# NUMERICAL METHODS WEEK 1

# CURVE FITTING 0

## OR SCIENTIFIC COMPUTING REFRESHER

This introduces the ideas of curve fitting - this week the simplest case of fitting a line to data we expect to be linearly related.

Learning outcomes:

- Revise some material from Scientific Computing last year.
- Code a working version of linear regression using C++.
- Check your code works correctly, via an external reference.


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## WHAT IS NUMERICAL METHODS?

Using computers to solve numerical problems in applied mathematics and physics.

## WHAT IS NUMERICAL METHODS NOT?

More programming training.

## WHY AM I LEARNING THIS?

Numerical competency will be one of the major skills you can bring to the market place alongside soft and professional skills.

# PHILOSOPHY

Break down problems into small chunks.

Use pen and paper and plan your work before attacking the keyboard.

Test, test and test again.

## NO REALLY - TRY AND TEST AFTER EVERY SINGLE LINE YOU ADD.

## SAVE - ON ONEDRIVE IT WILL KEEP BACKUPS TOO.

# LEAST SQUARES REGRESSION

suppose that you think a set of paired observations $(x_0, y_0), (x_1, y_1), \ldots, (x_{n-1}, y_{n-1})$ are related as

$$y_i = a_0 + a_1 x_i + e$$

where $e$ is the error, or residual, between the model and the observations.

We think there is a linear relationship between $x$ and $y$, but there is some error in the measurements.

# BEST FIT

given our assumption of a straightline

$$y_i = a_0 + a_1 x_i + e_i$$

the error at each point is given by

$$e_i = y_i - a_0 - a_1 x_i$$

So in some sense the some of the total errors would be given by the sum of the errors. We will take the sum of the squares of the errors

$$S_r = \sum_{i=0}^{n-1} e_i^2 = \sum_{i=0}^{n-1} (y_i - a_0 - a_1 x_i)^2$$

as our error criterion.

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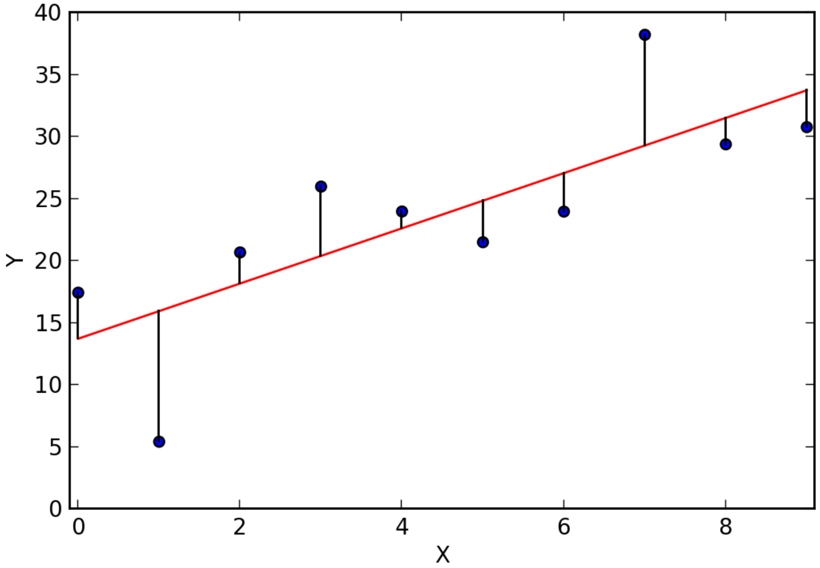

# OPTIMAL PARAMETERS

If we look at our model

$$S_r = \sum_{i=0}^{n-1} e_i^2 = \sum_{i=0}^{n-1} (y_i - a_0 - a_1 x_i)^2$$

we see that there are 2 parameters, $a_0$ and $a_1$ that control the slope and intercept of our model.

It is a model, we are assuming that there is a linear relationship between $x$ and $y$.

We want to minimize the value of $S_r$, so we differentiate with respect to our parameters

$$\frac{\partial S_r}{\partial a_0} = -2 \sum (y_i - a_0 - a_1 x_i)$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum [(y_i - a_0 - a_1 x_i) x_i]$$

where the summations go from $0$ to $n - 1$ (this is to agree with C style arrays).

Note that the points $(x_i, y_i)$ are not variables, they are things we have measured. What we can vary is the parameters of our model. So $S_r$ is a function of the two parameters $a_0$ and $a_1$.

For more general models we will have more parameters and a more complex relations ship than the straight line assumed here.

# OPTIMAL PARAMETERS

We want to minimize the value of $S_r$, so we differentiate with respect to our parameters

$$\frac{\partial S_r}{\partial a_0} = -2\sum(y_i - a_0 - a_1 x_i) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum[(y_i - a_0 - a_1 x_i)x_i] = 0$$

This gives us a pair of simultaneous linear equations, sometimes called the normal equations.

We can solve these for $a_1$ and $a_0$.

$$a_1 = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - (\sum x_i)^2} \tag{1}$$

and plug this into the first equation to get

$$a_0 = \frac{\sum y_i}{n} - a_1 \frac{\sum x_i}{n} = \bar{y} - a_1 \bar{x} \tag{2}$$

where $\bar{y}$ and $\bar{x}$ are the means of the $x$ and $y$ values.

# CODING UP LINEAR REGRESSION

You will want to use arrays to store data. Remember arrays are like a list, or ordered set, of numbers. The type of number is defined in the normal way.

Here is some code to allocate an array of size 100, place the numbers 0 to 99, in that order, into the array.

Then we add up the elements of the array, and print them out.

```cpp
/* C++ code*/
#include <iostream>
using namespace std;

int main()
{
  double x[100] ;
  for (int i = 0; i < 100; i++) {
    x[i] = i;
  }

  double sumx = 0.0;
  for (int i = 0; i < 100; i++) {
    sumx += x[i];
  }
  cout << "The sum of the numbers 0 to 99 is " << sumx <<"\n";
}
```

highlight: c++ hljs cpp

```python
# python code
# create an empty array
x = []

for i in range(100):
  x.append(i)

sumx = 0
for i in range(len(x)): # range(n) command creates a list of values from 0 to n-1
  sumx += i
  # print(i)

print("the sum of the numbers 0 to 99 is " + str(sumx)) # str(sumx) converts sumx into a strin
g
```

highlight: python hljs

# EXERCISES

Alter the previous code to answer the following questions:

- What is $\sum_{n=0}^{99} 2n^2$
- What is $\sum_{n=1}^{100} n$
- What is $\sum_{n=2}^{200} 2n$
- What is $\sum_{n=0}^{99} 2n^2$

# EXERCISES

Find the intercept ($a_0$)and slope ($a_1$) of the least squares best fit to the following data using the formulae given a few slides previously:

```
x = [
0.526993994,
0.691126852,
0.745407955,
0.669344512,
0.518168748,
0.291558862,
0.010870453,
0.71818573,
0.897190954,
0.476789102,
]

y = [
3.477982975,
4.197925374,
4.127080815,
3.365719179,
3.387060084,
1.829099436,
0.658137249,
4.023164612,
5.074088869,
2.752890033,
]
```

# TEST YOURSELF

That is it for the lecture! The really important thing this week is that you get a computer setup so that you can try the problems as we go forward.

If you have problems getting the software to work on your laptop or desktop let us know.