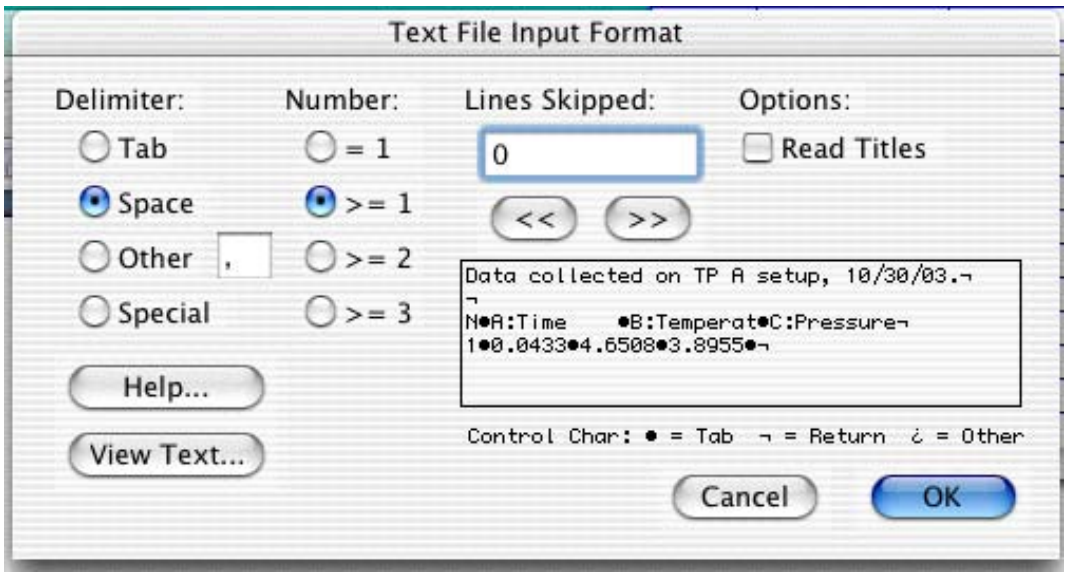
Chemistry 236 — Quiz 1
October 11, 2006 — Tellinghuisen

Honor Code Pledge: *I have neither given nor received aid on this exam.* _____

(Signature)

I. (24) Statistics and KaleidaGraph.

A. (4) Getting Started. You have recorded a boatload of data in the P Chem lab and now seek to plot and analyze them using everyone's favorite new tool — KaleidaGraph! You click on "Open" under the **File** menu and select one of your files, whereupon you see:



Precisely what do you select or enter in order to ensure that the resulting KG data sheet will contain all your data, in numerical format, with column headings?

Delimiter: __Tab_____ Number: ___1 or >= 1___ Lines Skipped: ____2_____

Options: (Check or don't check?)

B. (5) Having Fits. You encountered your first truly nonlinear least-squares fitting problem in Problem Set 3, where you fitted first-order kinetics data to a delining exponential function of time plus a background. The resulting function contained three adjustable parameters.

1. Write the fit relationship in mathematical form. Identify the independent and dependent variables and the adjustable parameters.

$f(t) = a + b\,e^{-kt}$ indep. — t; dependent — f; adj. params — a, b, k

2. Suppose you carry out the fit by defining the fit relationship in the "Define Fit" box of the **General** fit routine. Write below EXACTLY what you must enter there.

`a + b*exp(-c*x); a= ...; b = ... ; c = ...` (initial values)

C. (6) By the Numbers. You measure a quantity 57 times. You enter all the numbers in a column in a KG data sheet and click on the "Statistics" command. Let us suppose that the sum of squared residuals ($\Sigma\delta_i^2$, not included in the output of this command) is 113.771.

1. What values will the Statistics command show for (a) the variance, (b) the standard deviation, and (c) the standard error? [Hint: Recall definitions in terms of $\Sigma\delta_i^2$ in Statistics Notes 1. Also, this sum is the quantity called Chisq in unweighted KG fits.]

   (a) $s_y^2 = \Sigma\delta_i^2/(n-1) = 2.031625$

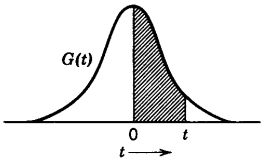
   (b) $s_y = 1.425351$

   (c) standard error = standard deviation in the mean = $s_y/\sqrt{n} = 0.188792$.

2. What uncertainty should you quote for 80% confidence limits on your mean value? (Use accompanying table.)

   By interpolation, we get $t = 1.28_2$. This is applied to the standard error, giving ±0.242.

Table 4-4. Error Function $\frac{1}{2}$ erf (t) from 0 to t and Ordinate Values
$G(t) = (1/\sqrt{2\pi})\, e^{-t^2/2}$



t	$\frac{1}{2}$ erf (t) Area	$G(t)$ Ordinate	t	$\frac{1}{2}$ erf (t) Area	$G(t)$ Ordinate
0	0	0.3989	2.0	0.4773	0.0540
0.1	0.0398	0.3970	2.1	0.4821	0.0440
0.2	0.0793	0.3910	2.2	0.4861	0.0355
0.3	0.1179	0.3814	2.3	0.4893	0.0283
0.4	0.1554	0.3683	2.4	0.4918	0.0224
0.5	0.1915	0.3521	2.5	0.4938	0.0175
0.6	0.2258	0.3332	2.6	0.4953	0.0136
0.7	0.2580	0.3123	2.7	0.4965	0.0104
0.8	0.2881	0.2897	2.8	0.4974	0.0079
0.9	0.3159	0.2661	2.9	0.4981	0.0060
1.0	0.3413	0.2420	3.0	0.4987	0.0044
1.1	0.3643	0.2179	3.1	0.4990	0.0033
1.2	0.3849	0.1942	3.2	0.4993	0.0024
1.3	0.4032	0.1714	3.3	0.4995	0.0017
1.4	0.4192	0.1497	3.4	0.4997	0.0012
1.5	0.4332	0.1295	3.5	0.4998	0.0009
1.6	0.4452	0.1109	3.6	0.4998	0.0006
1.7	0.4554	0.0941	3.8	0.4999	0.0003
1.8	0.4641	0.0790	4.0	0.5000	0.0001
1.9	0.4713	0.0656	4.4	0.5000	0.0000

D. (3) Picture it. In one of your exercises, you calculated and histogrammed 10^4 averages of two uniform random deviates. Sketch below the approximate appearance of your histogram. (Include values along the x-axis and approximate values on the y-axis.)

Review your results from PS 4, part 1a. Your histogram should be roughly triangular. For full credit, you need the x-axis extending from 0 to 1, and half-way reasonable values on the y (count) axis.

E. (6) Propagating Errors. Suppose that a quantity x is uncertain by 1.0% and y is uncertain by 3.0%. Under the usual assumption of random (uncorrelated) error in x and y, what is the percent uncertainty in z in each of the following cases? [Give numeric answers in those cases where you can, which is most; otherwise give expressions. Hint: Use the concept of relative error propagation to the extent possible.]

1. $z = 5y$

   3.0%

2. $z = 11x^2$

   2.0%

3. $z = \sqrt{7}y$

   1.5%

4. $z = 4xy$

   3.2%

5. $z = \ln y$

   $s_z = 0.030$ (can't convert to %)

6. $z = 2x - 3y$

   $s_z^2 = 4(0.010\ x)^2 + 9(0.030\ y)^2$
   (no simplification in s_z/z)

I. (12) Calibration.

A. (6) A Baratron pressure gauge reads 0.123 V when P = 0.0 and 5.321 V when P = 650 Torr. What is P in Torr when the gauge reads 1.652 V?

$P = a + b\ V \rightarrow$ solve for a and b from given data $\rightarrow$ $P = 191._2$ Torr.

B . (6) You carry out a fit of your thermistor calibration data and get the results shown here.

y = a + b*(x-25) + c*(x-25)^2		
	Value	Error
a	0.050861789	0.001247068
b	0.0036498518	0.0002037433
c	-0.00074572609	3.839555e-05
Chisq	0.00049905721	NA
R	0.96765516	NA

1. Properly state the correction and its error at 25°C.

Correction = y (25) = 0.0509(12) K.

2. If there are 31 data points, what is the estimated standard deviation (s_y) of the calibration data?

s_y^2 = Chisq/($n - p$) = ($4.99 \times 10^{-4}/28$) → s_y = 0.0042 .

3. What is the true temperature if the thermistor reads 32.37°C?

Correction = y(32.37°C) = 0.037256 → True = 32.37 + 0.037 = 32.41 (32.407).