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**Module DataFit: Data analysis and modelling – Tutorial / workshop 1**

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**Introduction**

This first workshop will not be formally assessed, but you will need to show that you have completed all the problems outlined in this worksheet. These are designed to give you some practice in error analysis, and are an essential part of the course.

These exercises should be carried out with the scientific data analysis software IGOR Pro.

To solve these problems, you can use online help and ask the postgraduate demonstrator to get you started.

You will also need to refer to your notes from the lectures.

**Problems**

*Problem 1*

A student makes six independent measurements of barometric (atmospheric) pressure  $P$  during a lab session. The values recorded were 762.2, 761.8, 760.0, 761.5, 762.2 and 762.0 mm Hg. Find the average value of  $P$  and the standard deviation of the data. Find also the standard error of the mean  $\sigma_{\text{std}}$  and the 95% confidence limit. (do this by calculator and check your result with Igor)

$\langle P \rangle =$

$\sigma =$

$\sigma_{\text{std}} =$

$t_{0.95} =$

*Problem 2*

For the data of Problem 1, quote the mean pressure below with this confidence limit and appropriate numbers of significant figures.

*Problem 3*

Take another look at the data presented in Problem 1. Are any points suspect? If so, apply the criteria given in the lectures to see whether this point may be eliminated. If so, recalculate the values for the standard deviation, standard error and the 95% confidence limit, and re-quote your answer below.

*Problem 4*

Calculate the molecular weight of an ideal gas if 5.05 g of the gas is contained in a 1.4 litre vessel at 765 mm Hg pressure at 295 K. The mass measurement is carried out on a triple beam balance that may be read to the nearest 0.01 g, the volume has a precision of 0.1 litres, the pressure is measured by a transducer with an absolute accuracy of 1 mm Hg, and the temperature is read to the nearest degree. State your answer with its uncertainty in the box below:

Useful equations:  $pV = nRT$  where

$p$  = pressure in Pa (750 mm Hg is  $10^5$  Pa) ;

$R$  - Universal gas constant =  $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$

$n$  (no. of moles) =  $m/M$      $m$  - mass of gas in grams

$V$  = volume in  $\text{m}^3$

$T$  - temperature in K

$M$  - molar mass in grams / mole

*Problem 5*

Into an Igor Pro Procedure, write a function to speed-up the calculation of problem 4. Using this function, calculate the molecular weight and its uncertainty for three different cases below.

	M (g)	T (K)	P (mm Hg)	V (L)	Result
Case 1	$10.5 \pm 0.5$	$77 \pm 1$	$765 \pm 1$	$1.4 \pm 0.1$	
Case 2	$7.5 \pm 0.1$	$77 \pm 1$	$356 \pm 1$	$1.8 \pm 0.2$	
Case 3	$4.5 \pm 0.1$	$295 \pm 0.5$	$356 \pm 1$	$2.67 \pm 0.01$	

*Problem 6*

Write a procedure to exclude any suspect points according to the criteria given in the lectures (Section 1.2.10).. Apply this procedure to the 1D waveform dataset of the problem 1.

*Problem 7*

The rate coefficient  $k$  for a reaction in the temperature range 278 K to 358 K is given by the Arrhenius equation:

$$k = A \exp\left(\frac{-E_a}{RT}\right)$$

where  $A = (1.4 \pm 0.1) \times 10^9 \text{ s}^{-1}$  and  $E_a = (103 \pm 1) \text{ kJ mol}^{-1}$ .

Find the value of the rate coefficient and its uncertainty at 336 K, assuming that this temperature is known to  $\pm 0.5 \text{ K}$ .

*Problem 8*

An experiment is performed to determine the virial coefficients  $B_0$  and  $B_1$  of a gas, given by the following expression for the compressibility,  $Z$ :

$$Z = \frac{PV}{nRT} = B_0 + B_1 P$$

The following dataset is obtained:

$P / \text{atm}$	$Z$
1.31	0.9950
9.76	0.9675
24.35	0.9489
49.38	0.9063

- Using Igor Pro, create a graph of  $Z$  against  $P$ , with appropriately labelled axes.
- With the built-in linear regression function (Analysis – Quick fit – Line), plot the regression for  $Z$  against  $P$  and note the fit values with their standard deviations.
- Now, using non-linear regression (Analysis – Curve Fitting) write a custom fit function to calculate  $B_0$  and  $B_1$  (i.e. the intercept and slope of a linear regression). The idea here is to get practice in coding so don't just use Igor's own built-in "line" fit function – write your own.
- Display on your graph the fit and the fitted values of  $B_0$  and  $B_1$  with their 95% confidence limits.
- How do the values for the standard deviation and the 95% confidence limits compare? How do you explain this?

