

A.1 Understanding the Output of Octave.

1. Let us take the example of fitting a curve with three parameters using non-linear least-squares (the “automatic” script process). You should get output which looks like this.

Estimated Coefficient

3.00000

-2.10001

0.28557

95% confidence intervals for parameters

2.99999 3.00000

-2.10002 -2.09999

0.28557 0.28558

rms error =

2.2140e-006

r2 value =

0.98

These are the estimated values of the three parameters A,B,C.

This means that for this fit of the function to the data, the chance of the parameters lying outside these ranges is 5%. So the chance of them lying in this range is 95%. All these ranges are small which is good.

The r2 value is a statistical measure. It tells us that 98% of the information in the original data is correctly represented by the chosen function.

A.2 How to decide if the curve-fit is good or not?

1. Well the first thing to do is look at the **r2 value** which is a number between 0 and 1; convert this to a percentage in your head. This number gives us the “confidence” that the chosen function correctly fits the data. So 0.98 means we are 98% sure that the chosen function is the right one. (Statistically speaking, there is a 2% chance, $100 - 98$, that the function was fit by pure chance).

So r2 needs to be close to 1.0. How close? Certainly above 0.9 and if we get 0.95 or above then we are very happy weebees indeed. Values less than 0.8 are troublesome.

If you fit two different functions to the same data, funcA gives 0.921 and funcB gives 0.953, then we conclude funcB is the better one, so we choose it.

2. The second thing to do is to look at the 95% confidence intervals for **each parameter** individually. Say we get the following:

estimated coefficient (parameter) 3.51

with confidence interval 3.49 3.53

This is good since the estimated 3.51 is bracketed by a small range. We are 95% sure that the estimated parameter is good for this fitted function. In other words only this small range of parameters would give us the fit (where we assume this is good). Compare this with the following:

estimated coefficient (parameter) 3.51

with confidence interval 1.51 5.51

Here the range is too large for us to be confident in the fit, since the function could be equally well fit by a huge range in parameters. Sure, there is an element of subjectivity that has crept in here, and that is mitigated by experience. The following one shouts out a clear warning

estimated coefficient (parameter) 3.51

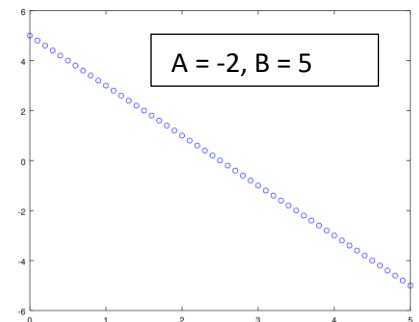
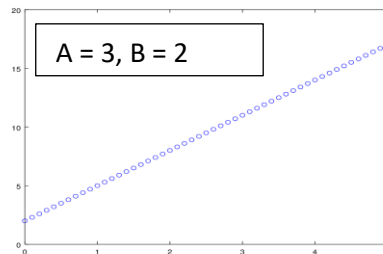
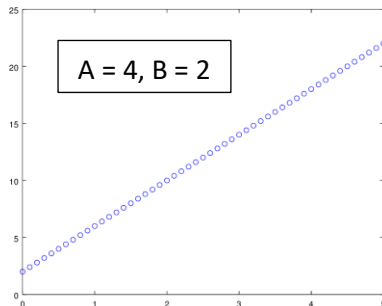
with confidence interval $-3.23 \ 3.61$

The range of parameters extends from negative to positive numbers. This includes zero which is therefore a possibility. A parameter value of zero means that the parameter is **not required** which tells us that we are fitting with the incorrect function.

B.1 Some Mathematical Functions

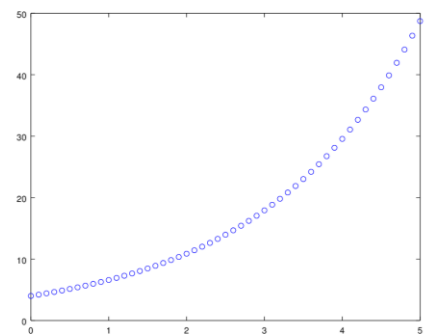
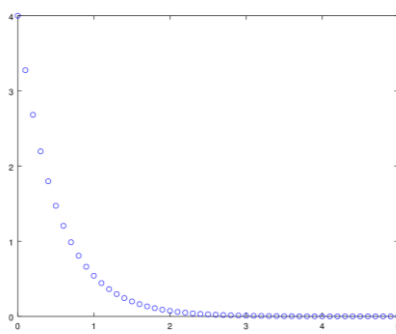
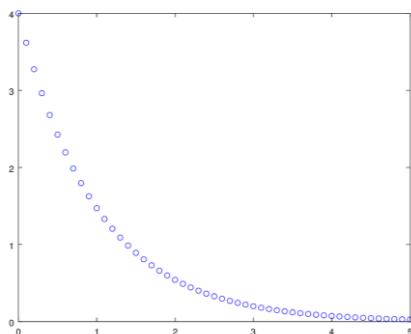
1. The Linear Function

This has the form $y = Ax + B$ where the parameter A controls how fast the line rises or falls ($A < 0$) and B tells you where the line hits the y-axis. Here's a couple of examples two on the left drawn to the same scale.



2. The Exponential Function

This has the form $y = Ae^{Bx}$. Here parameter A is the value of y when $x=0$. The parameter B changes how fast the exponential curve rises or falls (when $B < 0$). Here's some examples: From left to right, $[A=4, B=-1]$, $[A=4, B=-2]$, $[A=4, B=0.5]$.



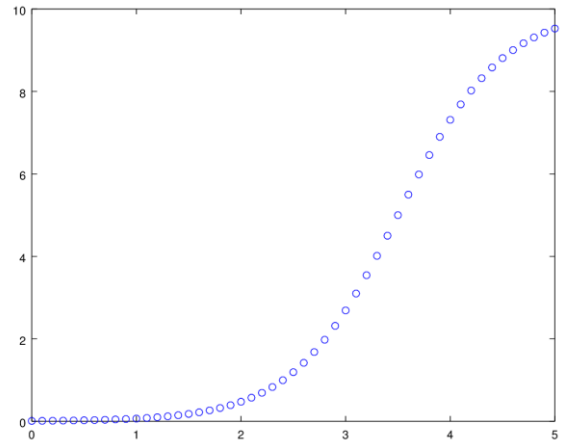
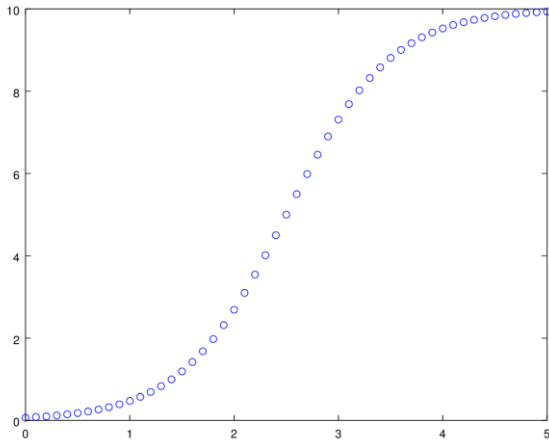
3. The Sigmoid (Logistic) Function

There are various ways of writing this mathematically; here I have chosen what I believe to be the most intuitive form,

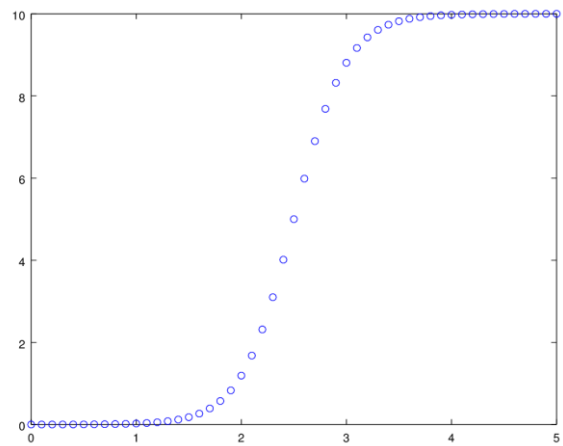
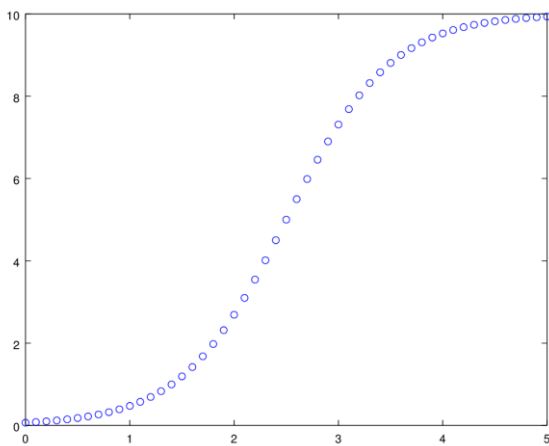
$$y = \frac{A}{1 + e^{-B(x-C)}}$$

There are three parameters here, so there is a little thought needed. Glance down at the graphs below. You will see that the function starts at $x=0, y=0$ then rises towards a maximum. This maximum is given by parameter A . Also you can see that as the graph rises it initially grows quickly then the growth slows, and between the two there is almost a straight segment. The centre of this segment on the x-axis is just C .

In the examples below we have, from left to right $[A=10, B=2, C=2.5]$ then $[A=10, B=2, C=3.5]$. You can see that both curves rise towards $A=10$. Also you can see the effect of changing C from 2.5 to 3.5 is to shift the centre of the curve to the right, from $x = 2.5$ to $x = 3.5$. This is the function of parameter C .



Let's have a look at how parameter B changes the curve. The examples below have on the left [A=10, B=2, C=2.5] and on the right [A=10, B=4, C=2.5]. You see that a large parameter B makes the transition much sharper.



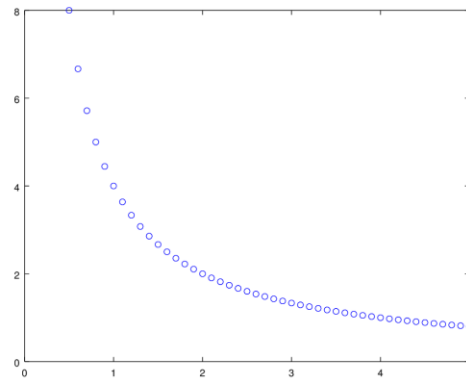
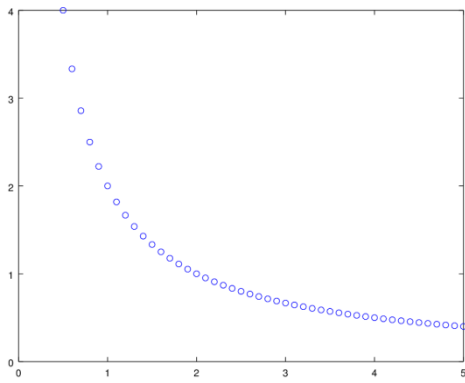
4. The Power Law Function

This has the mathematical form $y = \frac{A}{x^B}$

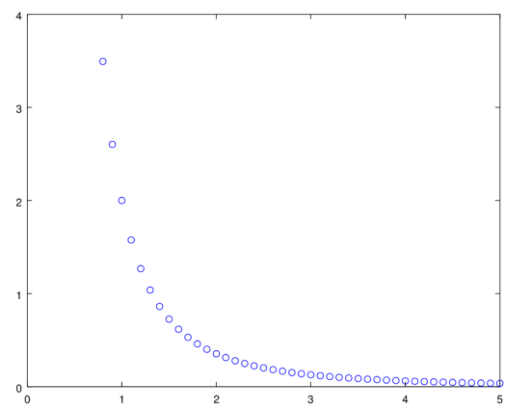
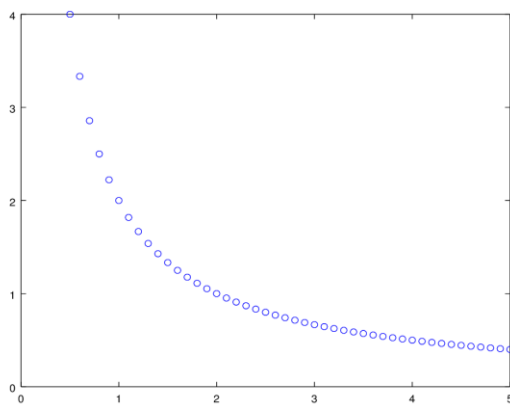
How can we understand this?

- (i) Well, clearly if A is large, then the values of y will be large whatever the value of parameter B is.
- (ii) For small values of x we will get large values of y since when we divide any number by a small number, the result is large. (Convince yourself that this is true by working out 10/2 then 10/0.5. Answers at the bottom of the page, hehe). And when $x=0$ we shall divide A by 0. Any number divided by zero is infinite. So when we are using the power law function **we must not have an x-value of 0**.
- (iii) When $x = 1$, the bottom of the above formula is just 1 (since 1 to any power is just 1), therefore the value of y for $x=1$ is just A.

Let's have a look at some plots for this function, bearing the above points in mind. First let's see what happens when we change the value of parameter A. In the graphs below, on the left we have [A=2, B=1] and on the right we have [A=4, B=1]. You can see that doubling the value of parameter A has doubled all the y-values.



OK, now we understand what parameter A does, it's time to see what parameter B does. On the graphs below we compare $[A=2, B=1]$ on the left with $[A=2, B=2.5]$ on the right. Note that I have scaled both axes to be the same in the two plots so we are able to make an objective comparison.



The curve on the right “drops off” much more quickly. That’s the effect of parameter B, the larger this parameter the quicker the graph drops off.

Also note that in both graphs, the value of y, for $x=1$ is 2. This is just the value of parameter A, as mentioned in point (iii) above.

B.2 Applications of the Mathematical Functions

Function	Applications
Exponential	* Many natural processes such as flow of water from a bucket with a hole, the voltage across a capacitor in an electronic circuit,
Sigmoid	
Power-Law	* Distribution of number nodes (y) with number of links (x) on a scale-free network.