Appendix ***C***

Data Analysis Using Origin on a PC

Origin is a data analysis and graphics package produced by OriginLab for the Microsoft Windows environment. Origin includes a nonlinear least-squares fitting routine based on an algorithm by D.W. Marquardt (see Bevington and Robinson, Section 8.6). Origin supports the use of Bessel functions in fitting functions, so it can readily be used to fit diffraction data from a circular aperture. Version 9.0 of Origin is installed on the hard drives of the lab computers, and when run, these installations obtain a license from an HMC server. We shall describe how to use Origin 9.0 to fit diffraction data from a circular aperture.

x	I	sigI
9	0.176	7.07107E-4
9.5	0.5222	0.00132
10	1.094	0.00245
10.5	1.886	0.0051
11	2.82	0.00447
11.5	3.76	0.00548
12	4.546	0.0103
12.5	5.064	0.00748
13	5.154	0.00678
13.5	4.87	0.00837
14	4.208	0.0086
14.5	3.326	0.01122
15	2.372	0.00374
15.5	1.484	0.00678
16	0.7944	0.0026
16.5	0.3302	0.00102
17	0.0862	3.74166E-4

Table C.1: data

Log on to a Windows computer in the Optics Lab (or in the computer labs on the HMC campus) and launch Origin 9.0. When the main Origin window appears, you will probably want to maximize the Book 1 worksheet window and type in your diffraction data or load it from a text file. To facilitate the discussion in this Appendix A, we have placed our diffraction data in a text file named CircularMoore2004.dat (data donated generously by Chris Moore HMC '05) that resides on our computer's hard drive, and we will use the Import feature of Origin to load our data into the Worksheet. Our data file CircularMoore2004.dat has three columns (see Table C.1): the first column contains the position of the detector (in mm), the second contains the intensity (in volts), and the third is the uncertainty (in volts) in the intensity. The intensity and its uncertainty are actually the mean intensity and the standard deviation of the mean (standard error) deduced from five scans through the diffraction pattern.

File—Import—Single ASCII That is, click on "File" to pull down the File menu, then slide the mouse down to "Import", then slide the mouse over to "Single ASCII..." in the Import submenu.

We then switched directory folders on our computer's hard drive to find the data file CircularMoore2004.dat; and double-clicked on CircularMoore2004.dat to open it.

Because our data file has headings on the columns, the import filter creates data columns with those headings. If you create a data file without headings, you can label the columns simply by double-clicking on the heading of the column and typing in a name. Our columns are labeled "x", "I", and "sigI." You can also add units for each column. (If "####" is displayed instead of a data value, just broaden the column width by grabbing the right vertical boundary line and moving it to the right. That will provide enough space in the column to display the full value in scientific notation.)

The position values in CircularMoore2004.dat are in millimeters. To convert the values to meters, highlight the x column (click on the heading) and then

Column—Set Column Values Type "col(x)/1000" and then click "OK". The values in the x column should now be in meters.

This is a good time to type into the row titled "Units" the appropriate units for each column. Origin will then automatically label graphs with the units appropriate for each data column. We typed in the units "meters", "Volts", and "Volts", respectively.

Next we tell Origin that the sigI column contains uncertainties for the I column. Highlight the sigI column and then

Column—Set as—Y Error The sigI column should now have (yEr±) behind its name.

To plot the data with error bars, highlight all 3 columns by clicking on the name of one column and dragging the mouse across the tops of the other 2 columns, then

Plot—Symbol—Scatter A plot will be created. (The System Theme is fine — click OK.) In order to see the error bars on the plot, we had to reduce the size of the data symbol from 9 points to 5 points — double-click on the data symbol in the legend and select the font size you want.

To change the label on the y-axis, double-click on the current label ("I (volts)" in our case) and replace it with your choice of label. Similarly for the x-axis.

We now prepare to fit the data by defining constants to be used in the fitting function.

Window—Script Window Type "lambda=632.8e-9" and then hit Enter. A semicolon will be appended to the line. (The wavelength of the laser is 632.8 nm.)

Type "k=2*pi/lambda" and hit Enter. (k is the wavenumber.)

Type "r=1.212" and hit Enter. (The distance from aperture to detector was 1.212 meters in Chris Moore's experimental setup.)

We now define the fitting function.

Analysis—Fitting—Nonlinear Curve Fit—Open Dialog...

In the NLFit window, click on the "f(x)" icon to create a new function (left-center on the screen).

In the Fitting Function Builder window, type "DiffCirc" into the Function Name box.

In the Description box, you might want to type in "Fit circular aperture diffraction pattern with Bessel functions".

Click on "Next" and in the Parameters box, type "Imax, a, xzero, Izero".

Click "Next" and in the large Function Body box, type the fitting function as an expression:

"4*Imax* (J1(k*a*(x-xzero)/r)/(k*a*(x-xzero)/r))^2 + Izero"

Now in the Parameters table, enter the initial values for the fitting parameters. Just double-click on the space where the value is to be entered, and type in the value. We entered 5.2 for Imax, 1e4 for a, 0.013 for xzero, and 0.001 for Izero. Note that an initial guess of zero for any parameter may give the nonlinear fitting routine trouble when it tries to calculate the derivative of χ^2 with respect to that parameter — it will not be clear what step size to use in the derivative.

You can now click "Finish", or simply click "Next" repetitively through the next few windows until you are forced to click "Finish". You will be dumped back into the NLFit window.

Next click on "Data Selection" (in the Settings tab of the NLFit window) and in the Weights box, select "Instrumental" which will weight the data with the values in the sigI column.

Now click on the button which is roughly in the middle of the window. The Messages tab will display the calculated value of (about 48,000 for Chris Moore's data and our initial guesses). The fitted curve will be superposed on the plot of the data — just move the NLFit window to see it.

Click on the "1 Iteration" button just to the right of the button. The Messages tab will display the new value after the single iteration (about 8000 for Chris Moore's data and our initial guesses).

Click on the "Fit until converged" button (just to the right of the "1-Iteration" button) and look for the results in the Messages tab and for the new fitted curve on the plot of the data (just move the NLFit window to see it).

Click "OK" and say "No" to the report sheet. You will be dumped into the "Graph1" window with the plot of the data and the fitted curve superposed, and the results box pasted onto the plot. You can click on the results box and drag it to a convenient place on the plot. The same is true of the legend box. See our plot of the fit to Chris Moore's data on the next page. You can always return to this "Graph1" window by double-clicking on the "Graph1" icon at the left-center of the Origin screen, or just use the Window menu at the top of the Origin screen.

If you click on the "Project Explorer" tab on the left side of the screen, and double-click on the "CircularMoore2004" icon (the name depends on the name you give to the data), you will return to the original data window (or you could have used the Window menu at the top of the Origin screen) which now has two additional tabs accessed at the bottom of the window. If you select the "FitNL1" tab, you can explore the results of the fit. If you select the "FitNLCurve1" tab, you will see a table of the fitted curve and residuals**.**

While viewing the "FitNLCurve1" window, "copy (full precision)" the column of residuals and paste them into the main datasheet tab in a new column. To create new empty columns in the main datasheet, go to

Column—Add New Columns Make two new columns, one labeled "Residuals" and one labeled "NormResid" into which you can place the normalized residuals.

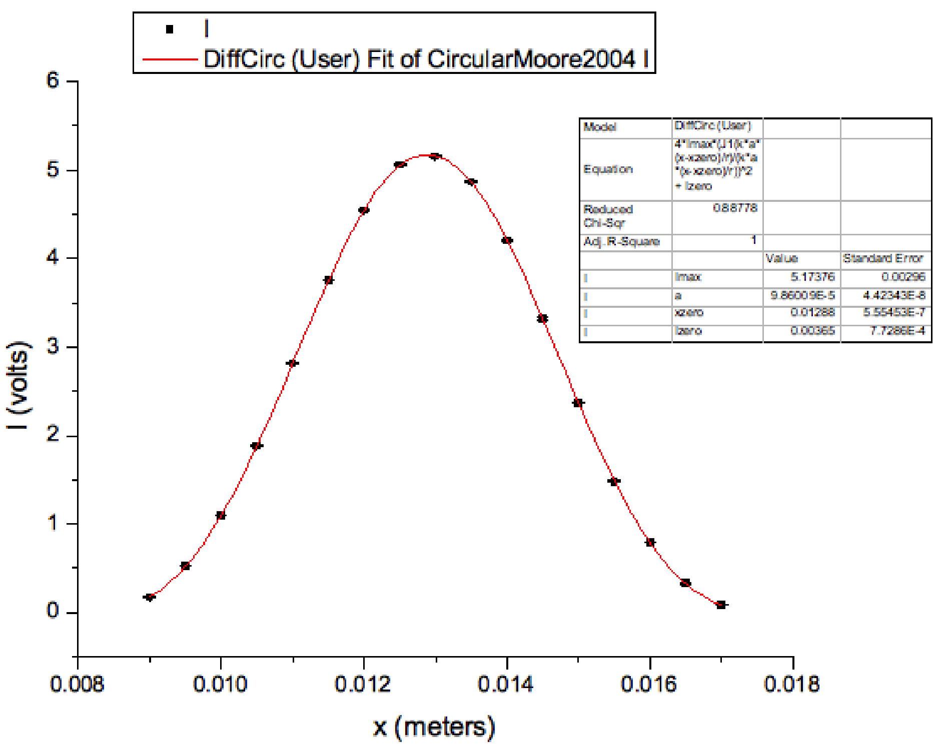
After you have pasted the residuals into the "Residuals" column, create the normalized residuals by clicking on the remaining empty column and using

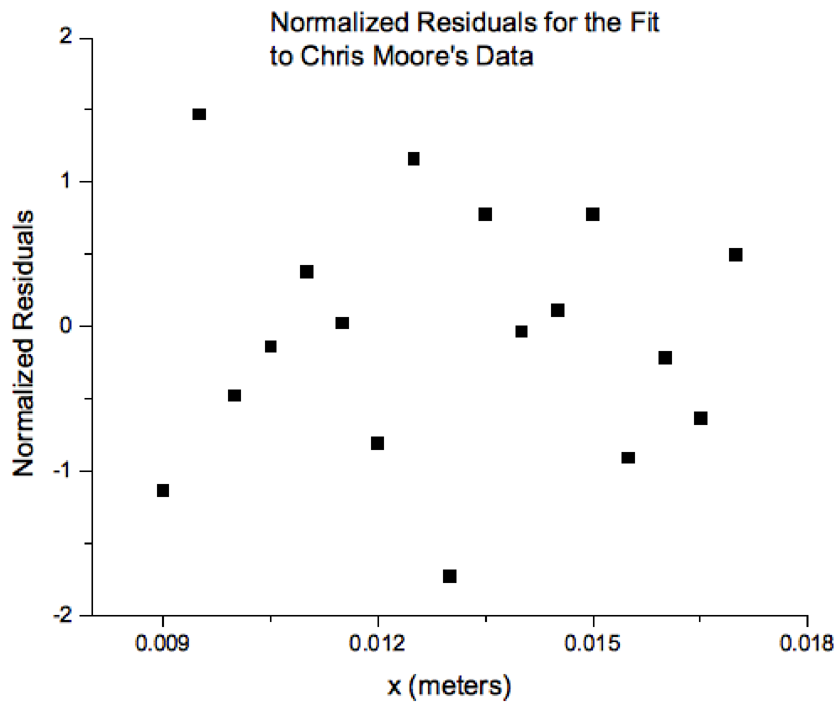
Column—Set Column Values Set the new column values equal to col(residuals)/col(sigI).

Plot NormResid versus x. This is your plot of the normalized residuals!

You can get a hard copy of the plot of the data with fitted curve (click on the graph and choose File—Print) or copy the plot to the clipboard (Edit—Copy Page) and then paste it into a document (as we have).

Our value of 0.89 for χ^2 per degree of freedom $(17-4=13$ degrees of freedom) indicates that our fitting function provides a fit to the data with a 55% chance of being exceeded if the measurements were repeated.




Normalized Residuals for the Fit
to Chris Moore's Data
Normalized Residuals
x (meters)
2
1
0
-1
-2
0.009
0.012
0.015
0.018