Graphing & Curve Analysis Using KaleidaGraph 4.5 Fall 2023

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-fit 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. *Bring these instructions to the lab each week*!



KaleidaGraph Icon

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 graphing and analysis tools of KaleidaGraph.

Entering the Data

1. When you start KaleidaGraph, you are presented with a spreadsheet (the "Data" window). As seen in *Figure 1*, data cells are designated by a row number (beginning with row '0') and a column title (A, B, etc.) A toolbar appears at the top of the Data window; labels in *Figure 1* show some of the more useful buttons (the name of the button will appear if you place the mouse cursor over it.) In addition, columns are referred to by a column number (c0, c1, etc.) that appears below the title*. The column number designation is not absolute, and its purpose will be more obvious later in 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).





A button that will expand or collapse the column header appears to the right of the column titles. *Click this button if needed to reveal or hide these column numbers.*

- The columns containing your data <u>must be labeled appropriately</u> 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!)
- 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 always save your data on a network drive; if you (or your instructor) need to recheck your results, you won't have to retype it, and you can check it from another computer.

Creating a KaleidaGraph Plot

- 4. Select *Gallery* from the menu bar, and 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 Scatter Plot window will appear (Figure 2).
- 5. You will next select the data to plot along the X and Y-axis of your graph (now you see why labeling columns is important!) As shown in *Figure 2*, click the box under the X next to your data column plotted along the x-axis; do the same for Y, then click the **Plot** button. Your graph will appear in a separate window.

 Scatter Plot

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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:
 - Increase the size of the graph by resizing the *plot frame*: first expand the plot *window*; next drag the lower right corner of the *plot frame* down and to the right (*Figure 3*). Drag the plot frame until it stops so that it will fill a single sheet of paper; note that it won't fill the entire window width!
 - From the *Plot* menu, look at the following options:
 - i. Uncheck **Display Legend**: you need to display the legend only when plotting more than one set of data on a single graph.
 - ii. Check **Display Equation**.
 - iii. Check **Auto Link**: The graph will automatically update if a data point is changed.



Curve Fitting

7. Now the graph you created needs to be analyzed. The first step is to determine which function best fits your data. Click the graph window *once* to select it, then select the **Curve Fit** menu. There are several possible fits to choose from; the ones that might be used in this course are "Linear" (for straight-line data in the form of y = ax + b), "Polynomial" (of 2^{nd} order: $y = ax^2 + bx + c$), "Exponential" ($y = ae^{bx}$), "Logarithmic" (y = alog(x) + b) and "Power" ($y = ax^b$). Select the appropriate function, *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, again choose the existing fit from the **Curve Fit** menu, 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 \rightarrow Display Equation). KaleidaGraph calculates the values of the appropriate coefficients *a*, *b*, *c*, etc.

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. <u>Your calculations should use all the significant figures presented</u> but remember to round *only* the final value that you record in your journal.

9. At this point your graph is complete. 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). If not, click the *Update Plot* button (second from left – see *Figure 1*) in the data window.



Figure 3 - Resize Plot

Evaluating Uncertainties in the Data

When evaluating data, it is important to be aware of the uncertainty of the calculated parameters. KaleidaGraph can provide this information when calculating the best fit with a user-defined function. *The following procedure details the analysis of linear data, but the same steps are followed for other functions.*

- 10. If you already have a best-fit line on your linear graph, remove it by selecting Curve Fit \rightarrow Linear, and clicking the **Deselect** button. Click **OK** to return to your graph.
- 11. Again select the Curve Fit menu, then choose General; you will see several "user-defined" fits that have been added by your instructor. Choose the desired fit, select the data column, and then click OK. (If you are performing the "Fitting Data to a Mathematical Function" exercise, then choose Linear Through Origin; this will be the only time in this course that you will choose this fit!) A best-fit line will again appear, along with a table of results, similar to Figure 4 (which shows the

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Linear	w/Uncerta	<i>inties</i> fit,	which	calculates	the slop	pe and

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

Figure 4 - Curve fit results from a user-defined linear function

intercept; your table will look different). If the table does not appear, choose $Plot \rightarrow Display Equation$. Click and drag the table of results to position it on your graph so that it doesn't obstruct axes or data points.

You'll notice that you get the same values for the coefficients (a, b, etc.) as you did with the first fit, but new quantities have now been calculated. The first row of the table contains the generic form of the fit, and the first column a list of the coefficients in your function. The second column ("Value") lists the numerical value of each coefficient. The third column ("Error") gives the *standard error* for each coefficient. (Ignore for the moment the rows labeled "Chisq" and "R" **).

Assuming four significant figures and units of velocity for the results shown in *Figure 4*, the value for the slope (coefficient *a*) and standard error would be:

Slope =
$$1.981 \pm 0.07781 \ m/s$$

The uncertainty in the coefficient is $\pm -t$ wice the standard error, so your final presentation in your journal of the velocity from the slope would look like this:

$$Velocity = 1.981 \pm 2(0.07781) = 1.981 \pm 0.156 \ m/s$$

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

** When applying a user-defined function, an *R*-value will always appear in the results table on the graph. *R* has nothing to do with the residuals; it is the *correlation coefficient*, another measure of the quality of fit. The value of *R* ranges from 0 (lousy fit) to 1 (most excellent fit). The experiments we will perform this semester will generally always have an *R* value very close to 1, so it isn't very useful for our purposes and does not need to be included in your journal.

Calculating Residuals

When you perform curve fitting, the line that KaleidaGraph draws won't necessarily go through each data point. The *residuals* are the differences 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 on the title for the 2nd column selects that column and changes its designation to c0. Always be sure that the *first* column is

selected in your data, 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. <u>For the "Fitting Data"</u> <u>exercise, be sure to choose the General fit "Linear through Origin"</u>.
- 13. With the fit in place, *again* go to the Curve Fit → General menu, then choose the function that you already applied to the graph (there will be a check mark next to the name). Click the down-arrow below "View" in the *Curve Fit Selections* window (*Figure 5*), and choose Copy Residuals to Data Window. This creates a column called "Residuals" in your data table (make sure you bring the data table back into view to see the residuals column). Click OK to dismiss the *Selections* window.

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

Since we have just calculated the residuals, we can create a simple formula in Kaleidagraph that can calculate the sum of the squares of those residuals (SSR). As you will see, KaleidaGraph automatically calculates the SSR for you when you apply a General fit for any function shape (linear or non-linear). 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; it appears grayed-out when selected. 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, *but don't do anything else yet*:

$$c3 = c2^{2}$$

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 (located 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! Therefore, you need not do this calculation if you apply a *General* fit. Click **OK** dismiss this window.

A Word about KaleidaGraph Plots

- 17. It is important to have your name appear on your graph since everyone in lab is working on the same experiment, so you want to make sure you get the graph of your data out of the printer. Select the graph and click the text tool (it looks like an uppercase 'T' on the small floating palette). Click anywhere near the top of your graph and type your name, as well as that of your lab partner. Click **OK** when finished.
- 18. To print your graph, click once to select it, and then choose **Print Graphics** (*NOT Print Setup!*) 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.