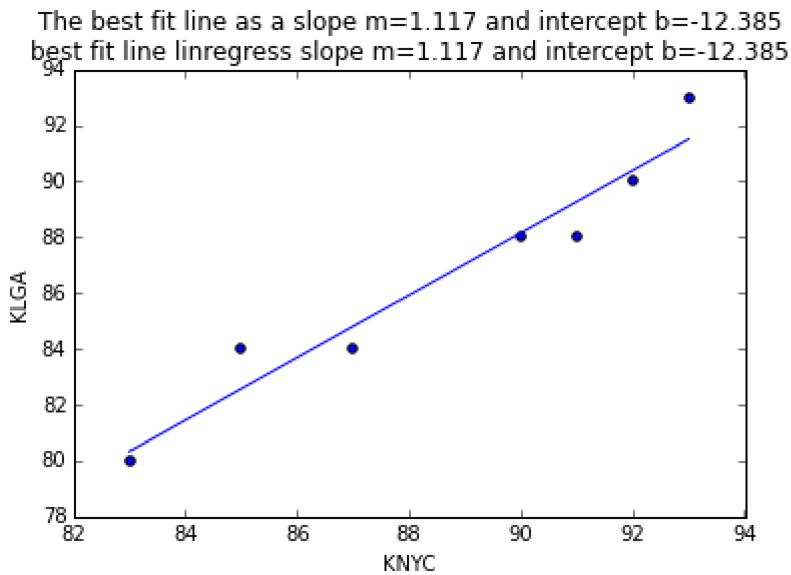
Class Assignment

Fit a line to the KNYC and KLGA data and plot it

Now can you go back and get the KNYC and KLGA weather data and see if they are correlated? I would use your program and then compare to linregress. Remember to use np.array([]) to enter the data as a numpy array. Also remember you need at least one float in your list to make it all floats. I like the second graph with the box!

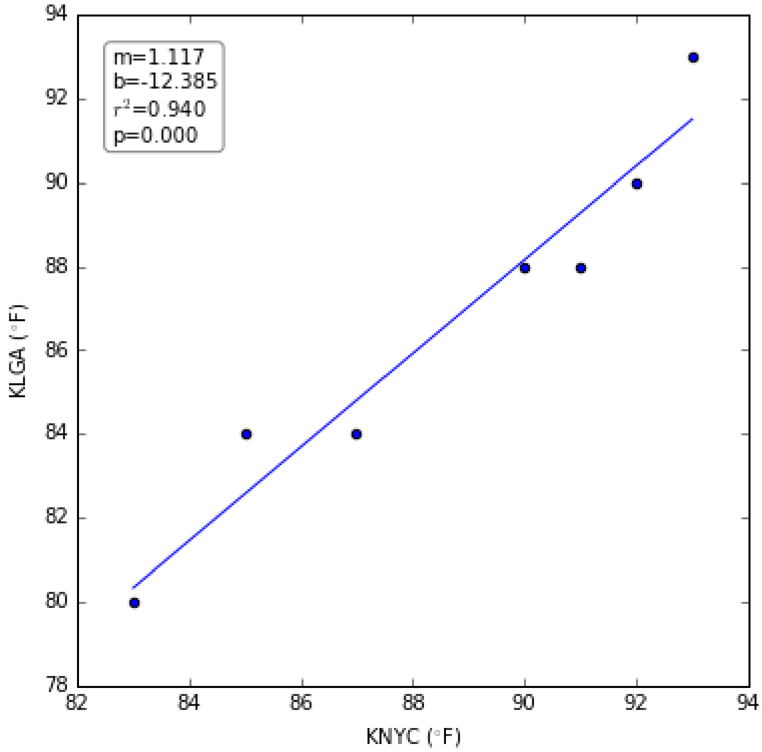
In [3]:

Out[3]: <matplotlib.text.Text at 0x15614fd0>



In [29]:

Out[29]: <matplotlib.text.Text at 0x9d05cf8>



What is a p-value?

Statisticians argue about p-values and what they exactly mean. We are going to do an exercise to help you understand.

In my simplistic world I think of a p-value as the chance of the result happening by chance.

a p-value of 0.05 means that result could happen by chance 5% of the time. It sort of but not quite means that the result is real 95% of the time.

a p-value of 0.01 means that result could happen by chance 1% of the time. It sort of but not quite means that the result is real 99% of the time.

you usually see people writing p<0.05 when they want to show the relationship is siginificant. We say it is significant because only 5% of the time it happens randomly.

This means if we randomly create data. 5% of the time we would get a p-value<0.05. 95% of the time our results would look like junk. so lets do it!

Use the nump function random to get random numbers from 0 to 1. it is np.random.random(size) and you give how many. lets do 50.

In [23]:
```
np.random.random(50)
```

Out[23]:
```
array([0.25275895, 0.03305665, 0.94104781, 0.6722305 , 0.23773632,
       0.93851915, 0.12961236, 0.10201882, 0.48071812, 0.49040787,
       0.75001889, 0.92054346, 0.93788928, 0.70639629, 0.02906303,
       0.70715162, 0.55801932, 0.75910762, 0.19028569, 0.03269578,
       0.13596112, 0.72398551, 0.65856306, 0.24053408, 0.81387377,
       0.60808716, 0.73752055, 0.79190437, 0.00365806, 0.93270819,
       0.12394915, 0.81827269, 0.61999088, 0.32774057, 0.87897003,
```

```
        0.12372507, 0.91374782, 0.93088581, 0.87484   , 0.4256022 ,
        0.27847397, 0.15926549, 0.26533697, 0.89631707, 0.98672037,
        0.69397302, 0.13111585, 0.33728261, 0.02734482, 0.05421295])
```

Now make your x and y data each with 50 numbers

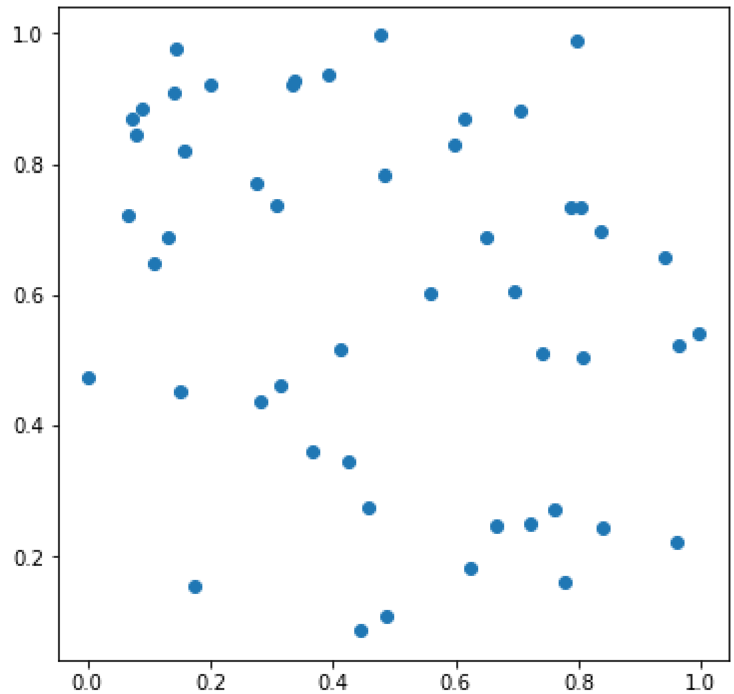
In [24]:
```
x=np.random.random(50)
y=np.random.random(50)
```

Now plot the data. Every time you run it your data will change. Run it a few times and see if the points move around!

In [26]:
```
x=np.random.random(50)
y=np.random.random(50)

fig,ax=plt.subplots()
fig.set_size_inches(6,6)  # I made a square graph
ax.scatter(x,y)

slope, intercept, r_value,p_value,stderr= stats.linregress(x,y)
```



Now add the best fit line

In [52]:
```
x=np.random.random(50)
y=np.random.random(50)

fig,ax=plt.subplots()
fig.set_size_inches(6,6)  # I made a square graph
ax.scatter(x,y)

#calculate the best fit line
slope, intercept, r_value,p_value,stderr= stats.linregress(x,y)

#plot the best fit line
x_fit=np.linspace(np.min(x),np.max(x))
ax.plot(x_fit,x_fit*slope+intercept)

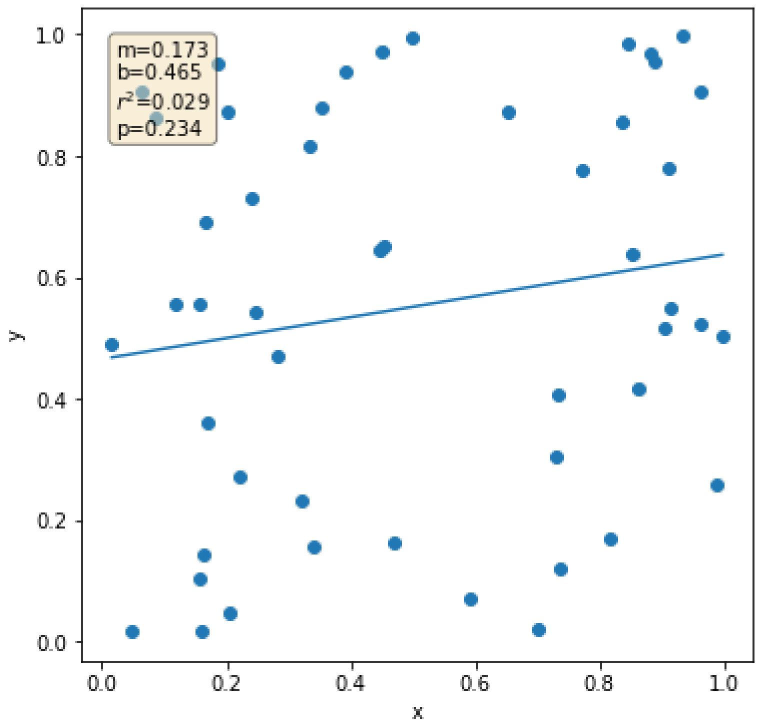
ax.set_xlabel('x')
```

```
ax.set_ylabel('y')

# This is the code I added to get the box below with the normal graphing
props=dict(boxstyle='round',facecolor='wheat',alpha=0.5)
textstr='m={:.3f}\nb={:.3f}\n$r^2$={:.3f}\np={:.3f}'\
        .format(slope,intercept,r_value**2,p_value)
ax.text(0.05,0.95,textstr,transform=ax.transAxes\
        ,fontsize=10,verticalalignment='top',bbox=props)
```

Out[52]:

```
Text(0.05, 0.95, 'm=0.173\nb=0.465\n$r^2$=0.029\np=0.234')
```



Now rerun the cell and count how many times it takes you to get a p-value less than 0.05. Then share with your breakout rooms It took me 27.

Now lets make the computer work for us. Think about this. We can ask the computer to make the graph above 1000 times. Then we can ask how many times we got a p-value less than 0.05. If it is random our answer should come about near but probably not exactly 50.

Now lets get rid of the graph and run the regression 1000 times and count how many times we get a significant result

In [58]:

```
num_sig=0

for i in np.arange(1000):
    x=np.random.random(50)
    y=np.random.random(50)

    #calculate the best fit line
    slope, intercept, r_value,p_value,stderr= stats.linregress(x,y)
    if p_value<0.05:
        num_sig+=1
        print('Loop Number {} with a p_value of {}'.format(i,p_value))

print('I ran the for loop 1000 times and the \
p_value was less than 0.05 {} times'.format(num_sig))
```

```
Loop Number 14 with a p_value of 0.013768191249915141
Loop Number 32 with a p_value of 0.010325587131925263
Loop Number 48 with a p_value of 0.04998574928702603
Loop Number 58 with a p_value of 0.011613259947481674
Loop Number 108 with a p_value of 0.013265557228705446
Loop Number 109 with a p_value of 0.024282603849346614
Loop Number 126 with a p_value of 0.028149764263222903
Loop Number 148 with a p_value of 0.017215378221889874
Loop Number 151 with a p_value of 0.03744735571244542
Loop Number 221 with a p_value of 0.01693622522281629
Loop Number 222 with a p_value of 0.04672332087508179
Loop Number 232 with a p_value of 0.02885611323628464
Loop Number 239 with a p_value of 0.04558808012319081
Loop Number 262 with a p_value of 0.02341930929481531
Loop Number 268 with a p_value of 0.03989203780271019
Loop Number 293 with a p_value of 0.031158267479432997
Loop Number 299 with a p_value of 0.025012441646863497
Loop Number 309 with a p_value of 0.01960985651839358
Loop Number 312 with a p_value of 0.048462735182921955
Loop Number 322 with a p_value of 0.012209025333444236
Loop Number 335 with a p_value of 0.026063543920688576
Loop Number 353 with a p_value of 0.04974052001790181
Loop Number 360 with a p_value of 0.03118879397133239
Loop Number 363 with a p_value of 0.03397917786757127
Loop Number 377 with a p_value of 0.021867928879286385
Loop Number 410 with a p_value of 0.0074251904712731
Loop Number 464 with a p_value of 0.019827242843665004
Loop Number 476 with a p_value of 0.02309036284730668
Loop Number 544 with a p_value of 0.0473919089091389
Loop Number 546 with a p_value of 0.0016485145587271672
Loop Number 549 with a p_value of 0.025498539161222442
Loop Number 556 with a p_value of 0.04234503983696942
Loop Number 614 with a p_value of 0.04961071483080715
Loop Number 633 with a p_value of 0.042187600493885646
Loop Number 660 with a p_value of 0.035531013241171645
Loop Number 686 with a p_value of 0.030139802705080338
Loop Number 687 with a p_value of 0.011015467120926728
Loop Number 711 with a p_value of 0.004031008343914578
Loop Number 729 with a p_value of 0.033784059453014464
Loop Number 747 with a p_value of 0.04368869470636622
Loop Number 798 with a p_value of 0.025582023294943128
Loop Number 826 with a p_value of 0.025288038285842685
Loop Number 839 with a p_value of 0.04970719406984716
Loop Number 915 with a p_value of 0.005864660421576615
Loop Number 929 with a p_value of 0.023040943147541418
Loop Number 933 with a p_value of 0.0428739647262823
Loop Number 935 with a p_value of 0.03652889883984372
Loop Number 946 with a p_value of 0.04585836355056982
Loop Number 982 with a p_value of 0.025960097663030125
I ran the for loop 1000 times and the p_value was less than 0.05 49 times
```

So hopefully this helps you with a p-values. the p-value tells you how often the result may happen randomly. So the lower the p-value the lower the probability of the result happening randomly. Therefore you can "trust" the result more. But really you report the p-value so people know how you are making your choice on the significance of the results. A lot of methods report a p-value so you will be seeing this!

In [ ]:

```

```

Foreshadowing.

If you are done early keep going and learn about polyfit. If not we will come back to this and don't worry.

Polyfit is from numpy.

In [30]:
```
?np.polyfit
```

Polyfit will return us the m and b. The strength of polyfit is two fold. First you can do higher order by changing the third parameter and also it makes it easy to fit your data.

In [31]:
```
np.polyfit(x,y,1)
```

Out[31]:
```
array([0.61538462, 1.34615385])
```

So you could do second order. where you get the best fit y=ax^2+bx+c

In [32]:
```
np.polyfit(x,y,2)
```

Out[32]:
```
array([1.77953990e-16, 6.15384615e-01, 1.34615385e+00])
```

Now how can we get the fit?

In [33]:
```
fit=np.polyfit(x,y,2)
print (fit)
```

```
[1.77953990e-16 6.15384615e-01 1.34615385e+00]
```

This is a cool polyfit function. Remember this as it can come in useful

In [34]:
```
eqn=np.poly1d(fit)
```

In [35]:
```
print (eqn)
```

```
           2
1.78e-16 x + 0.6154 x + 1.346
```

Now lets pass a value to eqn

In [36]:
```
eqn(10)
```

Out[36]:
```
7.500000000000015
```

In [37]:
```
eqn(np.linspace(-10,10))
```

Out[37]:
```
array([-4.80769231, -4.55651491, -4.30533752, -4.05416013, -3.80298273,
       -3.55180534, -3.30062794, -3.04945055, -2.79827316, -2.54709576,
       -2.29591837, -2.04474097, -1.79356358, -1.54238619, -1.29120879,
       -1.0400314 , -0.788854  , -0.53767661, -0.28649922, -0.03532182,
        0.21585557,  0.46703297,  0.71821036,  0.96938776,  1.22056515,
        1.47174254,  1.72291994,  1.97409733,  2.22527473,  2.47645212,
        2.72762951,  2.97880691,  3.2299843 ,  3.4811617 ,  3.73233909,
        3.98351648,  4.23469388,  4.48587127,  4.73704867,  4.98822606,
        5.23940345,  5.49058085,  5.74175824,  5.99293564,  6.24411303,
        6.49529042,  6.74646782,  6.99764521,  7.24882261,  7.5       ])
```

Poly1d doesn't do everything we want. But if you need to fit a higher order equation and print the equation it is really nice

Answer

I posted the answers in a seperate notebook. Don't cheat and look. Work through it.

In [ ]:

```
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In [ ]:

```
```