Week 1 Lecture – basic graph manipulation

Required reading: Ch. 8 and 9 of Monk & Munro, "Maths for Chemistry", 2^{nd} edition.

The objective of this lecture is to refresh graph plotting techniques in your memory, to give you some guidance on the appearance of the graphs that we would expect from you in your laboratory assignments, and to provide some training on extracting parameters of linear relationships from graphs.

1. Simple graphs in Cartesian coordinates

You have learned basic plotting techniques at school. Tabulated experimental data are usually easy to plot; for functions the method is roughly as follows:

1. Decide your X axis range by thinking about the interval (of time, concentration or any other independent variable) that you are interested in.
2. Decide your Y axis range by considering the biggest and the smallest value that your function takes within the interval you have selected in the previous step.
3. Decide how many points you need – the faster the function changes, the more points are necessary.
4. Create a table similar to the one below; do not forget the units.

t, seconds	0.0	3.5	7.0	9.5	13.0	17.6			
$f(t)$, metres	0	50	100	150	200	250			

5. Plot the points on a piece of graph paper.
6. Annotate the plot: draw tick marks, add axis labels and axis units.
7. Add a caption with the description of the content of the plot and all relevant parameters.

Steps 6 and 7 are commonly missed by beginner chemists, but they are very important – without that metadata, it is impossible to make use of the plot.

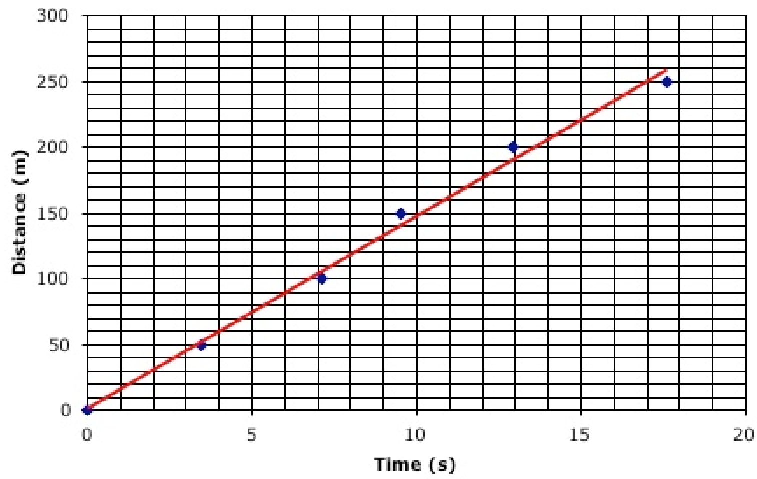

Figure 1. *A basic correctly scaled and annotated graph. Note the tick marks on both axes, the names of the variables and the units in which the variables are plotted. The points and the trend line are clearly visible. The plot makes good use of the graph area. Note also that this caption is clear and informative.*

As you gain more experience, particularly with computer software, you would be able to make more sophisticated plots. However, it is essential that you produce some of them by hand – this would allow you to understand the process that a computer goes through.

An important warning to make here is that, *when plotting experimental data, you should never connect points in any way*. The reason is obvious from Figure 1 – experimental data has uncertainties and measurement errors. The correct way of indicating a relationship between experimental data points is to draw a trend line using a physically appropriate function.

2. Transforming equations into a linear form

Laws of physics are rarely simple; you will come across many functions that do not look like the standard linear relationship:

$$f(x) = ax + b \tag{1}$$

where a and b are constants. A good example of a non-linear relationship is the dependence of the coordinate of a falling object on time:

$$h(t) = h_0 - gt^2/2 \tag{2}$$

where h_0 is the initial height at time zero and g is the acceleration of free fall. Equation (2) is not linear, but it is still possible to get a linear graph by plotting $h(t)$ against t^2 instead of t. This is illustrated in Figure 2. It is easy to see that the relationship between $h(t)$ and t^2 is linear:

$$h(t) = h_0 - \frac{g}{2}t^2 \tag{3}$$

with $a = -g/2$ and $b = h_0$.

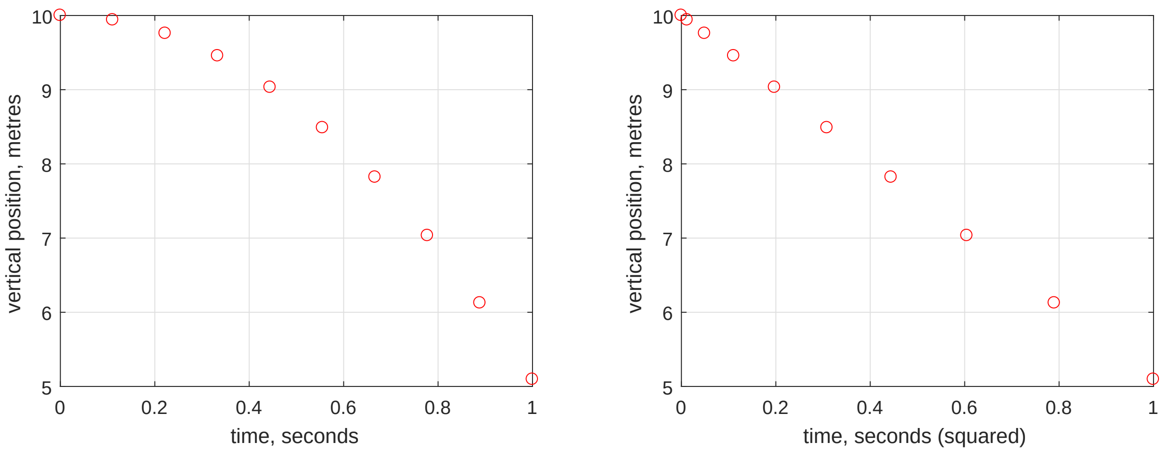

Figure 2. *An illustration to the fact that the non-linear relationship between the time and the vertical coordinate of a falling object in Equation (2) yields a linear plot when the vertical position is plotted against time squared.*

Example 1: linearizing equations of the type $y = ax^b$

1. Take a logarithm of both sides: $\ln(y) = \ln(ax^b)$
2. Simplify, using rules for logarithms: $\ln(y) = \ln(a) + b\ln(x)$

A plot of $\ln(y)$ against $\ln(x)$ would be linear.

Example 2: linearizing equations of the type $y = ab^x$

1. Take a logarithm of both sides: $\ln(y) = \ln(ab^x)$

2. Simplify, using rules for logarithms: $\ln(y) = \ln(a) + x\ln(b)$

A plot of $\ln(y)$ against x would be linear.

There is no general recipe for that process – it relies on your experience and creativity:

$$\begin{aligned} y = a\exp(-bx) \quad &\Rightarrow \quad \ln(y) = \ln(a) - bx \\ y = \frac{a}{b+cx} \quad &\Rightarrow \quad \frac{1}{y} = \frac{b}{a} + \frac{c}{a}x \\ y = ax^2 + 1 \quad &\Rightarrow \quad \sqrt{y-1} = x\sqrt{a} \end{aligned} \tag{4}$$

et cetera. In all three cases, plotting experimental measurements directly in $\{x, y\}$ coordinates would produce non-linear plots. However, plotting $\ln(y)$ against x in the first case, $1/y$ against x in the second case and $\sqrt{y-1}$ against x in the third case would produce linear plots.

3. Extracting straight line equation parameters from experimental data

The simplest method for extracting the parameters of a linear relationship is to plot the experimental data on a piece of graph paper and draw a line through it by hand. The process is illustrated in Figure 3.

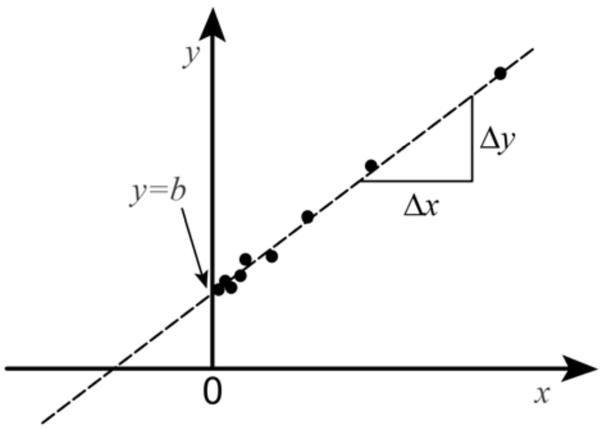

Figure 3*. A schematic illustration of the linear relationship parameter extraction process. The model equation is linearized, the experimental data is plotted in linearized coordinates, the slope and the intercept are extracted as shown, and then transformed back into physically relevant quantities.*

For a linear function $y = ax + b$, where a and b are constant parameters, the b parameter can be extracted from the value of y at the point where $x = 0$ (the so-called *intercept*) and the a parameter may be obtained from the relationship between increments:

$$a = \Delta y / \Delta x \tag{5}$$

This method is slow and prone to errors, particularly in situations where data points span several orders of magnitude in one or both coordinates. It also gives no quantitative measure of uncertainty in the resulting values of the parameters. It is, however, a good historical illustration and it is a good idea to practice with this method before starting to use modern statistics software, such as *Origin* and *Matlab*.

Class exercises

Monk & Munro, 2nd edition: problems 13.1-13.4; 8.6-8.10; 9.10