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Introduction

After collecting data it is usually necessary to display and analyze it. A two dimensional plot of the variables measured will show the relationship between them. Regression analysis will show the quality of fit and the degree of dependence of one variable on the other. There are many software packages available for this. One of the better ones available is called Grace, which has a home page <http://plasma-gate.weizmann.ac.il/Grace/>. It is available for many common operating systems at no charge, and widely used in scientific publications. The following tutorial will give you an introduction to using Grace for your physics labs. You will produce two plots of data and hand them in for marking.

17.1. The First Graph

Log-in to Linux and start the Grace program. The executable is called `xmgrace` (entered into a command line shell) and may also be in the menu under other.¹ This will present you with the main window of Grace as shown in figure 17.1. There are a few buttons on the left side of the main window. The most used ones are:

- AS = auto-scale all points to appear in the plot area.
- Draw = redraw the plot

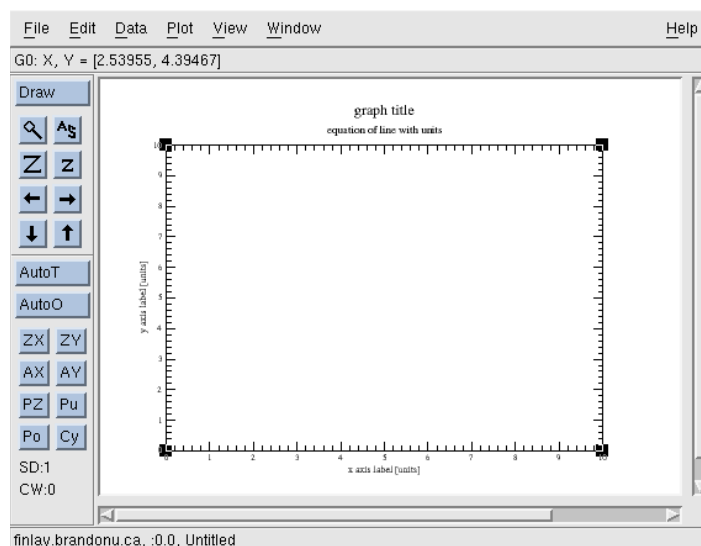


Figure 17.1.: Grace's main window

The process of creating a graph will take the following general steps:

- Choose which data is for the x-axis and which is for the y-axis. This will be explained more below.
- Enter the data into the spreadsheet contained in Grace. Calculations on this data may or may not be necessary and can be performed within Grace.

¹This depends on what linux distribution and desktop environment being used.

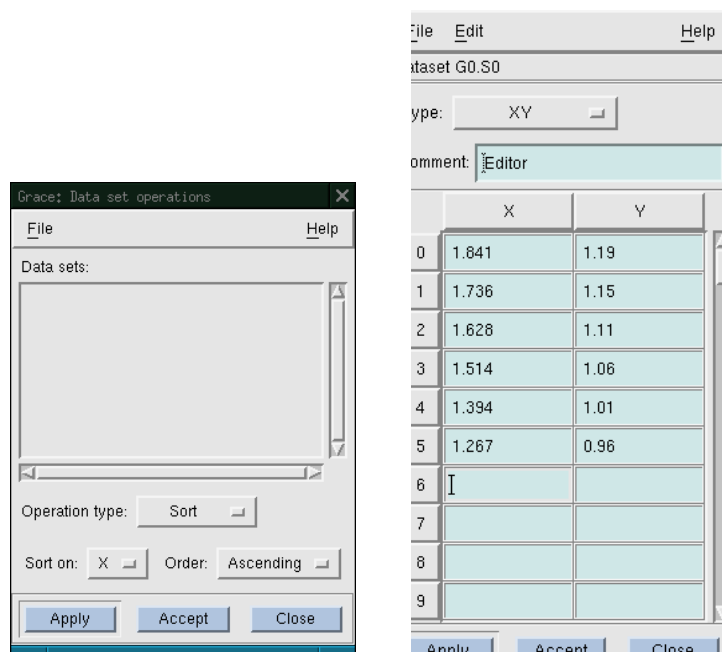


Figure 17.2.: Dialog windows for data entry

- Produce a scatter plot with Grace. This type of plot is one with just the data points showing; no line or lines are joining the points.
- Scale the graph as appropriate. The reader must know ahead of time if the the y-intercept or both intercepts should be shown. If only the slope is used in future calculations then, then showing the intercept(s) is not necessary.
- Perform a linear regression on the data and have Grace put this 'line of best fit' onto the graph
- Label the x and y axes with the variable plotted and its units.
- Put a title on the graph.
- Put the slope and intercept on the graph with their units.
- Print the graph and staple it into your lab report book for marking.

17.2. Entering Data into the spreadsheet of Grace

The Lab Instruction Book will ask that you graph two variables to produce a plot of your data. One of the first questions that arises is which variable goes on the x-axis and the y-axis. *All instructions for producing graphs are phrased in the form 'plot y as a function of x'. In other words you will always put the first variable (could be time, temperature, etc) on the y-axis and the second variable on the x-axis.* The first and second refer to the order of the names in the instruction. So if you are asked to 'plot phase shift as a function of temperature', phase shift values are on the y-axis and temperature is on the x-axis. In general the independent variable is plotted on the x-axis, the dependent variable goes on the y-axis.

The following example is to produce a plot of time T as a function of the square root of the sum of two distances (s+L). In fact this data is from an actual experiment, the measurement of g. However we have reversed the x and y-axis data to what is required for that lab.

1. To bring up the spreadsheet, click on 'data, data set operations'. This produces a window called 'Grace: Data set Operations' as shown in figure 17.2. This window will show the various data sets (empty now as none have been created) that the user has produced.

2. Hold the right mouse button down when clicking it in the data sets area of this window and select 'Create new, In spreadsheet'. This produces the 'Spreadsheet data set editor' window.
3. In this window, Type will be left as XY as we are dealing with just two columns of data. Enter the data shown in figure 17.2 . Use the tab key to move between cells of the spreadsheet. If you make a mistake, you must select and delete the row which contains the mistake using the Edit, delete selected rows drop-down menu. A row is selected by clicking on the row number on the left side of the data. **NB:** You must leave the last cell you have entered data into using the 'enter' or 'tab' key. Grace does not parse the data until you leave the cell. Failing to do so results in a zero being placed in the cell instead of you data. This will show up on the plot and throw the fit off considerably.
4. Comment can be changed to 'T and sqrt of (s+L)'. Now click 'Accept'. This will close the dataset editor window and bring you back to the data set operations window. The only difference between 'Apply' and 'Accept' is that Accept closes the window. Now you will see the data set operations window has a data set in it called G0.S0[2][6]. This is 'grace-speak' for 'graph 0, set 0 which contains 2 columns of values and 6 rows'. If you double-click on the set name G0.S0[2][6], Grace will load and display the data set in the spreadsheet editor again.
5. To see your comment right-click on the 'Data sets:' portion of the 'Data set operations' window. In this menu click on Selector operations, view set comments. Now your comment will be shown in the list of data sets. Labeling your data sets is helpful but not necessary.
6. Save your data to the hard-drive using the 'File, Save as' dialog. You have your own directory to store files in. If you are group 18, then your directory is /home/g18. This is the only directory you can use. **Save your file often as you work. Control-s will execute a save file operation.** To name your file use the 'Selection' field at the bottom of the 'Grace: Save project' window. So your file could be called tutorial1.agr. **Put .agr as the extension of your filename.** The 'Filter' field is for filtering out other files in the same directory so they are not displayed. Leave this alone, as the default extension for Grace files is .agr. Note that there are several useful areas of this window including the Directories list, the Files list and room for a description of the file. For more details see subsection 17.6.1.

17.3. Tuning a graph in Grace

Focus the main window again by clicking on it's title-bar and you will see that your data has been plotted. There will be a short black line on the graph, but this line is only using a small portion of the graph's area. Ideally, the axis should be scaled so that the data's range covers 80 to 90 per cent of the graph's area. Press the button labeled A_S to auto-scale the graph. Now you will see each axes' range has been adjusted. However the line shown is just segments that join from one data-point to the next. Such a 'join-the-dots' line is not desirable. We want to see the data points represented by small circles and then have the line of best fit drawn in. This can be done by:

1. In the main window click on 'Plot, Set appearance'. Go to Symbol Properties and change 'None' to 'Circle'. Change the symbol properties size to between 50 and 70 from 100. Click Apply and you will now see your data points represented by small, open circles.
2. Now remove the line by using the 'Set Appearance' dialog box and change the Line properties from 'Straight' to 'None'. Now there should only the circles representing the data. Click 'Accept' to close the Set Appearance window. Next we need the line of best fit.
3. In the main window, click on 'Data, Transformations, Regression'. The set S0 should be hi-lighted, the type of fit set to 'Linear', load should be set to 'Fitted values', Restrictions set to 'None'. (These are the defaults.) Click Accept and a red or black line will appear on the graph. This line is the best fit for the data as the vertical separation from it to all the points is a minimum. Also a window called 'Grace: Console' will open. Do not close this window until you have copied the necessary values from it.

There will be many windows up on the desktop during the use of Grace. On a smaller monitor, this makes life difficult. Use <alt-tab> to cycle through the windows. Also pressing F11 will bring up a complete list of open/minimized windows to select from. You can also shade the child windows (the main Grace window is considered the parent) by double-clicking on child window's title-bar. This will just leave the child's title-bar showing. To unshade it, double-click again.

In fitting the observations (your data), Grace has created a second data set called G0.S1[2][6], i.e. set one of graph 0. The console window contains messages, errors or information about the statistical analysis and the equation of your line of best fit. Scroll up and down in the console window to see what is there. You should see a detailed statistical analysis of your data set g0.s0. The main points of interest (and how to proceed) are:

1. the slope, the intercept, and the standard error of the line's slope and intercept. The equation of the line is also shown as $y = 0.44812 + 0.40419x$ in the console window. This equation is the same form as $y = b + mx$ with the intercept b and the slope m .
2. Cut and paste this equation into the graph *as follows*: Cut and paste in the X-Windows system is done using the middle mouse button if available. If your mouse does not have three buttons (which is the case for our lab) then 3-button emulation is used. To 'middle-click' using 3-button emulation, you simply press both buttons simultaneously. It takes some practice but is not difficult.
3. So first, wipe across or hi-lite/select the line's equation in the console window using the mouse. Now bring the focus to the main window (use the mouse or alt-tab until the main window has the focus) and double-click on the subtitle which reads 'equation of line with units'. This brings up the Graph Appearance window. Go to the field called 'Subtitle' and delete this text. Careful not to hi-lite this text with the mouse or you will have to go back and re-hi-lite the line's equation in the console window. Once this field is empty, perform a middle click as described above, then click Apply. You now have the equation of the line in the graph.
4. The default number of sig figs is six for the values of the slope and intercept. This is too many. As a general rule / compromise we will use three sig figs for the slope and intercept. Perform the necessary rounding to get three sig figs showing in the line's equation. Graphs with six sig figs showing will have marks deducted.
5. Back in the Graph Appearance window, change the title to 'T versus square root of (s+L)' by entering the text into the 'Title' field. Usually a more descriptive title is possible but not in this case.
6. In the Graph Appearance window you will see 6 tabs below the 'Graph:' internal window. These tabs allow you to control many settings of the graph's appearance. Usually the defaults are acceptable.
7. Click 'Accept' to close the Graph Appearance window.
8. The axes do not have labels (with units) yet. Bring up the 'Grace: Axes' window by double-clicking on the x or y-axis of your graph. Double-clicking on the existing axis title will not produce the 'Axes' window, clicking must be done on the axis line itself. Note that which axis is being modified is selected by clicking on the button beside 'Edit:'. Select 'X axis' if this is not the one showing.
9. Label the x-axis square root of (s+L) [$m^{1/2}$] by typing: square root of (s+L) [$m\backslash S1/2\backslash N$] into the 'Label string' field. To get the -1 superscript you have inserted font control escape characters which Grace interprets. Backslash tells Grace the next character is an escape character. S is for start superscripting. All characters after a $\backslash S$ will display and print as superscripts. The $\backslash N$ tells Grace to go back to the default font so that the final square bracket is the correct size and location. Click Apply to have the changes take affect and double-check them back in the graph.
10. Now change to the y-axis using the Edit: button and label the y-axis as T [s]. Click on the Accept button to close the Axes window.

11. Almost done, but our equation has no units in it. Both the slope and intercept have values with units. **The y-intercept is simple: it's units are those of the y-axis.** So 0.448 should be 0.448[s]. Make this change by double-clicking on the subtitle to get the Graph Appearance window up.
12. **The slope's units are determined by the units of the y-axis divided by the units of the x-axis:**

$$\text{units of slope} = \frac{\text{units of } y - \text{axis}}{\text{units of } x - \text{axis}}$$

due to the fact that the slope = rise/run. Thus in this example we have $\frac{s}{m^{(1/2)}}$. A quick way of making a fraction is to use superscripts and subscripts with a normal sized '/' between them.

13. In the Graph Appearance window, go to the subtitle field and behind the 0.404 enter: $[\backslash Ss\backslash N/\backslash sm\backslash S1/2\backslash N]$. At first this looks incredibly tedious but it allows you complete control and corrections are quick and easy. You are using the \S for superscript, \s for subscript and \N for normal text sizes. Fractions can also be achieved by using the \z (zoom) and \v (vertical shift) escape controls. Clicking on 'Apply' will allow you to check the results without closing the window. For example \z{0.5} will make a character 1/2 the size of normal text. \v{0.5} shifts text upward 1/2 a line, \v{-0.5} shifts the next characters downward 1/2 a line.
14. Finally change the y in the equation to T and the x in the equation to '(s+L)\S1/2', because these are the names of the values you plotted, not x and y.
15. **NB: Remember that the numbers in your best fit equation have units, but the variable names should not have units.** Think of the numbers for the slope and intercept as measurements you have made, so they require units. Even the units put behind the axis labels are in fact associated with the numbers along the axis.

Now your graph should appear as shown in figure17.3. **Please have your work checked by your lab instructor or demonstrator before proceeding.**

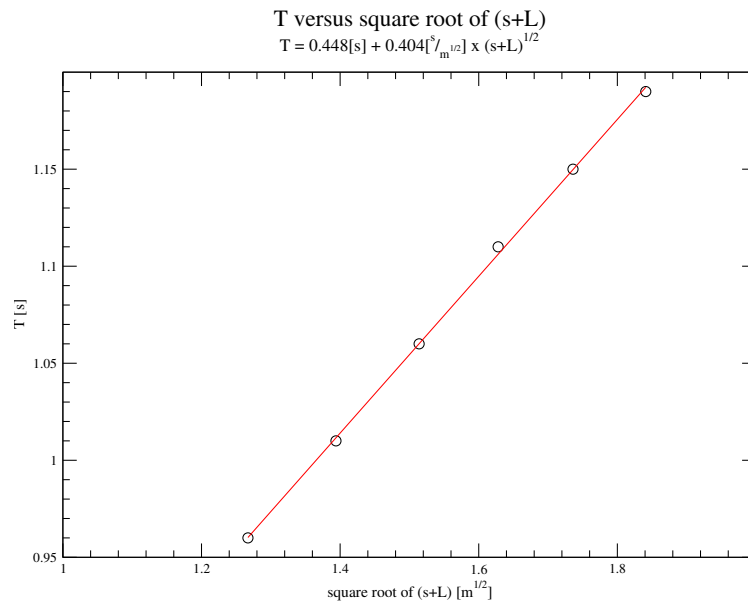


Figure 17.3.: Appearance of completed graph number 1

17.4. Correcting mistakes or view problems in Grace

1. To remove a point in the dataset editor, you must first select, then delete the row which contains the mistake by clicking on 'Edit, delete selected rows' in the drop-down menu of the 'Spreadsheet data set editor' window. A row is selected by clicking on the row number on the left side of the data.
2. To remove a line of best fit, delete the data set which was created for it. There is more than one location from which this can be achieved. One is to click 'Data, Set operations'. Then click on the appropriate set to select it, (not G0.S0; that will be your data) and then right-click on that data set to bring up a menu and click on 'Kill' or 'Kill data'.
3. If you plotted the wrong variable on the x/y axes: Oh no!! This cannot be easily corrected. The reverse x and y axis feature in the Graph Appearance window is not available yet. You must start again by removing the data set and re-entering it. This is still easier on a pc than a hand-made graph.
4. Sometimes you may not be able to re-size the window which contain Grace so that you can see all the graph. If you are not able to see the complete graph within the main window of Grace, you can change how many pixels Grace uses. Click on 'View', 'Page setup'. Confirm that X11 is the 'Device'. In the 'Page' section, change 'Size:' to Custom. Now you can modify the dimensions so that the complete graph is visible in the main window.

17.5. Using Grace's data set operations

Often data requires that mathematical operations be performed on it before plotting. For example, the experimenter measures diameter due to convenience but requires a plot involving the radius, or the measurements were made in centimeters but the plot must be in meters. The diameter needs to be divided by two before plotting and the centimeter converted to meter by dividing by 100. Grace's data set operations provide you with easy manipulation of data. A new data set is created: G0.S0 is generally the 'source' set and G0.S1 is the 'destination' set. Begin with entering the data shown in table 17.1.

$p_g[psi]$ <i>gauge pressure</i>	=	$t[F]$	P_A	$T[C]$
0.2		34		
0.7		44		
1.1		54		
1.3		64		
1.45		70		
1.65		74		

Table 17.1.: Data for second graph.

This data set shows values of temperature in Fahrenheit and pressure in psi (pounds per square inch). It was collected by cooling and heating a small volume of air in a closed container. Pressure and temperature sensors were mounted inside to record the changes in the air. This data set must be converted to metric units of Celsius (from the temperature t) and absolute pressure in pascals (from the gage pressure p_g) using the conversion equations below. This will complete table 17.1. The values are then graphed, fitted and the regression line extended to zero pressure. Absolute zero which is a value of temperature occurs when the pressure of gas is zero and we seek to find it's value. The conversion equations are shown below:

$$T[C] = \frac{5}{9}(t[F] - 32)$$

$$\text{absolute pressure } P_A = p_0 - (p_r - p_g)k$$

$$\text{where } p_0 = 98100[Pa] \quad p_r = 1.65[psi] = \text{pressure at room temperature} \quad k = 6894.6 \frac{Pa}{psi}$$

1. Open a new file in Grace by clicking 'File, New'. Enter the data shown in table 17.1. Put p_g in the X column and $t[F]$ in the Y column. Save this file to the hard-drive.
2. Click on 'Data, Data set operations' in the main window to open the 'Grace: Data set operations window. Right click on the inner window listing the Data sets and the click on 'Create new, By formula'. This produces a window call 'Grace: Load & evaluate'
3. We are going to create g0.s1, the new set of data by operating on g0.s0. Grace requires some information about which and how many points to operate on. We want to convert all the values in g0.s0, so the 'Start at:' field should have 0 in it and the 'Stop at:' field should have 5 entered into it. Enter 6 into the 'Length:' field. This instructs Grace to take values from g0.s0 starting at row 0, apply the formula to the data until reaching row 5, to create the new set. Grace begins numbering the spreadsheet rows at zero, not one.
4. In the field labeled 'X=' you must enter the conversion factor which will convert the readings of pressure from psi to pascals. Delete the \$t and enter (without the quotes) '98100 -(1.65-g0.s0.x)*6894.6' into the X field. Note that g0.s0.x represents the column of p_g or gauge pressure values you enter in the data set g0.s0. In the 'Y=' field you can convert the temperature reading from their Fahrenheit values to Celsius. Type in '5/9*(g0.s0.y - 32)'. Click Accept.
5. If you have any errors, then you will see the console window appear and a message will describe the problem. Often a typo results in a parse error, which means grace is expecting some type of value and not receiving it. Double-check your formula. When all goes well, you will see G0.S1[2][6] has been created and your graph will now contain a plot of the new set. The old set may still be visible and since we do not want to use it for fitting we will hide it. Bring up the 'Data set operations' window and hi-lite g0.s0. Then right click on it and select Hide. Now you will see a minus sign in front of G0.S0 instead of the plus sign. Note that Show is also in this drop-down menu. This allows you to select which data set(s) appears in the graph.
6. Next press AS to auto-scale the graph. Double-click on the 'join-the-dots' line, to bring up the Set Appearance window and change the symbol from none to a ~ 70 -point circle, and change the line properties to none. Make sure you make these changes to g0.s1.
7. Next scale the y-axis so that -300 C is the 'Start:' value. Click 'Apply'. Double-click on the y-axis and make this change in the 'Start:' field. If the x-axis does not start at 0, then make that change as well and click 'Apply'.
8. Next add the linear regression line. Click on 'Data, transformations, regression. In the 'Regression' window, hi-lite set S1, type of fit is linear, load must be changed to Function, leave restrictions as none. The 'Start load at' the value of 0, 'Stop load at:' should be set to the same value as the end of the x-axis. A value of $1e5$ is typical, although you should check your graph. ($1e5 = 1 \times 10^5$). '# of points:' can be set to 100. Click Accept. Grace will now produce g0.s2[2][100], which contains 100 xy pairs that fall on the linear regression line. The main window will now show this line, and the y-intercept has been plotted. Incidentally, the y-intercept coincides with the line's $x=0$ point.
9. The console window contains the line's equation and can be copied into the graph using the instructions from the first graph.

This second graph must be similar to the one shown in figure 17.4. Some changes to the major spacing may be necessary. Major spacing is the distance between points that are labeled with a value on each axis. Minor ticks are the marks between the major ticks. These are configured in the 'Tick properties of the 'Axes' window which appears when you double-click on either the x or y-axis.

Note that this data predicts a value of -205 degrees Celsius for absolute zero. The actual value is -273 Celsius. The standard error of the intercept is 17 degrees Celsius and is shown in the console window. Thus the data predicts a value of absolute zero of -205 ± 17 degrees Celsius. Since the range of this value (-222 to -188 degrees Celsius) does not include the true value, the experiment contained a systematic error which led to an unacceptably high value of absolute zero.

Again, **have your work checked** on screen before proceeding.

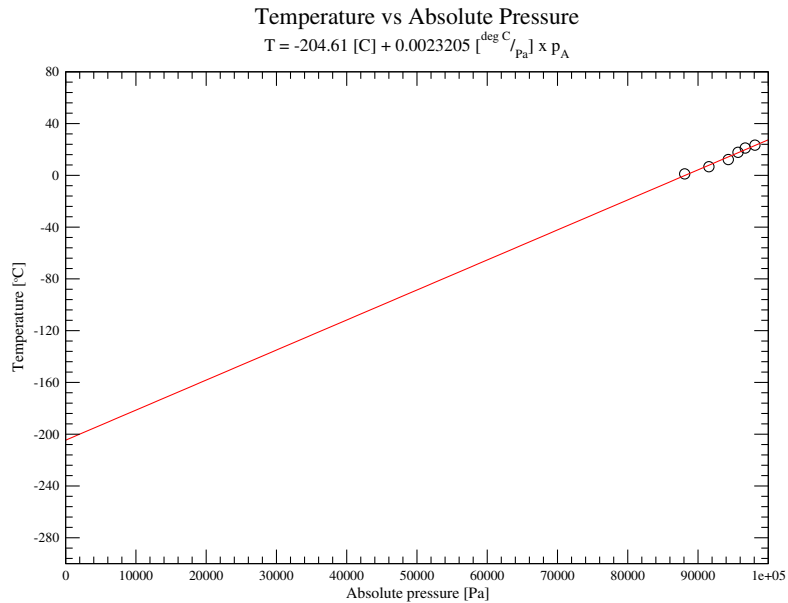


Figure 17.4.: Graph of Temperature vs Absolute Pressure.

17.6. Additional Features in xmgrace

17.6.1. Saving and Opening an Xmgrace File

Xmgrace's save file dialog has two fields that must be understood to avoid confusion. The top field is named 'Filter'. In that field will be the directory xmgrace was started from, usually the home directory of the user. In addition, the end of the filter has *.agr tacked on. This means the files list only shows files that end in .agr which is graces default file extension. Leave this as is.

To save a file, you type in the filename in the 'Selection' field. Do not remove the subdirectory names that are present, for example. /home/gx, where x is actually your group number. To save the file as test_graph1.agr in your home directory, you should have /home/gx/test_graph.agr. Then click ok.

Opening a files makes use of the filter as well. By default, only .agr files are shown in the 'Files' list. If your file is not present, you can remove the .agr in the 'Filter' field and press enter. Leaving the * means all files will be shown in the 'Files' list.

17.6.2. Greek Letters

Greek letters such are available for use in titles and labels of your graphs. They are accessed by changing the font to Symbol. This is done using the $\{\text{Symbol}\}$ or the $\backslash x$ escape control. Everything after will be displayed and printed in Greek characters. $\{f\}$ will return you the default or normal font. Use l (lower case L) for λ and 'D' for Δ , q for θ , etc.

17.6.3. Extending the line of best fit.

The line of best fit can be extended in either direction by using and adapting the instructions of step 8 in Section 17.5.

17.6.4. Importing Multicolumn Data From other Sources.

Xmgrace can import ascii or netcdf data files. If the source is multicolumn ascii data with columns separated by white-space it can be displayed in one graph using: 'Date, Import, ASCII' to display the

'Read Sets' dialog box. Here choose NXY as the 'Load as' setting. Then select your file from the Files list, adjusting the filter if required. Data sets can then be shown or hidden as necessary.

17.6.5. Non-Linear Curve Fitting

Xmgrace contains a number of preprogrammed, commonly used curve fitting functions. These are located in Regression window in the 'Type of fit' settings. But if the list does not contain your desired function, Xmgrace can be told what function you want it to attempt a fit with. Such a feature is not present on many graphing packages. After entering a data set, click on Data, Transformations, Non-linear Curve Fitting. Select the number of parameters (how many ways you want to use the x variable. In the 'Formula' field, enter your desired fit equation. For example $y=a_0+a_1*x+a_2*\cos(x)+a_3*x^{-1}$, which is not available in the 'Type of fit' list. Xmgrace then needs to know the source set that it is to fit. Select your data set in the left side list of sets. Then click apply. The console window will have the values for the a_n coefficients. Powerful, eh? Another example of this capability is illustrated in figure 17.5. The comments in figure 17.5 diagram provide the details for creating that graph.

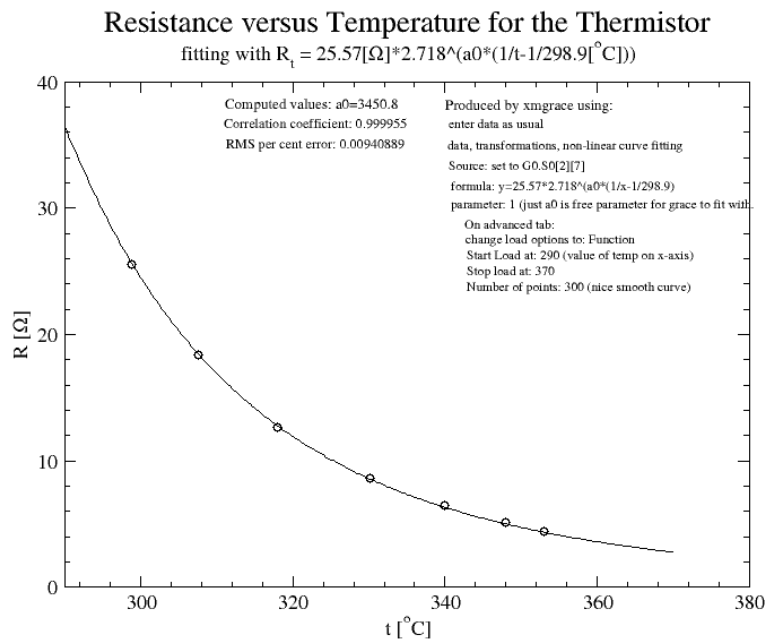


Figure 17.5.: Fitting a curve with a user defined function.

17.6.6. Plotting a function in xmgrace

To plot a theoretical function in xmgrace, use 'Dataset operations, Create new, By formula'. The 'start at' and 'stop at' are values of the x-axis which you will pick. For example to plot $y = x^2$ over the range of -1 to $+1$, set 'start at' to -1 and 'stop at' to $+1$. Length is the number of data-points grace will create in the new data set. Set it to 50. \$t is the variable name to be used in the formula you wish to plot. If plotting $y = x^2$, then leave the 'X =' field as \$t and put X^2 in the 'Y=' field. Click accept and you will have a plot of $y = x^2$ generated in the plot window. To edit the equation you have entered, repeat the steps above: 'Dataset operations, Create new, By formula'. Section 4.1 of the tutorial within grace itself has some more examples. Click on 'Help, Tutorial'.

17.6.7. Placing Additional Text and Other Objects on a Graph

Additional text like the authors name or the date can be added as follows. Once the graph is plotted, click on 'Window' then 'Drawing objects'. In the 'Objects' dialog box, click on the Text button. Now click on the graph at the location you want the text to appear. A dialog box will appear which is used to enter the text in the 'String' field. The 'Objects' dialog box also contains tools for drawing lines, moving objects, etc.

17.7. Final Graph.

The last exercise mimics what you will see in the lab. A set of data is available which you have collected. Next you are asked to plot the data. The first decision you must make is what column of data on the paper goes into the appropriate column of xmgrace. Reread the bold text in section 17.2 to determine this. Entering the data in the wrong columns results in the incorrect value for the slope. Correcting this requires the data to be re-entered in the correct columns. This does not take long but is easily avoidable. Consider this your warning.

17.7.1. Instructions for Final Graph

Make a plot of temperature T as a function of motor speed MS (rpm stands for revolutions per minute) for an electric motor for the following data. Fit the data with linear regression to obtain the line's equation. Use the error values to properly round the values of slope and intercept. Print one copy with your names. Hand this in for marking.

motor speed MS [rpm]	Temperature T °C
212	24.1
470	34.4
593	41.3
980	46.8
1427	53.1
1750	62.4
2230	74.4

Table 17.2.: Motor speed and temperature data.

17.8. Graphing with Grace: Quick Reference Guide

To create a graph with the required information:

1. Start grace, click on Data, Data Set Operations. Right click on the empty list area (no data sets listed yet), Create new, In spreadsheet, then enter the data. Exit the last cell, and click Accept. Set S0 is now created, and displayed in the graph. Click AS to scale the graph.
2. Double-click on one of the data line which will bring the Set Appearance window. Turn off the lines that are joining the data points using Line properties Type: None. Now display the data points using Symbol Properties Type: Circle.
3. Fit the data with a straight line. Click on Data, Transformations, Regression. Click accept if the correct set of data is hi-lighted in the Apply to set: list. (If S0 is the only set, it is already selected.) Click on Close to close the Regression window.
4. Double-click on the graphs title and make a title: 'your y-variable' as a function of 'your x-variable'.
5. Label each axis by double-clicking the existing label and modifying the label fields. Put the units in square bracket.

6. Delete all the text in the Subtitle field. Copy the equation of the regression line from the Console window by hi-lighting it and then middle-clicking in the Subtitle field.
7. Round the slope and intercept values using the errors for each number shown in the console window (scroll back in the console window to find them). State the error values rounded to one sigfig.
8. Put the correct units on the slope and intercept values (no square brackets).
9. Print as required.

17.9. Importing graphs to L_YX

Grace can produce output suitable for importing into L_YX or L^AT_EX software. Generally an encapsulated postscript version (.eps) of the graph is used due to that format's vector graphics, and inclusion of size information. This format is also closely associated with T_EX and as such works well.

To produce the eps file, use the Print setup dialog under File. Select EPS as the Device. The Output section should change and show a red square beside "Print to file". Enter your choice of filename in the appropriate field. Close that dialog and print the graph using "File, Print". Other formats of file are also available such as portable network graphics (.png) and scalable vector graphics (.svg).

L_YX will also directly import the native grace file format, typically the file uses the .agr extension.