Essential Mathematics for DTC DPhil Students
Michaelmas Term, 2019
PROBLEMS SHEET NUMBER 1
Graphs

GRAPHS:

Text relevant to these problems: Croft and Davison, 5th Edition, Chapters 17, 18.

19. The Lennard-Jones potential energy between two non-polar atoms may be simply given by the equation:

$$V(R) = \frac{A}{R^{12}} - \frac{B}{R^6}$$

where A and B are positive constants, $V(R)$ is the potential energy, measured in Joules, and R is the internuclear distance measured in Å.

a) For which values of R is $V(R)$ positive? Negative? Zero?
b) Plot a graph showing the potential energy between the two atoms as a function of R (in Å) given that $A = 0.06$ and $B = 0.03$.
c) What is the potential energy between the two atoms at infinite separation?
d) What would happen to the two atoms if they were brought very close together?
e) What is the physical interpretation of the sign of $V(R)$, and of its slope?
f) What are the dimensions ([Length], [Mass], [Time]) and units of the constants A and B?
g) (Extension) Use Python to plot the graph of V versus S for $A = 0.06$ and $B = 0.03$. Remember to add relevent axis labels. Plot on the same graph the line of $V = 0$, so you can verify your answers in (a) and (b).

20. How should these equations be rearranged to allow the plotting of a suitable **linear** graph, assuming that the constant parameters a and b are unknown, and we wish to use the graph to find them? Write down expressions for the gradient, X-intercept and Y-intercept of each rearranged equation:

(a) $y = \frac{a}{x}$
(b) $y = b - a\sqrt{x}$
(c) $y = \frac{b}{1 + ax}$

21. (Extension) The rate at which a given enzyme catalyses a reaction is dependent upon the substrate concentration:

$$V = \frac{S}{m + cS}$$

where V is the rate of the reaction, S is the substrate concentration and m and c are *unknown* constants. How can we transform V and S to derive a straight line graph relating them? What will be the gradient and the ordinate intercepts?

22. The OSMOTIC PRESSURE of a solution of a protein is related to the concentration of that protein by the equation:

$$Z = R\ T\ b$$

where Z is the osmotic pressure in kPa, T is the temperature in Kelvin, R is the gas constant ($R = 8.314$ kPa.dm^3.mol^{-1}.K^{-1}) and b is the molarity of the protein (mol. solute per dm^3 solution). Plot a suitable graph to determine, as accurately as possible, the molecular mass (take care with units!) of the protein given the following data taken at room temperature (usually taken as 21°C):

Protein Concentration (in g dm^{-3})	7.3	18.4	27.6	42.1	57.4
Osmotic Pressure (in kPa)	0.211	0.533	0.804	1.236	1.701

(Hint: compare the function with the equation of a straight line, $y = mx + c$, and think about the relationship between concentration, molar concentration and molecular weight)
(Extension) Use Python to plot the graph and confirm your pen&paper solution.