

Essential Maths for DTC DPhil Students

Michaelmas Term 2022

Problem Sheet 1: graphs

Introductory problems

1. Sketch the following graphs. First, use pen & paper, then use Python to check your answers.

a) $y = 3x + 5$ $x \in [0, 10]$

b) $y = \frac{x^2}{2} - 4$ $x \in [-4, 4]$

c) $y = \sqrt{x}$ $x \in [0, 25]$

d) $y = \sin(t)$ $t \in [0, 2\pi]$

e) $y = \sin(2t)$ $t \in [0, 2\pi]$

f) $y = \frac{1}{x}$ $x \in [0.1, 5]$

g) $y = \frac{-1}{x^2}$ $x \in [0.1, 5]$

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# hint
import numpy as np
from matplotlib import pyplot as plt

x = np.linspace(0, 10, 100)
y = 3 * x + 5

plt.plot(x, y)
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2. For which values of x are the following functions positive? Negative? Zero?

a) $x^2 - 9$

b) $\sin(x)$

c) $\sin(3x)$

d) $\frac{2}{x} - \frac{1}{x^2}$

Main problems

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

1. The Lennard-Jones potential energy between two non-polar atoms may be 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) Use Python to plot the graph of V versus R for $A = 0.06$ and $B = 0.03$. Remember to add relevant axis labels. Plot on the same graph the line of $V = 0$, so you can verify your answers in a) and b).
2. 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) $y = \frac{b}{1 + ax}$

3. 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 ($R = 8.314 \text{ kPa} \cdot \text{dm}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$) 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).

Use Python to plot the graph and confirm your pen & paper solution.

Extension problems

1. 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?