Graphing & Curve Analysis Using KaleidaGraph 4©

Fall 2008

The following instructions guide you through the process of using KaleidaGraph to create a graph from a set of data, and to calculate and draw a line or curve that best fits your data. The information determined from this best-fitting line will be used to analyze your data. These graphing techniques will be used in most of the labs this semester, so it is important that you understand them. You will also find that these techniques are useful for analyzing data from other disciplines. *Bring these instructions to lab each week!*

It is important to note that KaleidaGraph can open Microsoft Excel worksheets, or you can copy and paste data from Excel into KaleidaGraph. This allows you to use Excel for data acquisition and calculations, and then use the powerful graphing tools of KaleidaGraph to render your final plot.

Entering the Data

1. When you start KaleidaGraph, you are presented with a spreadsheet (the "Data" window). As seen in Figure 1 below, data cells are designated by a row number (beginning with row '0') and a column title (A, B, C, ...). In addition, columns are referred to by a column number (c0, c1, etc.) which appears below the title. The column number designation is not absolute, and its purpose will be revealed as you perform this exercise. A *Formula Entry* window appears at the bottom of the screen; this is where you enter equations to act on your data (if this window isn't visible, choose **Formula Entry** from the **Windows** menu).

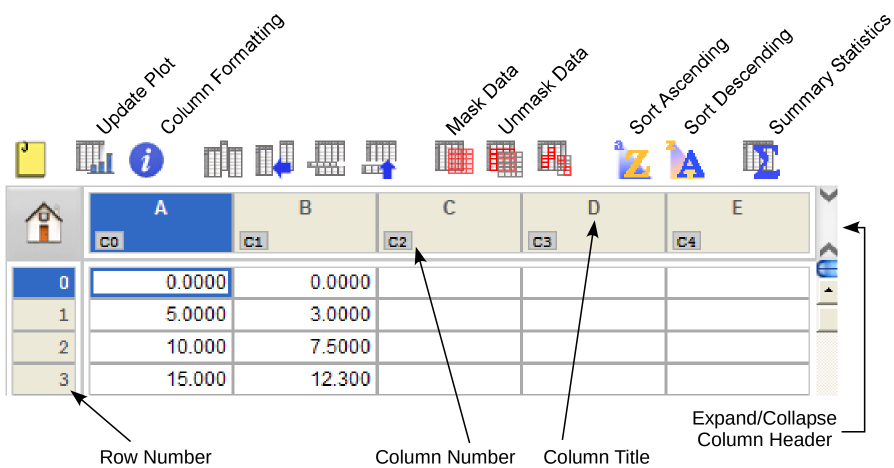

Figure 1 - The KaleidaGraph 4 Data window

A toolbar appears above the Data window; some of the more useful ones are labeled above (the name of the button will appear if you place the mouse cursor over it). To the right of the column titles is a button that will show or hide the column numbers.

2. The columns containing your data must be labeled appropriately to ensure the proper orientation of your graph. Double-click the letter above a column and type the title for each column you will use, replacing A, B, C, etc. (Be sure to include units in the title!). *In general, you will find it easier to have the first column contain the values to be plotted along the 'X' axis.*

3. Enter your data in the spreadsheet. Generally, you will only need to include the data that will actually be plotted, not your raw measurements. Be sure to save your data; if you need to recheck your results, you won't have to retype it.

Creating A Graph

4. If you select *Gallery* from the menu bar, you will see that there are several different types of graphs available. In this course, you will be creating scatter plots of X and Y data. From the **Gallery** menu, choose **Linear**, then **Scatter** (*do not choose "Line"!*). The *Plot* dialog box will appear.

5. In the Plot dialog, you will select the data that will be graphed along the X and Y-axis of your plot (now you see why it was important to label your columns in step 2!). As shown in Figure 2 at right, click the radio button (the circle) under the X next to your data column to be plotted along that axis; do the same for Y, then click the **New Plot** button. Your graph will appear in a separate window.

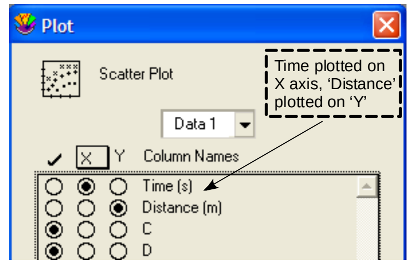

Figure 2 - Selecting data to graph

6. Click the window containing your plot once to select it. You may now change the appearance of the graph. You might need to change the following:

   - You can resize the graph by first dragging a corner of the *window* to expand it, then drag the lower right corner of the *graph* itself.
   - From the *Plot* menu, look at the following options:
     i. Uncheck **Display Legend**: you should display the legend when plotting more than one set of data on a single graph.
     ii. Check **Display Equation**.
     iii. Check **Auto Link**: If you change a data point, the graph will automatically be updated.
   - Double-click the title of the graph (it probably says "DATA 1", unless you saved your data in step 3), and replace it with a clear, descriptive name.

Curve Fitting

7. Now that your graph is created, you'll need to analyze it. The first step is to add a best-fit line or curve. Click the graph window *once* to select it, then select the **Curve Fit** menu. There are 10 possible fits to choose from, including "Linear" (for straight-line data in the form of $y = mx + b$), "Polynomial" (of 2nd order: $y = ax^2 + bx + c$), "Exponential" ($y = ae^{bx}$), and "Power" ($y = ax^b$). (There is also a "General" menu that we'll use later to select user-defined fits.) Other fits are available, but they won't be used in this course. Select the appropriate fit, *click the box next to the name of your data column*, then click the **OK** button.

   *If you wish to change the type of fit, first choose the existing fit, click the **Deselect** button, then click **OK**; you can then choose the correct fit. If you don't remove the incorrect one, two fits will appear on your graph.*

8. The best-fit line appears on your graph, as well as the appropriate equation for the fit chosen (if the equation does not appear, choose **Plot ⇒ Display Equation**). KaleidaGraph calculates the values of the appropriate coefficients *a*, *b*, *c*, and *m*.

   *If the best-fit line ends at the extreme data points, choose **Curve Fit ⇒ Curve Fit Options**; checking **Extrapolate Fit to Axis Limits** will extend the line across the graph.*

   You will note that more significant figures are presented in the evaluation of the coefficients than may be dictated by the accuracy of your measurements. It is from these coefficients that you will be performing your analysis.

   - Note that the procedure just performed does not give estimates of the *errors* in the coefficients. You will learn how to do this below.

9. At this point your graph is complete. Your instructor can show you how to edit portions of the graph if they need to be changed. If you find that a data point is incorrect, change the number, or delete the point, and the graph will update automatically (if **Auto Link** is selected under the **Plot** menu).

Evaluating Uncertainties In The Data

When evaluating data, it is important to be aware of the uncertainty of the measurements. KaleidaGraph can provide this information when calculating the best fit. The following procedure details the analysis of linear data, but it can be calculated for other fits as well.

10. If you already have a best-fit line on your linear graph, remove it by selecting **Curve Fit ⇒ Linear**, and clicking the **Deselect** button. Click **OK** to return to your graph.
11. Again select the **Curve Fit** menu, choose **General**; you will see a series of custom fits that have been added by your instructor. Choose the desired fit, select the data column, then click **OK.** *(If you are performing the "Fitting Data to a Mathematical Function" exercise, then choose **Linear Through Origin** for data set #1; this will be the only time your choose this fit!)* A best-fit line will again appear, along with a table of results, similar to Figure 3 at right (which shows the *Linear w/Uncertainties* fit, with slope and intercept). If the table does not appear, choose **Plot ⇒ Display Equation**. Click and drag the table to position it on your graph so that it doesn't obstruct the data points.

y = b+a*x		
	Value	Error
a	1.9809	0.077808
b	-0.061496	0.26263
Chisq	0.18429	NA
R	0.99769	NA

Figure 3 - Curve fit results

At the top of the table you'll see the generic form of the fit chosen. In the first column you'll see a list of the coefficients (a, b, etc.). The second column ("Value") lists the numerical value of each coefficient. The third column ("Error") gives the uncertainty (the *standard error*) for each coefficient. *(Ignore for the moment the rows labeled "Chisq" and "R").*

For the results shown, the value for the slope (coefficient *a*) would be presented – assuming four significant figures and units of velocity – as:

$$1.981 \pm 0.07781 \; m/s$$

Frequently we will display the uncertainty in the coefficient as +/- *twice* the standard error:

$$1.981 \pm 0.1556 \; m/s$$

Twice the standard error provides a 95% confidence level concerning the data, i.e. there's a 95% chance that the data will fall within twice the standard error of 1.981 *m/s*.

Calculating Residuals

When you perform curve fitting, the line that KaleidaGraph draws won't necessarily go through each data point. The *residuals* are the difference between the actual *y* values of the data, and the corresponding points on the line.

If you've used a spreadsheet program before (such as Microsoft Excel), the difference you'll notice when using KaleidaGraph is that you don't reference cells *individually*, but by column. Columns are designated by a column number that appears below your titles in the data window, as seen in Figure 1. The first column is c0, then c1, c2, etc. The interesting thing about KaleidaGraph is that these column references are not absolute; clicking the mouse on the title for the 2^{nd} column selects that column and changes its designation to c0. For our purposes, always be sure that the *first* column is selected, so that it will be referred to as column *zero*. If you forget to do this, you'll get an error message or incorrect results when trying to execute a formula.

12. Click on the graph window to select it, and make sure it contains a curve fit. For "Data Set #1" of the "Fitting Data" exercise, be sure to choose the General fit "Linear through origin".

13. With the fit in place, *again* go to the **Curve Fit ⇒ General** menu, and *again* click the fit you just chose (there will be a check mark next to the name). In the dialog box that appears, click the down-arrow that appears below "View", and choose **Copy Residuals to Data Window**. When you click **OK**, a column called "Residuals" is added to your data.

Calculating SSR (also known as χ^2, "Chi Square")

Now that the residuals have been calculated, they need to be squared, and these squares added up. As you'll see, KaleidaGraph will automatically calculate the SSR for you when you apply a General fit. You will create a short formula to calculate the SSR from the residuals calculated in step 13, and then compare the result with that obtained by applying a curve fit.

14. In the *Formula Entry* window, click the **F1** button (note that you can enter 8 different equations). KaleidaGraph refers to the first column of your data as `C0`, the zeroth column. The residuals are located in the third column (`C2`), and we want the square of the residuals to appear in the fourth column (`C3`). Type the following in the Formula Entry window:

```
c3 = c2^2
```

15. The *sum* of the squares of the residuals (SSR) can now be calculated; KaleidaGraph will display the sum in a separate window. The command to sum the squared residuals (in the *fourth* column, `C3`) is: `sum(c3)`. KaleidaGraph allows you to create several formulas at once; a semicolon need only separate them. Add the Sum command to the commands typed previously, and the formula entry window will read as shown:

```
c3 = c2^2;sum(c3)
```

16. Click the **Run** button at the bottom of the Formula Entry window. If all goes well, a *Macro Results* window will appear, containing your SSR value.

    Note that the value that of the SSR you calculated is *the same* as the "Chisq" (*Chi Square*) value that appears in the results table on your graph!

A Word About KaleidaGraph Plots

17. Since everyone in lab is working on the same experiment, and their graphs will be similar, it's important to have your name appear on the graph. Click the text tool (it looks like an uppercase 'T'), click anywhere on your graph, and type your names. Click **OK** when finished.
18. To print your graph, click once to select it, then choose **Print Graphics** from the *File* menu.
19. KaleidaGraph saves the data in the same file as the *plot*, so be sure to save your graph! If you reopen a saved graph, choose **Extract Data** from the *Plot* menu. A "new" data window will appear, containing your original data and calculations. You can then edit this data, and changes will be reflected on the graph.