INTRODUCTION TO ORIGIN
(DATA ANALYSIS AND PLOTTING SOFTWARE)
(UPDATED 01/12/09)

Origin (Microcal Software, Inc., One Roundhouse Plaza, Northhampton, MA 01060) is one of several software packages designed specifically for plotting and analyzing quantitative data. You will be using Origin for a variety of applications in this course. Purposes of this document are to introduce you to two of the primary capabilities of ORIGIN software, namely plotting and curve-fitting capabilities, and to illustrate applications of Origin in conjunction with spread-sheet programs such as Microsoft EXCEL.

Data for the spectrophotometric determination of ferrous iron (Table 1, Columns A – E) and masses of paper clips (Table 1, Columns F and G) are used to illustrate applications of the Origin software to both linear and nonlinear data sets. Data in the first three columns represent experimentally determined values of absorbance and percent transmittance for different Fe(II) concentrations treated with 1,10-phenanthroline under appropriate conditions (See text.). Data in the fourth column represent realistic absorbance errors for a spectrophotometer good to $\pm$ 0.2 %T. Data in the fifth column are exaggerated (x 10) transmittance errors; exaggerated values are used to aid in visualization. The data are to be entered into columns A(X) and B(Y) through E(Y) of an Origin worksheet using procedures described below. Origin will be used to plot the data and to fit suitable models to the plotted data. The figure at the end of this presentation illustrates a formatted plot of absorbance vs. concentration with a least-squares line included.

Table 1. Numerical data used to illustrate basic applications of data analysis and plotting software.

Concn. (10^{-4} mol/L)	A (au)[a]	T (%)	Error (au)	Error (%T)	Mass (g)	Number of values
A(X)	B(Y)	C(Y)	D(Y)	E(Y)	F	G
0	0.000	100	0.00087	2	0.4621	1
0.0226	0.0438	90.5	0.00095	2	0.4632	7
0.0458	0.0615	86.8	0.001	2	0.4644	17
0.0915	0.1238	75.2	0.0011	2	0.4655	16
0.229	0.292	51	0.0017	2	0.4667	9
0.458	0.595	25.4	0.0034	2	0.4679	1
0.915	1.167	6.8	0.013	2		
1.84	2.22	0.6	0.12	2		
2.5	3.01	0.1	0.48	2		

[a]Although absorbance is a unitless quantity, it will be helpful to imply units, au, in expressions involving absorbance.

Notes: 1. Throughout this discussion, **"click"** means a <u>single click</u> with the <u>left mouse button</u>; **"double click"** means <u>two quick clicks</u> with the <u>left mouse button</u> and <u>right click</u> means one click with the <u>right mouse button</u>.

2. One of the figures you are to produce is included at the end of this tutorial.

A series of sequential selections from one or more sequential menus will be represented in italics as "*Step1/Step2/Step3*", etc**.** in which the slash marks are separators and are not entered from the keyboard. For example, to open Origin click on "*start/course software/science/chm/microcal origin 6.0*" . User-added text, numbers, etc. are represented by **bold** type.

I. OPENING ORIGIN/ENTERING DATA

The first time you use Origin, you must click on "*start/course software/science/chm/Copy client files*" in sequence. To start Origin, click on "*Origin 6.0 client*". For all subsequent uses, click on "*start/course software/science/chm/Origin 6.0 client*".

When Origin opens on screen, you should see a "*menu*" bar (in light gray) and two rows of toolbars (to which we will refer as "*toolbars*") at the top of the screen, a worksheet with two empty data columns, A(X) and B(Y), and a toolbar near the middle or bottom of the screen we shall call the "*plotting toolbar*".

To enter **concentration** data in Column A(X), click on cell A-1, type the first concentration value, click the "*Down arrow*" or "*Enter*" on the keyboard, type the second concentration value, and repeat the process until all concentration data are entered in column A(X). Repeat the process to enter absorbance data in column B(Y).

It will be necessary to add columns for the other data in Table 1. To add a column, click on "*Column/Add new columns/OK"* from the menu bar at the top of the screen. Enter data from Table 1 in Columns A – E.

Use "*File/Save project" as* options from the menu bar to save your worksheet onto a floppy disk as "*File name"* **ORIG1_A.ORG**.

SUGGESTIONS: It is strongly suggested that you save your work on a floppy disk after major steps below. This will save you grief in case you accidentally lose a file and it will permit you to explore capabilities of Origin other than the minimum essential features described below.

II. PLOTTING DATA (Linear plot)

Data for absorbance vs. concentration in Table 1 are used to illustrate how to plot data and format plots using Origin 6.0.

A. Unformatted scatter plot

To generate an unformatted "Scatter plot" (plot of individual data points) of Absorbance vs. Concentration:

a. Click on "*Plot/Scatter plot"* in the menu at the top of the screen.
b. Click on "*A(X)/<->X"* in the drop-down menu to select concentration data in the A-column as the independent variable (X-axis).
c. Click on "*B(Y)/<->Y"* in the drop-down menu to select concentration data in the B-column as the dependent variable (Y-axis).
d. Click on "*OK*"; an unformatted or partially formatted scatter plot should appear with data in Column A on the abscissa (X-axis) and data in Column B on the ordinate (Y-axis).

Notes: There will be two small icons in the upper left corner of the plot, one colorful one next to "*Graph1*" and one gray one below it with a number (probably "1") in it. The colorful icon is called the "***Hide/delete***" icon herein; the numbered icon is called the "***Layer icon***".

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e. Double click on the "*Hide/delete*" icon and note the options in the pop-up menu; Click on "*Cancel"* so that the figure will not be hidden or deleted. This function permits you hide or delete unwanted plots.
f. Double click on the "*Layer icon*" and note the options; then click on cancel. This icon permits you to add other data (such as error bars) to a plot.
g. The *Screen-reader* tool (small square with cross-hairs in it near the center of the screen) is used to read values of X/Y coordinates. With a plot in the foreground, click on the Screen-reader tool, place the cursor somewhere on a plot and Click the left mouse button. Numerical values of the X/Y coordinates should appear on the screen. Click on the *Pointer* tool to return to the normal mode. Help can be used to learn more about this and other tools.

B. Error bars
   It is always good practice to include error bars on data plots. The following procedure illustrates how to add the absorbance errors in Column D(Y) as error bars on your plot; a similar procedure can be used to add errors in any column to a plot.

   a.   Double click on the "*Layer icon*"; click on "*Plot association*".
   b.   Click on (Select) "*Data 1: A(X),B(Y)*" in the **bottom box**.
   c.   Click on "D(Y)/<->YEr/Replace/OK/OK"; the plot should reappear with error bars on it.

Notes: For multiple plots in a window, click on the data for the plot to which error bars are to be added, click on "*<->YEr*" to add error bars in the Y direction (the usual case) or "*<->Xer*" to add error bars in the X direction.

C. Window control
   1. Screen layout. Origin permits a variety of window options controlled by the *Window* option in the menu bar. To examine some of these options, click on:
   a.   "*Window/Tile horizontally*".
   b.   "*Window/Tile vertically*".
   c.   "*Window/Cascade*".
Using the screen in the "*Window/Cascade*" format, click anywhere on the edges of the worksheet and note that it is brought to the forefront. Then click on the graph to bring it back to the forefront.
   2. Sizing figures/worksheets. To change the size of the graph display on the screen, move the cursor to the gray frame at the bottom of the graph until a double vertical arrow ($\downarrow\uparrow$) arrow appears; Click and Drag the edge of the frame to increase or decrease the size of the graph. Adjust the size to your liking and proceed.
   3. Zoom/Suppress. The first three icons in the second row of the toolbar can be used to zoom in or out on a graph. To *zoom in* on the graph, click on the "*eyeglass +*" icon, place the cursor on the figure and click. Use the position arrows at the corners of the frame to view different parts of the figure.
   To restore to the normal view, click on the "*full-page icon*" (third icon in the set). To *zoom out* on the graph, click one or more times on the "*eyeglass -*" icon, then restore to full page using the "*full-page*" icon.

D. Formatting figures
   Data plots should always have axes with tick marks on all four sides; the following stepwise procedure will help you format the figure plotted above.
   1. Abscissa. With the plot in the foreground, click on "*Format/Axes/X Axis*" from the menu bar and:
      a.   Choose "*Scale/Horizontal*" notecard and set: "*From*" to **-0.25**, "*To*" to **2.749**, "*Type*" to **linear**, "*Rescale*" to **manual**, "*Increment*" to **0.5** "*# Minor Ticks*" to **1**, "*First tick*" to **0**. (This sets parameters for the X-axis.)
      b.   Choose the note card "*Title and format/Bottom axis*" and: **check** "*Show axis and ticks*", Change"*Title*" to **Concentration**, set "*Color*" to **black**, "*Thickness*" to **1.5**, "*Major ticks*" to **In**, "*Minor ticks*" to **In**.
      c.   Click on "*Top axis*", set "*Major ticks*" to **In**, "*Minor ticks*" to **In** and leave other settings as they are.
      d.   Click "*Apply /OK*" to view the modified graph.
   2. Ordinate. Use a similar procedure (Steps a - d) to format the ordinate of your graph, replacing "*X axis*" with "*Y axis*", "*Horizontal*" with "*Vertical*", and '*Bottom*" and "*Top*" with "*Left*" and "*Right*". The ordinate title should be **Absorbance (au)** the scale should be from **–0.25** to **3.6**.

NOTE: After making appropriate settings, your figure should have axes and tick marks on all four sides; bottom and left axes should have titles and numbers on them; and each axis should extend in each direction slightly beyond data points and numerical scales.

E. Sizing and positioning

The small square in the top left corner of your figure with a number in it (the *Layer icon*) can be used to adjust the size and position of your figure.

     a. Double-click on the "*Layer icon*"; click on "*Layer properties*" in the pop-up menu and select the "*Size/speed*" note card.

     b. Make sure the "*Units*" box reads **% of page**; set both "*Left*" and "*Top*" to **20**, "*Width*" to **65** and "*Height*" to **50**; click on "*OK/ OK*". The figure should be sized and positioned nicely on the page.

F. Relabeling the X axis

The purpose here is to illustrate how to use subscripts/superscripts, etc. and how to control font sizes. The abscissa is to be relabeled **Concentration (10^{-4} mol/L)** and set to "*font size*" **24**.

    1. To insert the 10^{-4} mol/L unit:

     a. Double click on "*x axis label*", a pop-up box will appear with the title, **Concentration,** in the top and bottom sub-boxes. (This is the title you gave the X axis earlier.)

     b. Place the cursor just after **Concentration** in the top box, insert a space and type **(10 mol/L)**.

     c. To insert the -4 power, locate the cursor just after the 10, click on "x^2" at the top right side of the label square and type **-4** in the parentheses that appear.

     d. Click on "*OK*".

    2.To set the font size of the X axis to 24, replace any number in the "*Size*" box with 24.

    3. Follow the same procedure to set the font size of the Y-axis title to 24.

Note: B, I, U and Γ correspond to bold, italics, underline and Greek; x_2 refers to subscript.

G. Numbers on axes

    1. To change the font size for the numbers on the abscissa to 24 points, place the point of the cursor carefully on one of the numbers on the X axis, double click and select the "*Tick labels*" note card from the choices. Change the "*Point*" setting to **24**. Note the "*Divide by factor*" box on this card before you check "*OK*" and see the note below.

    2. Repeat the process for numbers on the ordinate.

Note: The "*Divide by factor*" feature is used to change very large or very small numbers to small whole numbers on the axes. For example, if the numbers on an axis were in the range of 0.000013, etc., which would clutter the axis, setting the "*Divide by factor*" to 1e-5 would change the numbers on the axis to 1.3, etc. The factor should of course be included in the axis label as **10^{-5} units** or **units x 10^5** (not "x 10^{-5} units"). (Ask if you do not understand this latter point.)

H. Data-point format

Origin permits the selection of a wide variety formats for data points and lines. To select a format for data points in the plot just constructed:

     a. Use the "*Zoom*" function described earlier to observe the data symbols used in your plot (Probably closed squares) and use the "*View*" function to return to the "*Whole page*" format.

     b. Click on "*Data/ Data1 A(X), B(Y)/Symbol*".

     c. Click and release on the large black "down triangle" (∇) and select the open square option from the many choices.

     d. Use the "*Size*" function to set the point size to 8.

     e. Click on *"Apply/OK"*.

     f. Use the "*Zoom*" function described earlier to observe the data symbol.

I. Text

All figures should include identifying information; the text feature of Origin makes it easy to add identifying information to figures. The text function is illustrated by adding a title to the figure prepared above.

    a. Click on the "*T*" (for text) on the toolbar and place the cursor at a point above and slightly to the left of the figure and click one time.

    b. Type **Figure 1A. Absorbance vs. concentration for spectrophotometric determination of ferrous iron**.

    c. Set the font size to 24 and change the color to black.

    d. Click "*OK*".

NOTES:

1. The text will likely run over the side of the figure. Decide on a place or places to split the title; double click at any point on the text; place the cursor at the point in the text box at which the text is to be split; press the "*Enter*" key on the keyboard and click on "*OK*".

2. Text can be moved either by dragging it with the left mouse button held down or by clicking on it and using the "up/down", "left/right" arrows on the keyboard.

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    e. Use the "Text" procedure to place an upper-case **A** in the upper left-hand corner of your figure and to label the figure in the lower left hand corner of the page as follows:

DISK: CHEM XXX ; FILE: ORIG1_A; PLOT1, COLUMNS A AND B in which XXX is your course number.

J. Printing a figure

    a. Make sure the figure is in the forefront of the screen.

    b. To format your figure for printing, Click on "*File/Page setup/ Portrait/OK*".

    c. To print your figure, click on "*File/Print/OK*".

SAVE YOUR FILE ON A FLOPPY DISK AS ORIG1_A.ORG BEFORE PROCEEDING WITH THE NEXT PART.

K. Preparing a template

This section explains how you can prepare and save a template that will help you avoid having to repeat some of the steps above each time you prepare a new figure.

    a. Bring the worksheet to the forefront and double click on the green button in the upper left corner and select delete from the menu. The worksheet will disappear and the data will disappear from your figure.

    b. Click "*File/New/Worksheet*/OK"; a new worksheet will appear.

    c. Use "*Save As*" to save this template as "Formatted Template" on your disk.

    d. To illustrate the use of the template, Click File/Close. Then Click "*File/Open/A/FORMATTED TEMPLATE*". Click "*File/New/Worksheet*/OK"; a new worksheet will appear. Enter the numbers 2, 4, 6, 8 in rows 1 – 4 of **Columns** A and B of the worksheet. Then highlight data in column B, bring the blank figure to the forefront, Click "*Graph/Add Plot to Layer/Line + Symbol*"; a Line + symbol plot should appear.

    e. Close this file without saving changes before proceeding to PART III.

Note: You can use the FORMATTED TEMPLATE for any of the plots you will do in the remainder of this tutorial or this course. It will usually be necessary to ranges of axes, axis labels, titles, etc., but the template should save you significant amounts of time.

III. LEAST-SQUARES FIT OF A LINEAR MODEL
      The Origin software includes built-in least-squares fitting routines for several types of functions, including linear relationships such as that represented by the absorbance vs. concentration data plotted above. The purpose of this section is to illustrate the use of the linear fitting function and subsequent plotting of results.

A. Rationale
      The absorbance vs. concentration data are expected to follow a linear relationship of the form

$$A = a + bC \tag{1a}$$

in which A is absorbance, a and b are the intercept and slope, respectively, and C is concentration. This expression can be written in the more general form

$$Y = a + bX \tag{1b}$$

Either way, the goal of a fitting process is to obtain best-fit values of the intercept, a, and slope, b as well as other statistical quantities to be discussed in class.

NOTE: Use a different file name, e.g. ORIG1_B, to save modifications made to this plot in subsequent steps.

B. Fitting process - built-in algorithm
      There are different ways to use Origin to do a least-squares fit of a linear model to a data set. One of the simpler options is illustrated here.
      Numerical values of slopes, intercepts etc. will be displayed on the screen below the "*plotting toolbar*" near the middle or bottom of the screen. It may be necessary to "drag" the "*plotting toolbar*" up to free some screen space below it after you complete the fitting process.
      1. Linear fit using the "*Tools*" menu. The purpose of this section is not only to illustrate how to use the "*Tools menu*" to obtain a least-squares fit of a data set but also to illustrate how to format the resulting figure to conform to good scientific and engineering practices.
      a. Open the figure saved above as ORIG1_A. (Click "*File/Open/A/ORIG1_A*")'
      b. With the plot in the forefront, use the "*Format/Axes/X axis*" sequence on the menu bar to set the X axis range from 0 to 2.75.
      c. Click on "*Tools/Linear fit*" from the menu bar. The drop-down "*Fit*" menu in the upper left corner has two options, "*Operation*" and "*Settings*".
      d. Click on "*Settings*" first and set "*Points*" to **9** (there are nine sets of points in the data set), "*Confidence level*" to **95**, and "*Range margin*" to **0**, clear "*Residuals data*" if it is set, and click on the box "*Span X Axis*".
      e. Return to "*Operation*" and click on "*Fit*"; a fitted line should appear on your figure and numerical values of least-squares statistics (slope, intercept, etc.) should appear below the plotting toolbar. Click on the small x in the upper right corner of the "*Linear fit*" dialog box to close it. If the numerical data for slope, intercept, etc. do not appear below the plot:
        i. Click on *"View/Results log"*. If results still do not appear:
        ii. Place the cursor on the bottom of the frame of the colorful toolbar at the bottom of the screen and drag the toolbar up to about midscreen. If the numbers still do not appear:
        iii. Click on *"View/Results log"* again; fitting results should appear.

      f. Click on the X in the upper right corner of the "Fit" dialog box to close it.
      g. Save the figure on your disk as **ORIG1_B**.
      h. After saving the figure, zoom in on it and note that the fitted curve passes through the points; this is not good form. We will modify the figure later to pass the fitted curve "under" the points.

     i. Bring the plot to the forefront again.

  2. <u>Handling fitting parameters</u>. The following procedure illustrates how to put the fitting parameters (i.e. the numerical data below your figure) onto your figure and into a script window to be saved or printed.

    a. To put the fitting parameters onto your figure:
      i. Put the cursor anywhere on the fitted parameters and click the RIGHT mouse button.
      ii. Click "Select all".
      iii. Put the cursor anywhere on the fitting parameters again and click the RIGHT mouse button; then click "Copy" in the dialog box (with the LEFT mouse button).
      iv. Click "*Edit/Paste*" on the menu bar; the fitting parameters will be pasted onto your figure. You can reduce the size by double clicking on the text and removing spaces etc.
    b. To put the fitting parameters into a script box:
      i. Copy the parameters as described immediately above (a. i – iii).
      ii. Click on "*Window/Script window/Edit*" from the drop-down menu.
      iii. Click on "*Edit/Paste*" in the script window; parameters should be pasted into the script window.
      iv. Use the "*File*" function in the script window to **save** and/or **print** the fitting parameters.

    c. Save the figure as ORIG1_B and print the figure and script window.

  3. <u>Replotting the figure</u>. It was noted above that it is bad form to have a fitted line overlay experimental data. The following procedure will illustrate how the data points can be removed from the graph and replotted over the fitted line.

    a. With the figure in the forefront, click on "*Data/Data A(X),B(Y)*" from the menu bar.
    b. With the "*Data A(X),B(Y)*" highlighted, press the delete key on the keyboard; data points will disappear but the line will remain.
    c. Double click on the small square with a number in it near the top left corner of the graph frame.
    d. Highlight (click on) "*Data1 B*" in the "*Data available box*", click on the arrow ($\Rightarrow$) toward the "*Layer contents*" box and click on "*OK*".
    e. Zoom in on the resulting figure to observe that the fitted line does not pass through the points.
    f. Save the figure as ORIG1_B.

C. <u>Fitting process – Custom model</u>
  Although Origin has many built-in fitting algorithims, you will need to use custom designed algorithms from time to time. The linear data set is used here to illustrate how custom fitting programs can be used.
  Close the active window, open the first window saved (e.g. ORIG_A) and be sure the plot is in the forefront.

  1. <u>Creating a user-designed fitting algorithm</u>. As noted earlier, the absorbance vs. concentration data conform to a linear relationship of the form

$$A = a + bC \hspace{4cm} (1b)$$

When custom fitting algorithms are used, Origin automatically assigns default parameter symbols, P1 and P2, for the fitting parameters, unless one specifies otherwise. In this case, the resulting expression will have the form

$$Y = P1 + P2*C \hspace{4cm} (1c)$$

2. <u>Selection of correct mode</u>. The Origin software includes an "*Basic mode*" and an "*Advanced mode*"; you will use the "*Basic mode*" in this exercise.
   a. Click on "*Analysis/Nonlinear curve fit*" from the drop-down menu; a "*Nonlinear curve fitting*" dialog box will appear.
   b. Move the cursor to the bottom of the dialog box until a double up/down arrow appears, then click and drag the bottom line of the dialog box down to its maximum vertical expansion.
   c. If either "*Close*" or "*Accept*" buttons appear, you are in the "*Basic mode*" dialog box; go to the next step. If a "*Basic mode*" button appears in the lower right corner of the dialog box, click on it to change to the "*Basic mode*" and go to the next step.
   d. If the "*Accept*" button appears, click on it and proceed to the next step; if the "*Close*" button appears, proceed to the next step.

3. <u>Implementing a custom fitting algorithm</u>. The above sequence should set the dialog box to the "*Nonlinear curve fit:Select function mode*". Click on "*New*" and proceed as follows.
   a. In new menu box, change: "*Name*" box to "**LINFIT**", "*Form*" to "**Expression**" and "*No. of Parameters*" to **2**. Origin will insert P1 and P2 for "*Parameter names*".
   b. In the "Definitions" box, type P1+P2*X and click on "Save/Accept".
   c. Click on "Start fitting" and then on "Active data set" in the new dialog box.
   d. A new dialog box will appear in which you must insert initial values for the fitting parameters, P1 and P2. Clear the dashes in the boxes and set "*P1*" to **0.01** (see Note 4 below) and "*P2*" to **1** and click on "*1 Iter*"; numerical values of fitting parameters will appear.
   e. Be sure both boxes under "*Vary ?*" are checked.
   f. Click on "Done"; fitting parameters will be pasted onto the figure and entered below the figure. The procedure described above (III-B-2-b) can be used to paste these parameters into a script window.

NOTES: 1. Both a and b were used in the fitting described in III-C above. It is sometimes desirable to fix one or more parameters. For example, the above fit can be forced through zero by clearing the "*Vary* ?" box (III-C-3-e) adjacent to the intercept, a, and inserting zero in the "*Parameters*" box. Try it.
  2. This feature is particularly useful when complicated expressions are being fit to complex data sets for the first time.
  3. For complex relationships with poorly defined initial estimates of fitting parameters, it usually is best to do approximate fits initially by clicking on "*1 Iter*" one or more times before asking for a full fit.
  4. Never set the initial estimate of the intercept to zero (III-C-2-d). Values of some fitting parameters smaller than about 1×10^{-15} interfere with procedures used to obtain numerical estimates of derivatives.

IV. USE OF ORIGIN WITH A SPREAD-SHEET PROGRAM
    It is often necessary to use best-fit parameters to compute expected curves to be compared with experimental data or to extend the range of computed data beyond the range represented by the data set. This is easily done using a spreadsheet. The purpose of this section is to illustrate how a spreadsheet can be used in conjunction with Origin to recalculate and replot data with the data points superimposed on the best-fit line.

A.   <u>Using Excel</u>
1. After doing a linear fit in Origin (Part III-B or III-C), look at the Results log and write down values of A (should be about A = 0.0204) and B (should be about B = 1.201). These are the slope and intercept of your data.
2. Copy Column A of your origin worksheet, open an Excel worksheet and paste Column A from Origin to Column A of Excel. Type 2.75 after the last entry in Column A. You should have data in rows A1 thru A10.
3. Highlight cells B1 thru B10 of the Excel worksheet.

4. With Excel cells B1 thru B10 highlighted, click in the Excel formula bar and type =0.0204+1.201*A1:A10. Then press CTRL/Shift/Enter simultaneously. Calculated best-fit values of Absorbance should appear in Cells B1 thru B10.
5. Minimize the Excel worksheet for the time being.

B.   Plotting data using Origin
     The purpose here is to first plot data calculated using Excel as a line and then to superimpose the original data as discrete points on top of the line. We shall use the FORMATTED TEMPLATE (Part II-J) to plot a formatted figure.
1. Preparing the Origin worksheet
     a.   Highlight and Copy data in Columns A and B of the ORG1_A worksheet and close the file.
     b.   Open the FORMATTED TEMPLATE file and open a new worksheet. (See Part II-K-d).
     c.   Paste data copied from the ORG1_A worksheet into Columns A and B of this worksheet (or type in the data from Table 1). Type the value 2.75 in Cell A-10 of the origin worksheet.
     d.   Click "Column/Add New Column/OK" to add a new column.
     e.   Deemphasize Origin, reemphasize the Excel worksheet and copy data in Column B of the Excel worksheet.
     f.   Deemphasize the Excel worksheet, emphasize the Origin worksheet and paste the calculated data in Column C of the Origin worksheet.

2. Plotting the line
     a.   Highlight Column C in the Origin worksheet.
     b.   Bring the formatted graph to the forefront and Click "*Graph/Add plot to layer/Line/OK*"; a line plot should appear.

3. Adding scatter points
     a.   Bring the worksheet to the forefront and highlight Column B.
     b.   Bring the formatted graph to the forefront and Click "*Graph/Add plot to layer/Scatter/OK*"; Data points should be superimposed on the line plot.
     c.   Change the X/Y scales so that the line and points fall inside the axes. (See Part II-D-1 and 2).
     d.   Change points to open symbols to visualize that points are superimposed on the best-fit line. (See Part II-H.)
     e.   Save using a suitable file name and print.

V. NONLINEAR DATA SET (GAUSSIAN FUNCTION)
     An attractive feature of Origin and other data analysis programs is that they permit fits of user-selected models to nonlinear data sets. This section illustrates the use of Origin to fit a Gaussian model to a data set (Table 1, Columns F and G) similar to that obtained for paper clips in the laboratory.

A. Mathematical model
     The data are expected to conform to a model of the form

$$f = \frac{k}{s\sqrt{2\pi}} Exp\left[-\left(\frac{(x-x_{Av})}{2s}\right)^2\right] \tag{2a}$$

in which f is the frequency of occurrence, k is a constant, s is the standard deviation, x represents individual values of the mass and x_{Av} is the average value of the masses. Assigning P1 = k, P2 = s and P3 = x_{Av}. The equation in Origin syntax can be written as

$$(P1/(P2*(2*pi)^0.5))*Exp(-((x-P3)/(2*P2))^2) \tag{2b}$$

This is the model we shall fit to the data in Columns F and G in Table 1.

B. Plotting the data

Open the FORMATTED TEMPLATE file prepared in Part II-K. Bring in a new worksheet (Part II-K) and enter data from columns F and G of Table 1 into Columns A and B of the Origin worksheet. Highlight Column B, bring the formatted graph to the forefront and Click "*Graph/Add plot to layer/Scatter/OK*". A peak-shaped plot should appear.

C. <u>Fitting a model to the data</u>
    The following is an abbreviated version of the procedure described in more detail in Part III-C.
1. With the plotted curve in the forefront, Click "*Analysis/Nonlinear curve fit*".
2. Click "*New*" and set the "Number of parameters" to 3.
3. Type Eq. 2b above into the "Definition" box; DO NOT INCLUDE AN = SIGN.
4. Click "Accept".
5. Click "Select data set/B/Assign/Start fitting".
6. Set P1 to 0.05 and P2 to 0.001, P3 = 0.46 and Click "1 iter".
7. If there is no error message, Click "10 Iter" several times until values of the fitting parameters do not change.
8. If there is an error message, Click "OK" and check initial estimates of parameters. If initial estimates are as suggested above then Click "Select function"/Edit" and look for errors in the equation entered into the Definition box. Then follow steps 4 – 7 above.
9. Successful completion should give a fitted bell-shaped plot through the data.
10. Label the abscissa (Mass(g)) and ordinate (Number) and save and print the figure.
11. Compare best-fit values of P3 and P2 to the calculated average (0.4649 g) and standard deviation (0.00116 g).

VI. NONLINEAR DATA SET (TRANSMITANCE)
    Data for percent transmittance vs. concentration (Columns A and C) will be used to illustrate application of the curve-fitting process to a nonlinear data set.
    Based on the following relationships among absorbance, A, concentration, C, and percent transmittance, T (%),

$$A = a + bC = -\log \frac{T(\%)}{100} \qquad\qquad (3a)$$

it follows that percent transmittance is related to concentration as follows

$$T(\%) = 100 \text{ x } 10^{-(a+bC)} \qquad\qquad (3b)$$

Use the following steps to illustrate the use of Origin software to fit this nonlinear relationship.
    1. Close the current Origin file and open FORMATTED TEMPLATE.
    2. Bring in a new worksheet (Part II-K). Enter data from columns A and C of Table 1 into Columns A and B of the Origin worksheet. Highlight Column B, bring the formatted graph to the forefront and Click "*Graph/Add plot to layer/Scatter/OK*". A scatter plot of Transmittance vs. Concentration should appear. (Transmittance should decrease nonlinearly with concentration.)
    3. Add values in Column E of Table 1 as error bars (Section II B).
    4. Use procedures described in Part V to fit the two-parameter model in Eq. 3b to the plot of percent transmittance vs. concentration. (You can use either the Origin-defined parameter names (P1 and P2) or check the "User defined parameter names" box and use a and b (or any other symbols you choose) as the parameter names.

NOTES: 1. The expression in the "Equation box" should be 100*10^(-(α+βX)) if you use user-defined symbols, α and β, or 100*10^(-(P1+P2*X)) if you use Origin-generated symbols, P1 and P2, for fitting parameters.

2. Use values close to the intercept (a ≅ 0.02) and slope (b = ≅ 1.2) values obtained from the linear fit of absorbance vs. concentration as initial estimates of the fitting parameters. (For some unknown reason, the version of Origin used to write this tutorial does not like "0" as an initial estimate.)

3. Best-fit values of a and b are not expected to be exactly the same for the linear and nonlinear fits because these are experimental rather than ideal data.

5. Use Eq. 3b, a spread-sheet program and computed values of parameters, a and b or P1 and P2, to compute values of transmittance for values of concentration between 0 and 2.75 with a step size of 0.025 i.e. T (%)$_n$ for C$_n$ = 0.000, 0.025, 0.050, 0.075 .... 2.70, 2.725, 2.750 (x 10^{-4} mol/L). (NOTE: Because the x 10^{-4} mol/L unit is not included in the Origin worksheet, do not include it in the spreadsheet calculations.

These calculations are done most easily using a spreadsheet and data can be transferred from the spreadsheet to an Origin file using the "Copy"/"Paste" operations. With Microsoft EXCEL, the "Edit"/"Fill" (pull-down menu) can be used to generate the series of concentration values. Ask for help if you need it.

6. Construct a formatted graph (Part IV-B) containing plots of computed and experimental data for Transmittance (%) vs. Concentration (10^{-4} mol/L). For the concentration range from zero to 2.75 x 10^{-4} mol/L. (Use a dashed-line for computed values and an open-triangle scatter plot for experimental data and remember that the line should not overlay the experimental points (Part IV-B).)

VII. **USING "*HELP*"**

Origin includes an excellent "Help" section; you should learn to use it. For example, to get information about adding error bars to a graph:

1. Click on "*Help*/*Search*" and type "error" in the dialog box.
2. Select "*Error bars dialog box*/*Display*".
3. Click on the double arrows right, ">>" until you find "Adding Error Bars using the Select Columns for Plotting Dialog Box" which gives the procedure summarized in the tutorial.

You will probably need to use "*Help*/*Layer*" to learn how to use the "*Layer n*" dialog box.

H. Pardue, 1/02

Experimental and fitted values of absorbance vs. concentrationfor the spectrophotometric determination of Fe(II).
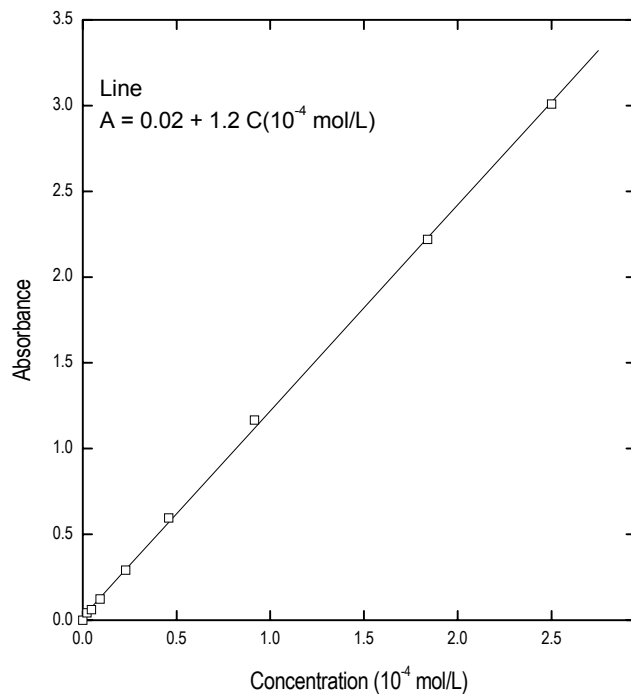
This figure was generated using a FORMATTED TEMPLATE as described in Parts II-J and IV-B.

COMPUTER: HOME, FOLDER:CHEM 321/323_FALL_OO, SUBFOLDER: SPECIAL TOPICS, FILE: ORIGIN TUTORIAL_F00

REPORT
    No narrative report is required. You should print and turn in four figures, Figures to be turned in are those associated with:
    Part II-J
    Part III-B-3-f
    Part IV-B-3-e
    Part V-C-10