Appendix IV. *ORIGIN*

revised August 12, 2009

A. Introduction

Origin is a data analysis and technical graphics program for computers running the Windows operating system. It is designed for professional use and is far more sophisticated for data analysis and display than are, for example, *Logger Pro*, *MPLI* or *Microsoft Excel*.

Licensed copies of *Origin* version 8 are available over the campus network. *Origin* is already installed on all of the intro lab computers. If you cannot finish in lab any analysis that requires the use of *Origin*, you may use the lab computers at other times as posted on the lab web site.

You may also access *Origin* from any other computer connected to CWRUnet. If you have trouble doing this, don't ask the Intro Lab staff for help, ask the CWRUnet help desk. The instructions in the next section for accessing *Origin* were correct at one time, but CWRUnet policies and file locations are changed too often for us to guarantee that these instructions will work when you try them.

B. Accessing ORIGIN on Your PC

You can install *Origin* from the Case Software Center. To navigate to this site, start at the University Home Page (http://www.cwru.edu/) and select *Computing–Softwarecenter* or navigate directly to http://www.cwru.edu/softwarecenter From there, you are on your own.

After downloading and installing Origin 8, you will have to register your copy on Origin's website. Follow the installation directions to do this.

If you have difficulties installing *Origin*, you should contact the *CWRUnet HELP* desk and not your laboratory instructors.

C. Some Basics

Origin is similar to a spreadsheet such as Quattro Pro or Excel, but is designed specifically for scientific and engineering applications.

Adding Columns

Origin starts a session with a default of two columns. If you might require additional columns, you should select the *Column* item from the main tool bar and select *Add New Columns.* It's a good idea to add a few to get started.

Renaming Columns

You can rename columns from the default letters to something more meaningful if you wish. Meaningful names will make it easier to keep track of these variables but may complicate writing formulae for *Origin* calculations. To rename a column, double click on the top of a column to bring up the column menu. Several options are available.

i. You can change either the *Short Column Name* or the *Long Column Name* to something descriptive of the variable in that column. The short versus long column names differ only in that only the long name will appear when plotted, whereas the short name will appear when left in the spreadsheet. For example T for temperature. Further reference to these variables will be of the form COL(T) in the *Short Label.*. **Note that the *Column Name* must include only letters and numbers.** *Origin* will

ignore any special characters you type in.

ii. You can add a *Unit Label* to describe the variable. For example, you might label the column "Temperature (deg C)". Labeling a column has no effect on how you refer to it in *Origin* calculations.You may also leave *Comments* for your own future reference; again, this will not affect your data.

iii. You can set the column to be *X, Y* or *Err Bar* (*as well as other choices*, *but you can redefine the columns for different calculations or plots*) via the *Plot Designation* drop menu. It may be better not to use this method for setting columns as either *X, Y* or *Err Bar* for plotting, a more flexible technique is described elsewhere.

iv. You can set the column width.

v. You can adjust the number of *significant decimal places, the display type and the format of the data*. Only the number of decimal places may be useful to prevent the computer from rounding a value such as 3.0 to 0.

Setting Numbers in Columns

You can enter numbers in the columns by simply typing them into the cells. You can also load data from a file by using the *File-Import* option. A third way to enter data is to "copy and paste" from another program.

Setting Column Values

If you right click on the top of a column, say column D, and select *Set Column Values* from the menu you will see an entry box for Column Values. An example of an entry would be

Col(D)=Col(B)-Col(A).

This means that the numbers in the rows of column D will be set to the differences between the numbers in the corresponding rows of column B and A. You can enter other formulae to set the column values. Enter and/or edit the equation you wish to use and click "OK". To avoid computational errors resulting from empty cells or division by zero, you may need to set the range of rows for the calculation. This range can be changed within this menu.

You can refer to constants set in the Script Window. (*Using a script window to set a value for X is described in Section D below.*) For example, type

Col(D)=Col(B)-X.

To refer to a specific row of a column, enclose the row in square brackets, following the column address. (*Warning: Do not use square brackets for any other purpose.*) The currently active row is referred to as row I. (*Note: The letter* I *is reserved for the row number and should never be used in a Script Window calculation as a variable or constant.*) Thus, COL(A)[I-1] refers to the previous row in column A. To set the rows of Column B to the difference between adjacent rows of column A, use *Set Column Values* with

COL(B) = COL(A) - COL(A)[I-1].

Note that for this calculation you must start with row number 2.

To set the rows of Column A to the values 0, 2, 4, 6, ..., use *Set Column Values* with COL(D)=2*I-2.

Functions

Many functions are available. The default angle argument for trig functions is radians, so to set the variable x = sin(20°), type

X=sin(20*pi/180)

or reset the default under TOOL-OPTIONS-NUMERIC FORMAT.

D. The Script Window

You can set constants in the *Script Window.* The constants are then available for use when you *"Set Column Values"*. If the Script Window is not open, select it from the *Window* menu item. To set the variable *X* equal to 2, type

```
X=2
```

and the window will display

```
4*PI=12.56637
```

In fact, you can write an entire program with loops and branches.

To write a series of instructions without executing them, turn off *Script Execution* in the *Edit* menu. Then, type in your instructions. Each instruction must be terminated with a semicolon. To run the entire set of instructions, turn on *Script Execution*, select the instructions and hit enter.

The *Script Window* is not automatically saved when you save your *Origin* project. You must save it separately and reload it when you need it.

E. Plotting

To make a simple plot of *Y vs. X*, right-click on the top of the *Y*-column and select *Plot → Symbol → Scatter* to plot discrete points. (*Plot-Line will show a line joining the points but not the points itself and should not generally be chosen*.) While it is often tempting to select *Line* so that you have a line connecting your data points but still see the data points themselves, the line it shows does not have any deep significance and can sometimes be confused with a least-squares fit to the data.

If you want to make more complex plots, for example including error bars on one or both axes, or if your worksheet has several columns, it is best if no columns are highlighted when you are about to make a plot. Selecting *Scatter* will then call up a window that lets you define any given column for any given purpose.

You can also change the data point display by double-clicking on any data point. One reasonable change is to change the size of the default data points, which tend to be overly large, to something such as 3 point circles. You can also change the symbol used to display the data as well as the color of the symbol. This can be helpful when a plot contains several different datasets. Note however that colors other than black may not be distinguishable after printing.

To make changes in the plot axes, double click on them. This brings up a menu that lets you customize them, including features like the type of scale (*linear, log, etc.*) and the placement of tick marks.

Right clicking on an empty region of the plot will bring up an additional menu which includes information on the plot and an option to add text to label the plot.

There are many other features and shortcuts that you may choose to use, but it is not necessary to become an expert in *Origin* to succeed in this laboratory.

F. Least-Squares Fitting

Origin offers several choices of fitting methods**.** Under its *ANALYSIS* menu, you can find under the sub-menus *LINEAR FIT*, *POLYNOMIAL FIT, NON-LINEAR CURVE FIT,* and several other options. Be sure to select the graph before starting a fit.

in the *Script Window* and hit enter. A semicolon will be added to the line. (*The program does not distinguish between upper and lower case characters*.)

Another example:

```
fourPi=4*pi
```

sets fourPi to 12.56637.

You can also use the *Script Window* as a quick calculator. Type

```
4*pi=
```

F.1. Linear Fits

In its *Analysis* menu, click on *Fitting → Fit Linear* to make a least-squares fit of a straight line to the data. The line will be plotted on your graph. If you defined a column of uncertainties in *y*, the fit will be weighted by the inverse square of these uncertainties.

The results of the fit will appear in the *Result Window*. The intercept *A* and the slope *B* will each be represented by two numbers corresponding to the value and uncertainty. The uncertainties are calculated statistically from the scatter of the data points about the fitted line and not from your estimates of the uncertainties in the measurements. The standard deviation SD is described below; its value should be approximately 1 for a good fit with uncertainties.

Origin will often show its calculations with an excess number of significant figures. If, for example, it gives A = 1.3429764 ± 0.0347632, it is incumbent upon you, the user, to edit this appropriately, as in A = 1.34 ± 0.03, before submitting your work.

F.2. Statistics-SD and Chi-square

For a linear fit without error bars, the quantity *SD* displayed in the *Results Window* is the standard deviation of the fit, defined as

$$SD = \sqrt{\frac{\sum\left[y_i - \left(A + Bx_i\right)\right]^2}{N-2}}$$

where *x* and *y* are the variables plotted on the abscissa and ordinate respectively, *N* is the number of measured points on the graph, and the sum is taken as *i* goes from 1 to *N.* For a reasonably large data set with uniform uncertainties in *y* and negligible uncertainties in *x*, *SD* is a good estimate of the average uncertainty in individual measurements of *y*.

If error bars δ_i are used to weight the fit, then the quantity calculated as *SD* is the square root of chi-square per degree of freedom, *DOF*,

$$SD = \sqrt{\frac{\sum\left[y_i - \left(A + Bx_i\right)\right]^2}{\left(N-2\right)\delta_i^2}}$$

$$\Rightarrow SD = \sqrt{\frac{\chi^2}{N-2}} = \sqrt{\chi^2_{DOF}}$$

where $\chi^2_{DOF} \equiv SD^2$ is the *"goodness-of-fit"* parameter, which is minimized in the least-squares fitting procedure. On the average, we should expect $\chi^2_{DOF} \sim 1$. See the Appendix VIII on *Least-squares Fitting* for more information.

F.3. Uncertainties in the Parameters

Origin calculates the internal *statistical* uncertainty in the parameters, *i.e*., it uses the standard deviation of the fitted curve from the data points (σ=*SD*) as an estimate of the uncertainty in the measurements. This means that *Origin* ignores your own estimates of uncertainties in your measurements when it calculates errors in its fitted parameters, except to use them as weighting factors. For a fit to a straight line, the uncertainties in the intercept *A* and slope *B* are given by

$$\delta_A^2 = \frac{\sigma^2}{\Delta}\sum x_i^2 \ , \ \delta_B^2 = \frac{\sigma^2}{\Delta}N$$

with $\Delta = N\sum x_i^2 - \left(\sum x_i\right)^2$, where the sums are over the *N* measured values of *x*.

Students who use a spreadsheet instead of *Origin* for their calculations should use these equations to find the uncertainties in the parameters.

F.4. Non-linear Fits

Non-linear fits are those in which the fitting equation is not linear in the parameters. Unlike linear fits (*which include fits to polynomials*) the parameters in non-linear fits cannot be determined analytically but require a trial-and-error method. *Origin* pro-

vides many different types of fitting procedures in the *Analysis* menu. The *Non-linear Curve Fit* method is a general purpose routine useful for many different formulae that are either stored in *Origin* or defined by the user.

Follow these steps to make a non-linear fit. First, load and plot your data file. Make sure the graph is active.

1. Select ANAYLSIS / NON-LINEAR CURVE FIT/ ADVANCED.
2. Click the Create/Edit Function Button.
3. Select one of the pre-programmed fitting functions (*editing it if necessary*) or click Function/New to write your own. Skip steps 4 and 5 if you are using a pre-programmed equation.
4. Type the fitting equation in the Definition Window. Assuming that the "Use Origin C" menu is **un**selected, the equation should be of the form
   fn(*x*, *P1*, *P2*,...) **not** *y*= fn(*x*, *P1*, *P2*,...)
   where fn(*x*, *P1*, *P2*,...) is the fitting function with independent variable *x* and parameters *P1*, *P2*,...
5. Be certain to set the number of parameters to the correct values. If you select *User Defined Parameter Names*, you don't have to define the number of parameters and you can replace *P1*, *P2*, etc. by your own parameters, separated by commas.
6. Click OK, then *Initialize Paramters* button..
7. Select *Active Data Set* when this option appears.
8. You must set each parameter to a suitable non-zero value to get started. Do not set any parameters to 0!
9. Click *1 iter.* You should see a curve appear on your graph. It probably won't be a very good fit. If you don't see a curve, you have either made a poor initial estimate of the parameters or have an error in your equation.
10. Click *Fit Until Converged* to finish the fitting process. The parameters are now set unless you choose to go back to step 4.
11. Click *Fit* to see the *Results Window*, which will be pasted into your plot and can then be moved to a convenient position. Note that the significant figures won't be correct for your fitted parameters; you will have to correct this manually.

G. Curve Simulations

It is sometimes useful to be able to plot a curve with no variables, for example when the theoretical expression that should describe your data has no free parameters. The easiest method to do this to go to the Menu bar and select *Graph → Add Function to Graph*. You can then write an equation and show it on your plot. Note that the independent variable in this routine is referred to as *x* and not by its column name.

The following procedure is also useful when *Origin's* fitting routine seems to be malfunctioning. You can use the simulation routine to plot the equation you have defined with various parameters to see if you have made an error in your equation or in your guesses of the parameter values.

To simulate a curve, follow the first 5 steps as described for non-linear fits. You can still have parameters in the simulation and you can vary these parameters to adjust the simulation At step 6, click *Action/Simulate*. Enter values for any parameters and then click *Create Curve*. You are done. If you were doing a simulation to check your fitting procedure, the appearance of a good curve now is reassurance that you were doing things correctly. If a proper curve appears in the simulation but the same equation and parameter values don't work in the fitting routine, the problem lies with *Origin*.

H. Layout Page

It is often convenient to summarize and display your *Origin* results in a *Layout Page*. A Layout Page might include your name and your partner's name, one or more graphs, selections of data from the beginnings of tables of data which were plotted and parameters listed in the *Results Window.* To create a Layout Page:

i. Click on *FILE-NEW.*
ii. Select *LAYOUT* from the menu that pops up.
iii. A new menu appears at the top of the page. You may either use this menu or right click on the Layout area to access the commands that control the Layout Page. For example, right click and select *ADD GRAPH* or *ADD WORKSHEET*. Move the cursor to place the object in the desired position on the page.
iv. You can then adjust the size of a graph and decide how much of a worksheet you wish to show. You can copy and paste text directly to the Layout Page using *COPY* and *PASTE* commands.

Note that if you make changes in your data or graphs, the Layout Page will be updated automatically.

I. Help

Origin has very good *Help* files, accessed by clicking on the menu icon, or pressF1.