Getting Started with OriginPro 7.5 (Part 2)

An introduction to OriginPro, a scientific charting package.

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EDITION 2.1

TUT 77

Contents

Format Conventions

In this document the following format conventions are used:

Input which must be replaced by your details is given in bold italics.	LOGIN ***server/username***
Menu items are given in a bold, Arial font.	**Windows Applications**
Keys that you press are enclosed in angle brackets.	**<Enter>**
Toolbar buttons for some menu commands are displayed in the left hand margin.	

Feedback

If you notice any mistakes in this document please contact the Information Officer. Email should be sent to the address info-officer@leeds.ac.uk.

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Print Record

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This document continues from 'Getting Started with OriginPro 7.5 (Part 1)'.

Task 9 Curve Fitting: Pre-defined

Objective To introduce the concept of curve fitting.

Instructions You will use a pre-defined function as an example.

When you are in a graph window, OriginPro's automatic fitting commands are located in the **Analysis** menu. Parameter initialisation and fitting is carried out automatically when fitting from these menu options. A fitted curve is displayed in the graph window while the fitting parameters and statistical results are recorded in the Results Log window. The **Analysis** menu contains the following automatic pre-defined fitting models:

- Linear
- Polynomial
- Exponential Decay (First Order, Second Order, and Third Order)
- Exponential Growth
- Sigmoidal
- Gaussian
- Lorentzian
- Multi-peaks (Gaussian and Lorentzian)

Users can have more control over fitting parameters of a pre-defined function or can add their own fitting function by using the **Non-linear Curve Fit** option from the **Analysis** menu. This option contains over 150 pre-defined functions which are divided into the following categories:

- Origin Basic Functions
- Chromatography
- Exponential
- Growth/Sigmoidal
- Hyperbola
- Logarithm
- Peak Functions
- Pharmacology
- Polynomial
- Power
- Rational
- Spectroscopy
- Waveform

Activity 9.1 We will now consider a curve fitting session using one of the pre-defined functions. To try this example you should open FITEXMP1.OPJ, an OriginPro project file which can be found in C:\Program Files\OriginPro75\Tutorial. Click on **File** > **Open** to open the project file. As you can only have one project file open at a time, you will be asked if you want to save any existing work first.

Figure 22 shows the plot in FITEXMP1.OPJ which will be used for this example.

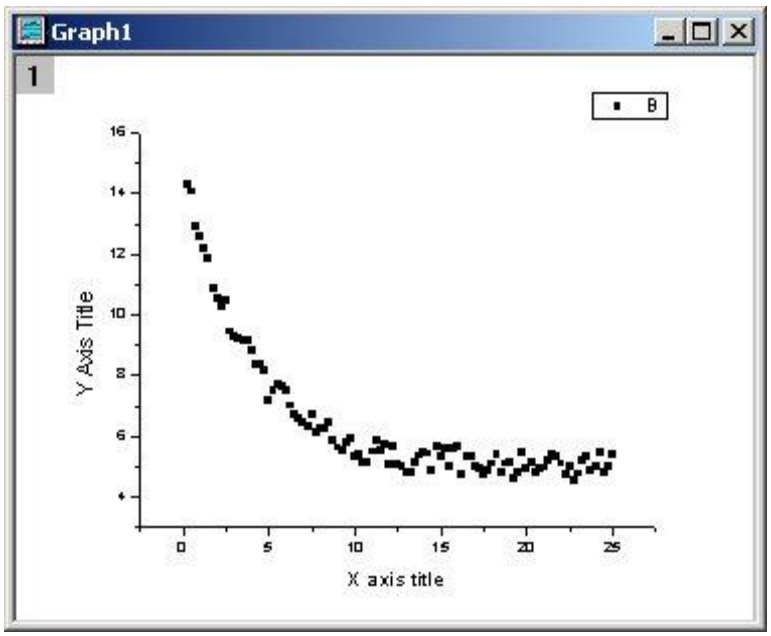


Figure 1. A scatter graph

Click on the graph and choose **Fit Exponential Decay** > **First Order** from the **Analysis** menu. OriginPro will do the necessary initialisation and fit a curve to the data. The result of this operation is shown in Figure 23.

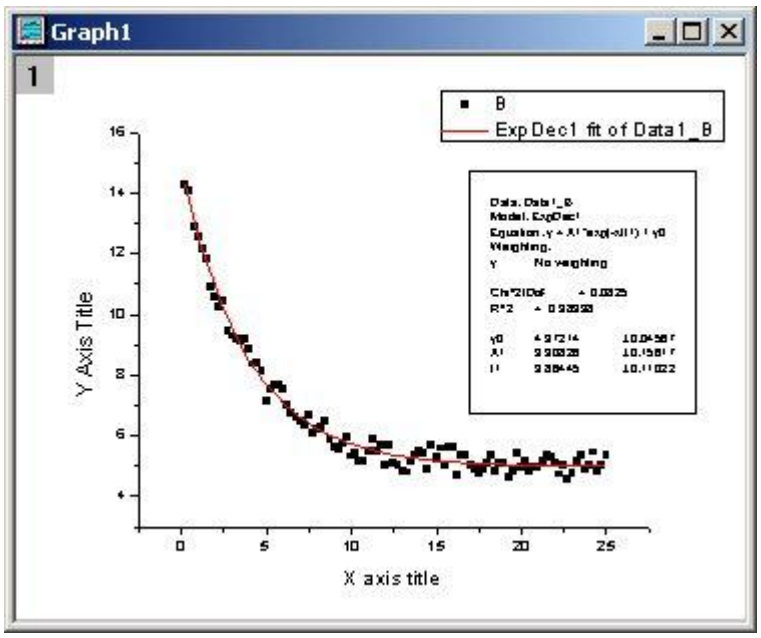


Figure 2. First order exponential decay curve fitting

Details of the fitting parameters appear in both the graph window and the Results Log window.

Activity 9.2 The above case fits the following exponential equation to the data:

$$y = y0 + A1*\exp(-x/t1)$$

This is a specific case of the equation:

$$y = y0 + A1*\exp(-(x-x0)/t1)$$

where x0, the x offset, is assumed zero. To allow an x offset you should choose the **Non-linear Curve Fit** > **Advanced Fitting Tool** option from the **Analysis** menu. The NonLinear Curve Fitting: Fitting Session dialog box should appear containing details of the fitting session just performed. If this box does not look like Figure 24, click on Basic Mode at the bottom.

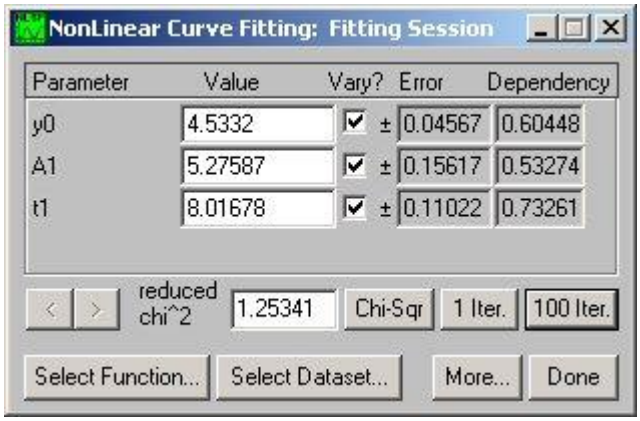


Figure 3. Fitting Session dialog box

- Click Select Function and choose ExpDecay1 from the Functions list.
- Click Start Fitting, followed by Yes.
- Make sure the Vary? check box for x0 is checked and set the following values: y0 to 0, x0 to 0, A1 to 10, and t1 to 1.
- Click the 100 Iter. button and then click Done.

This will update the plot with a new curve and the new fitting parameters will appear in both the graph window and the Results Log window.

Figure 24 shows the Basic NLCF Mode. The Advanced NLCF Mode can be accessed by clicking on the More button at the bottom of the Basic Mode (see Figure 25). While both modes enable you to fit a curve to your data, they differ substantially in the options they provide as well as in the degree of complexity they entail.

The Basic Mode is simpler and is used for selecting or defining your own function, selecting a dataset for fitting, performing an iterative fitting procedure and displaying the results on the graph.

The Advanced Mode includes the above and allows you to define a LabTalk script or Origin C code to initialise parameters, impose linear constraints, specify a weighting method and termination criteria, display the residue plot, parameter worksheet, variance-covariance matrix and confidence and prediction bands. It also allows the user to fit multiple datasets with a choice of shared parameters and change parameter names.

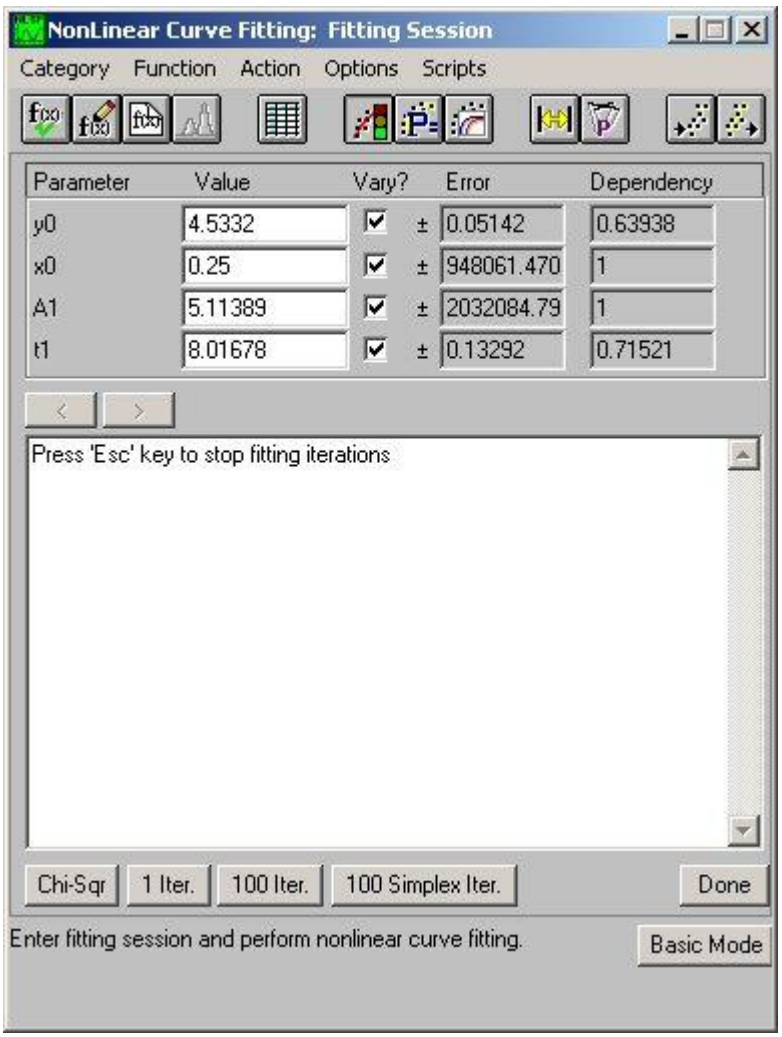


Figure 4. Advanced NLCF Mode

Task 10 Curve Fitting: User-defined

Objective Curve fitting using a user-defined function.

Instructions You will use an example of a user-defined function.

Activity 10.1 Consider a curve fitting session using a user-defined function. To try this example you should open the file FITEXMP2.OPJ which is available under C:\Program Files\OriginPro75\Tutorial.

To enter a new fitting function, from the **Analysis** menu choose the **Non-linear Curve Fit** > **Advanced Fitting Tool** option and then select Basic Mode. The following dialog box will be displayed:

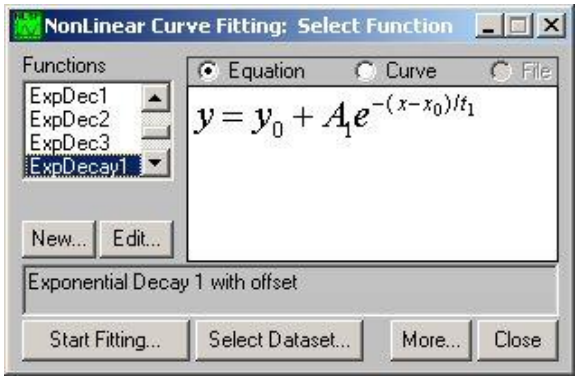


Figure 5. Select a new function

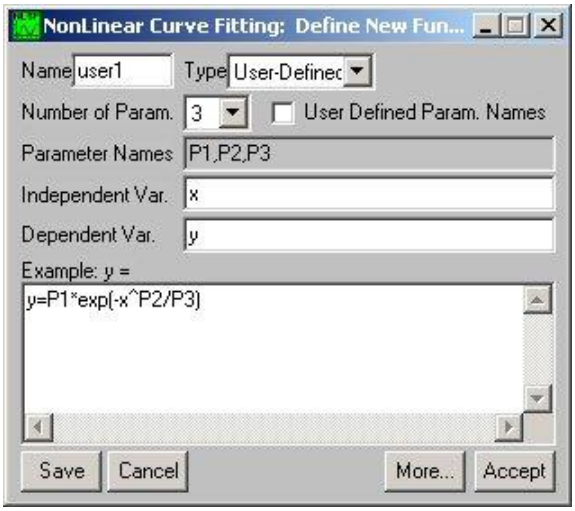


Figure 6. Define a new fitting function

Click on the New button. Enter 3 in the Number of Param. box. Next enter the following into the box at the bottom:

y=P1*exp(-x^P2/P3)

and click the Save and then the Accept button.

Activity 10.2 To start the fitting session from the dialog box in Figure 26, click on the Start Fitting button. You will be prompted for a choice of fitting the curve for the active dataset or any other. Choose the active dataset. The Fitting Session dialog box appears (see Figure 28) and you need to set the starting values for P1, P2, P3 in the boxes adjacent to the parameters e.g. try P1=7, P2=2, P3=2.

If you want to fix the value of any of the parameters you must clear the box next to the value box that says Vary?. If the Vary? boxes are checked it allows the parameters' values to change during the iterations.

Click in the 1 Iter. or 100 Iter. box to do the curve fit. Repeat the iterations until you get a satisfactory fit. Once you are happy with the curve, click the Done button to terminate the fitting session.

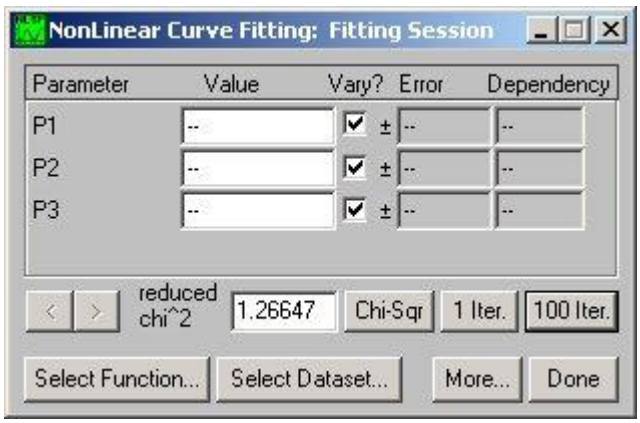


Figure 7. The Fitting Session dialog box

Figure 29 shows the result of fitting the function to the plot.

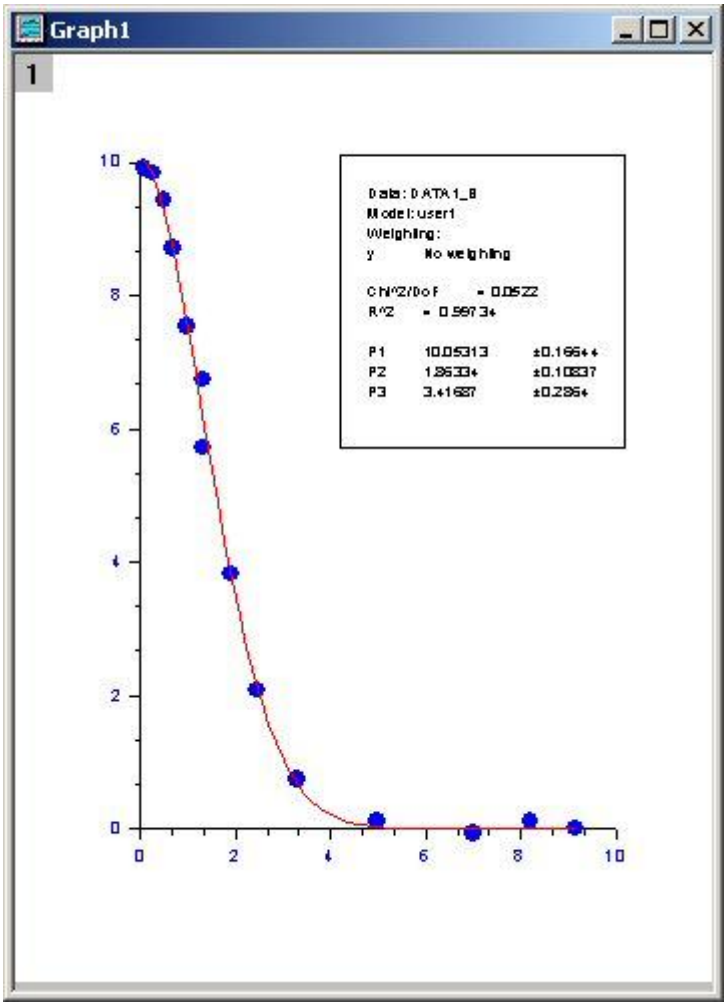


Figure 8. Fitting a function to a plot

Note: The option More during the fitting session provides the user with more sophisticated options to control the fitting parameters. See the NLCF (Advanced Mode) **Options** > **Constraints** menu item.

Close FITEXMP2.OPJ by clicking on **File** > **Close**.

Task 11 Creating a 3D Graph

Objective To create a 3D graph.

Instructions Enter data into a worksheet and produce a 3D plot.

Comments Enter the data as shown.

Activity 11.1 Add a third column to an OriginPro worksheet as done in Task 2 previously.

Activity 11.2 You will need to change the name of the third column to C(Z). To do this, click on the column heading and then click on the **Column** menu. Choose the **Set as Z** option. Enter the data shown in Figure 30.

Data1

	A(X)	B(Y)	C(Z)
1	4	7	5
2	5	6.7	6
3	6	6.2	7
4	7	6	8
5	7.3	5	9
6	7.9	4	10
7	8	3	11
8	8.1	2	12
9			
10			

Figure 9. 3D graph data entry

Activity 11.3 To draw a 3D scatter graph, click on the C(Z) heading in the third column of the worksheet. Next click on the **Plot > 3D XYZ** menu and choose the **3D Scatter** option. The data will be plotted into a new plot window and the 3D Rotation toolbar will also appear.

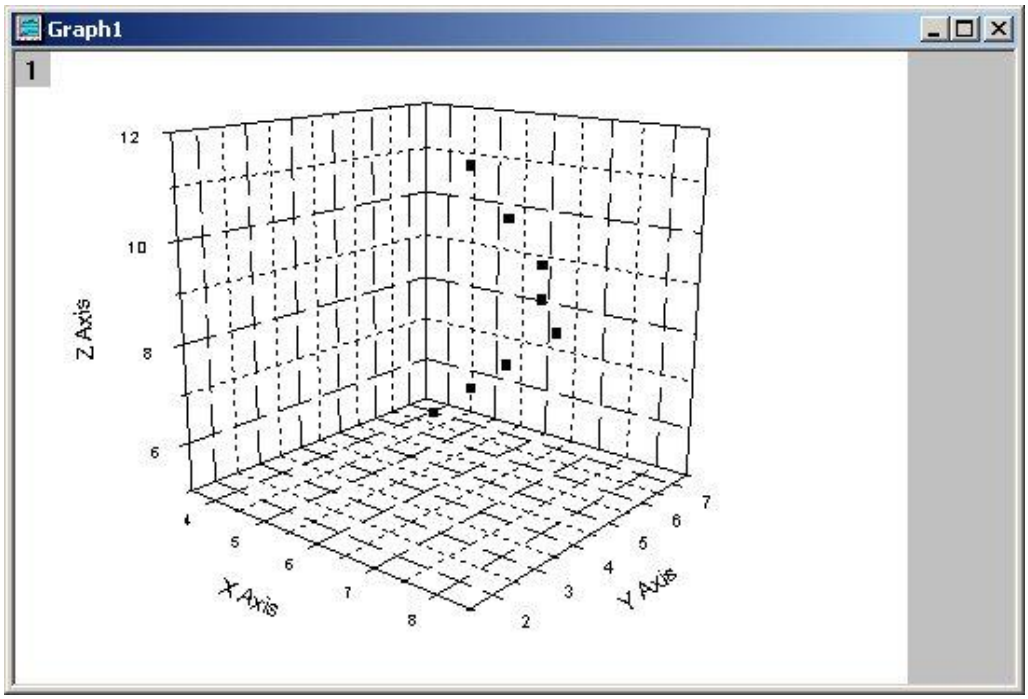


Figure 10. Scatter plot

Activity 11.4 The Plot Details dialog box allows you to choose and change various parameters of a 3D scatter plot.

To open the Plot Details dialog box you can either double-click on a plotted data point or click on the **Format** menu and choose the **Plot** option. The following dialog box appears:

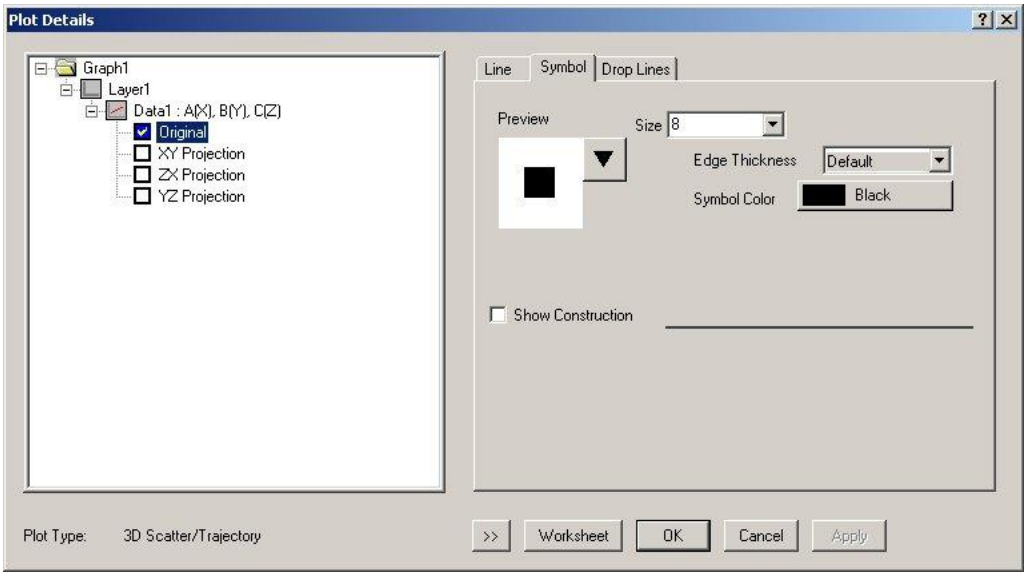


Figure 11. The Plot Details dialog box

If the left-hand side of the Plot Details dialog box looks different from above, expand the graph structure by clicking on the +'s. Make sure that Original is selected.

As you can see, the 3D plot is not particularly easy to interpret at the moment. The following formatting procedures should be carried out:

1. To join the points with straight lines (a trajectory plot) click on the check box next to Connect Symbols in the Line tab. (Alternatively you could have chosen the **3D Trajectory** option, instead of the **3D Scatter** option, when creating the plot.)

2. To add drop lines choose the Drop Lines tab and select Parallel to Z Axis.

3. To remove the grid lines from all three axes click on Layer 1 in the left hand side of the Plot Details dialog box and choose the Display tab. In the Show Elements section de-select the X Axes, Y Axes, and Z Axes options. Then click OK. The plot should now resemble that in Figure 33.

4. To make the points bigger and to number them you should re-open the Plot Details dialog box as before. Select Original from the left hand side of the dialog box. Click on the Symbol tab. Choose Show Construction, Row Number Numerics, select the Outline box and choose Size 24 from the drop down list. Then click OK.

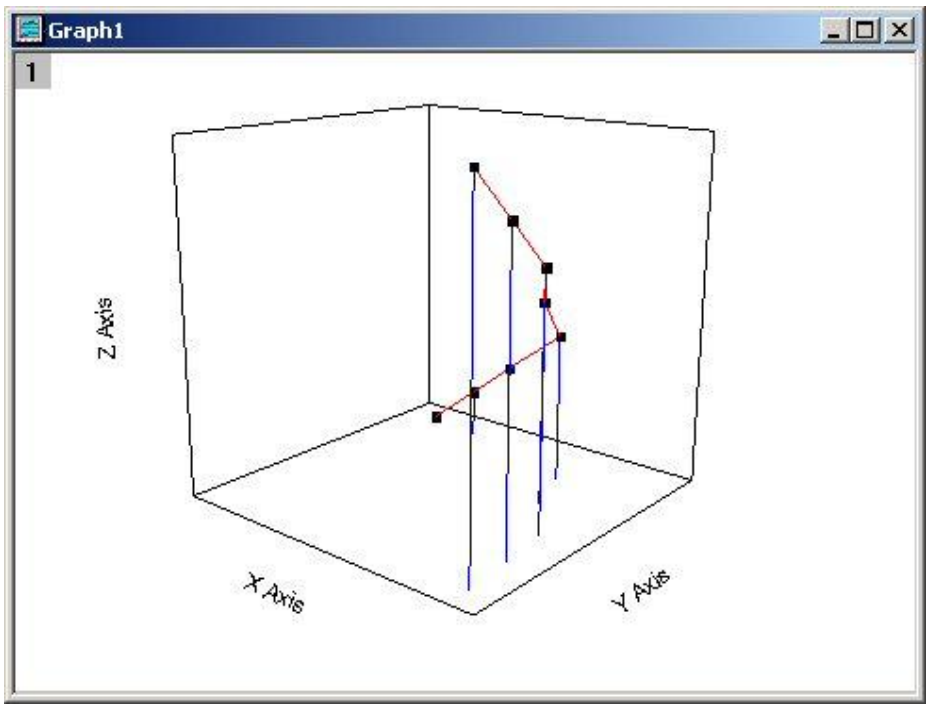


Figure 12. Trajectory plot, no grid lines

5. To trace a line onto the bottom of the graph, open the Plot Details dialog box again and select Original from the left hand side. Turn off the Parallel to Z Axis in the Drop Lines tab. Then click on the XY Projection check box in the left hand side of the Plot Details dialog box, so a tick shows. Finally click on the check box next to Connect Symbols in the Line tab. Click on OK and the graph should now resemble Figure 34 below:

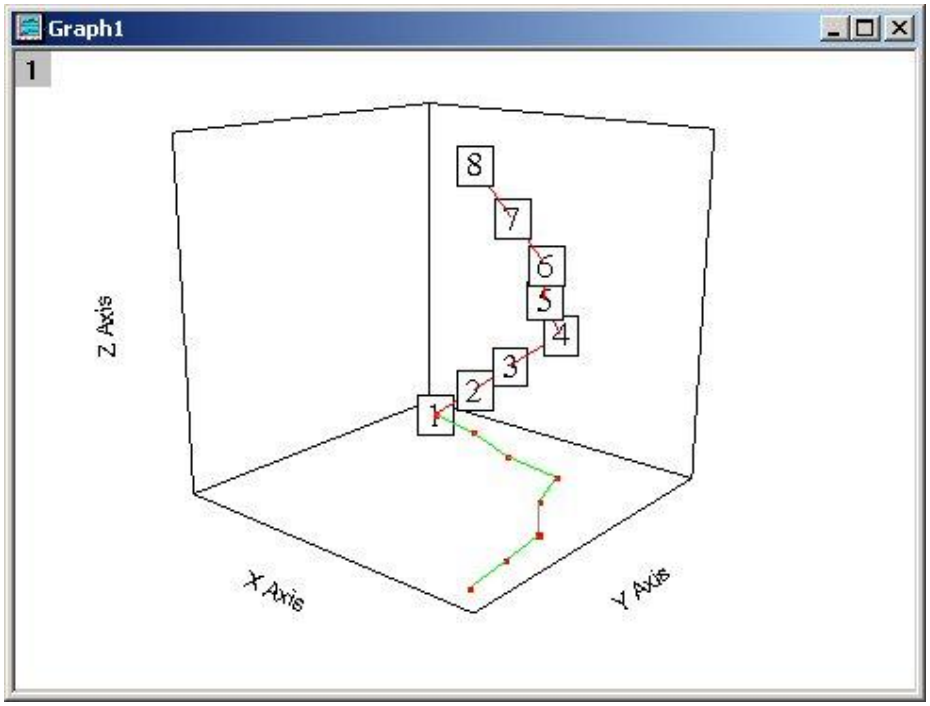


Figure 13. Formatted 3D plot

The 3D Rotation toolbar (see Figure 35) has several buttons that can be used to rotate and change the perspective of the 3D graph. The six buttons on the left rotate and tilt the 3D plot by the specified rotation angle, in this case 10°. The next two increase and decrease the perspective angle by 3°. The last two fit the graph to the layer frame and reset the rotation angles. If the 3D Rotation toolbar is not displayed, open it by selecting **View** > **Toolbars** and then 3D Rotation.

Figure 14. The 3D Rotation toolbar

Task 12 Creating a Surface Plot

Objective To create a surface plot from 3D data stored in a matrix window.

Instructions Create a matrix from worksheet data and plot as a 3D surface.

Comments Use the matrix details given.

Surface plots can only be plotted from matrix windows. Matrix data can be input in several ways: it can be created from a formula, copied and pasted from another application, imported, or created from an existing worksheet as in the following example.

Activity 12.1 Open a new worksheet and import the ASCII data file Tutorial_5.DAT from C:\Program Files\OriginPro75\Tutorial. The worksheet displayed should have three columns A(X), B(Y) and C(Y). Change the name of the third column to C(Z), as in Activity 11.2.

Activity 12.2 Highlight column C(Z) and select **Convert to Matrix** from the **Edit** menu and choose **Random XYZ**.

Activity 12.3 Select the Correlation gridding method. The box shown in Figure 36 should now appear. Select the number of rows and columns, search radius and amount of smoothing required for the data.

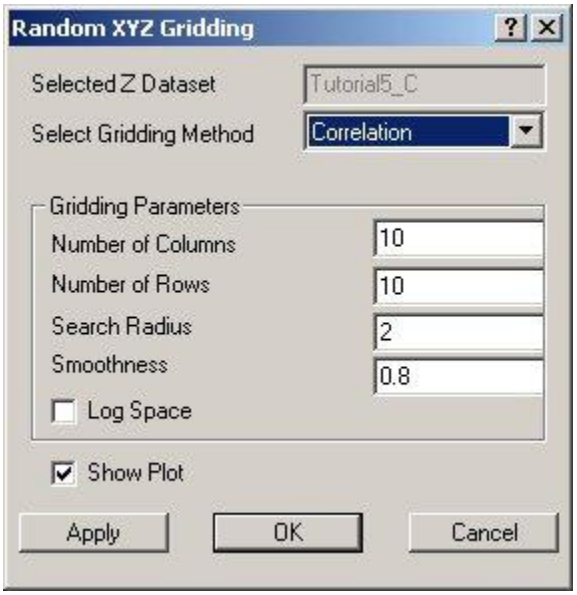


Figure 15. Adjusting the number of cells

The values selected will determine how fine/blocky your plot will be. From your XYZ data, OriginPro will interpolate values for each cell in the matrix - the more cells, the finer the plot but too many cells will take much longer to calculate and could be meaningless if there is not sufficient data. The search radius value is used to determine which of your XYZ data points will be used to compute each cell value - this needs to be big enough to cover small gaps in the data but should not be so big that values at one end of the dataset have an effect at the other end.

If you are not sure about values for your dataset, try several different ones. For this example, accept the default values as above, de-select Show Plot and click OK. The following matrix shown in Figure 37 appears (note, you may need to increase the column width to display the values).

Matrix1 - Correlation Gridding for Tutorial5_C

	1	2	3	4	5	6
1	-2.83098E-6	-8.48322E-7	-1.31178E-6	-2.34499E-6	-1.20524E-6	6.9745
2	-1.4735E-6	7.00171E-7	1.24064E-6	-3.26447E-7	1.18853E-5	5.5669
3	-7.12961E-7	1.08393E-6	2.01817E-6	4.19444E-6	4.38622E-5	1.223
4	1.35644E-7	2.48755E-6	4.22418E-6	6.49572E-5	9.47342E-5	1.7614
5	1.28077E-6	4.54625E-6	8.87785E-6	1.62926E-4	2.63362E-4	2.5799
6	1.88983E-6	5.76902E-6	1.14287E-5	1.15833E-4	2.82467E-4	2.7529
7	1.95357E-6	5.72978E-6	1.12235E-5	4.61702E-5	2.1638E-4	2.6610
8	1.59485E-6	5.51987E-6	1.09936E-5	3.1159E-5	1.4384E-4	1.8575
9	7.4891E-7	4.21159E-6	1.04578E-5	1.89809E-5	6.57137E-5	3.1081
10	-2.32641E-6	-1.30004E-7	3.94956E-6	7.01337E-6	2.05707E-5	-8.878

Figure 16. The Matrix window

Activity 12.4 The graph is now ready to be drawn. Open the **Plot** menu and click on the **3D Color Map Surface** option. The graph which is plotted is shown in Figure 38.

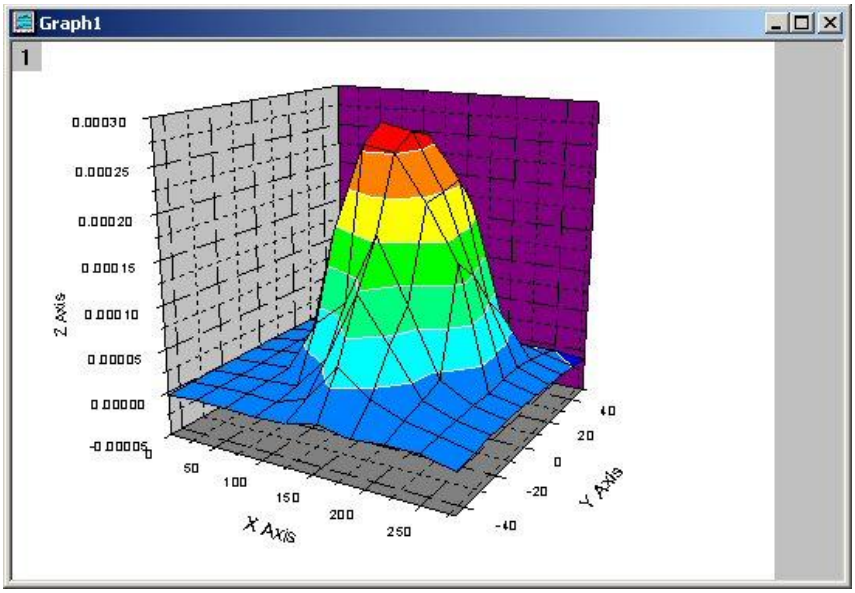


Figure 17. Surface plot

Activity 12.5 Now open the Plot Details dialog box by double-clicking on one of the grid data points. If Matrix1 is not selected on the left-hand side of the Plot Details dialog box, expand Layer1 by clicking on the + and then select it. Most of the options are self-explanatory so try and play around with them, especially experimenting with the Plot Type options at the bottom left of the dialog box.

Task 13 Quitting OriginPro

Objective To quit OriginPro.

Instructions You will use the **Exit** option from the **File** menu.

Activity 13.1 Select the **Exit** option from the **File** menu.

Note: If you have not saved the project, you are now given the opportunity to do so before exiting.

Further Information

Documentation

To find out more about OriginPro 7.5 the following documents are available for reference or loan from the ISS Help Desk (these manuals can also be purchased, for more information please contact ISS Sales):

Getting Started Manual

Peak Fitting Module Manual

There are also the following manuals available for previous versions:

Microcal Origin User's Manual

Microcal Origin 3D/Contour Manual

Microcal Origin LabTalk Manual

Programming Guide

Documentation is also available as pdf files under C:\Program Files\OriginPro75:

GettingStarted.pdf

Origin_V75_User's_Manual.pdf

PFM_Manual.pdf

(The first is available on the OriginPro 7.5 CD whilst the second and third can be downloaded from OriginLab's website.)

Help

OriginPro incorporates an on-line help system which includes a search facility. You can access help by choosing the **Help** menu.

You can also contact the ISS Help Desk if you have any questions about using OriginPro (e-mail helpdesk@leeds.ac.uk or phone ext. 33333).

Appendix 1 Types of Graph Available under the Plot Menu

2D Line and Symbol Graphs

 Line

 Scatter

 Line + Symbol

Special Line/Symbol:

 Vertical Drop Line

 2 Point Segment

 3 Point Segment

 Vertical Step

 Horizontal Step

 Spline

 Double-Y

 Line Series

 Waterfall

 Zoom

 Y Error

 XY Error

2D Bar, Column and 2/3D Pie Charts

 Bar

 Column

Special Bar/Column:

 Stack Bar

 Stack Column

 Floating Bar

 Floating Column

 Pie

3D XYY

 3D Bars

 3D Ribbons

 3D Walls

 3D Waterfall

3D XYZ

 3D Scatter

 3D Trajectory

3D Surface/2D Contour Plots (only available for Matrix windows)

 3D Colour Fill Surface

 3D X Constant with Base

 3D Y Constant with Base

 3D Colour Map Surface

 3D Bars

 3D Wire Frame

 3D Wire Surface

 Image Plot

Contour Plots:

 Contour – Colour Fill

 Contour – B/W Lines + Labels

 Gray Scale Map

 Histogram

 Profiles/Image and Profiles/Contour

Bubble/Colour Mapped

 Bubble

 Colour Mapped

 Bubble + Colour Mapped

Statistical Graphs

 Box Chart

 QC (X Bar R) Chart

 Histogram

 Histogram + Probabilities

 Stacked Histograms

Panel

 Vertical 2 Panel

 Horizontal 2 Panel

 4 Panel

 9 Panel

 Stack

Miscellaneous

 Area

 Fill Area

 Polar

 Ternary

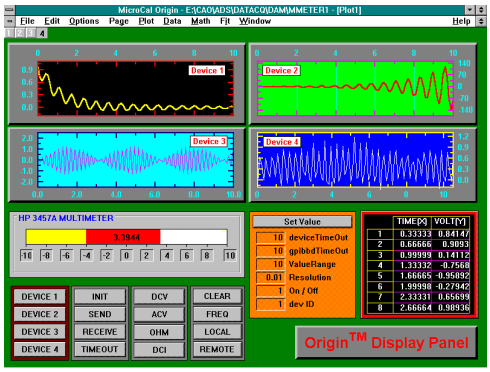
 Smith Chart

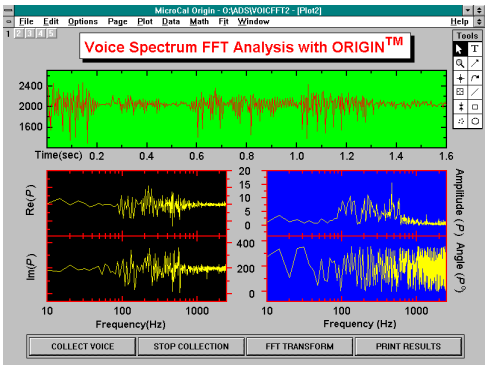
 High-Low-Close

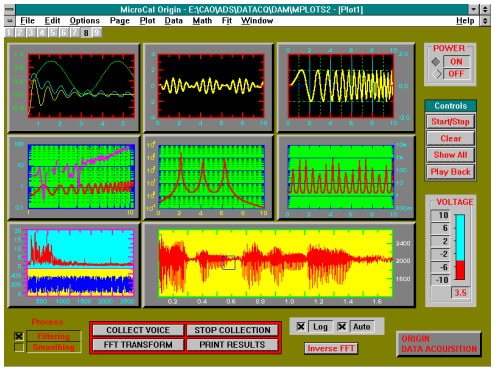
 Vector XYAM

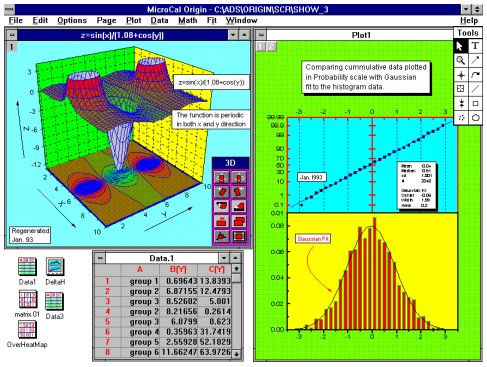
 Vector XYXY

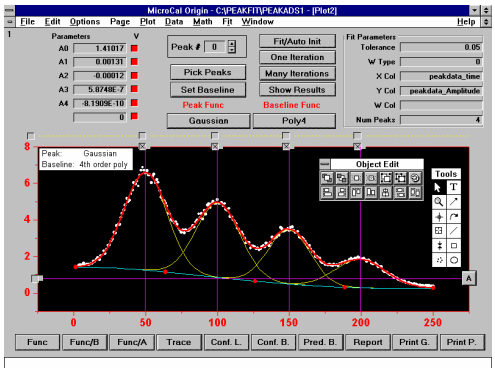
Appendix 2 OriginPro Examples

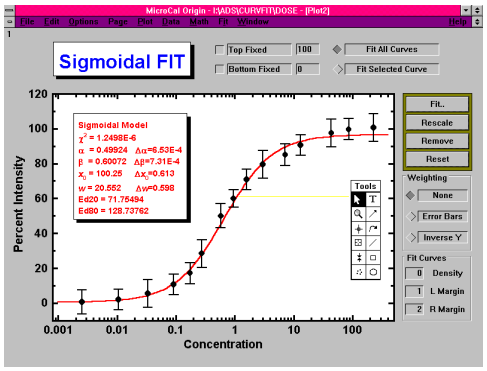


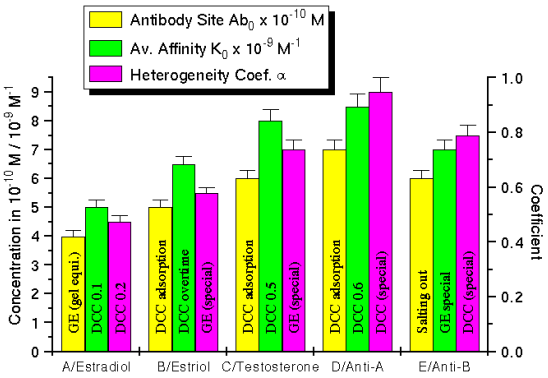


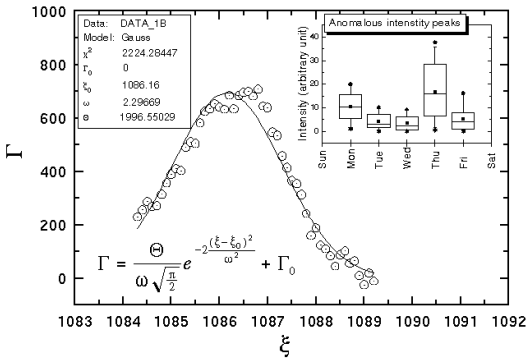


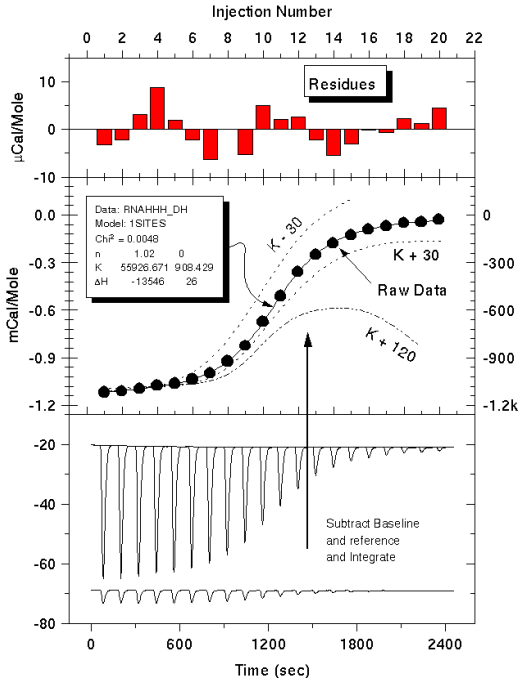


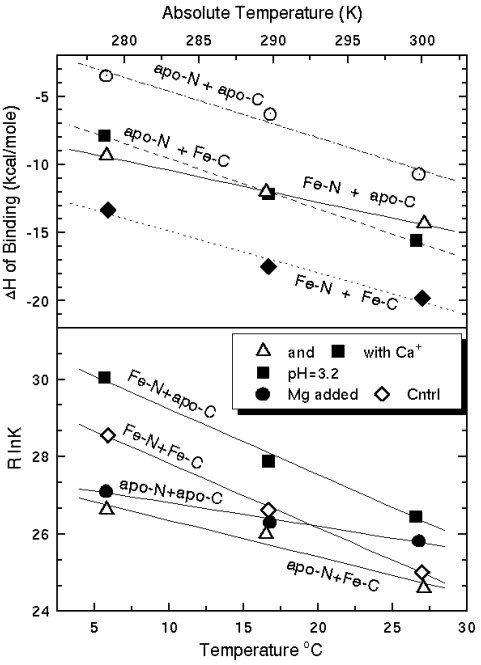


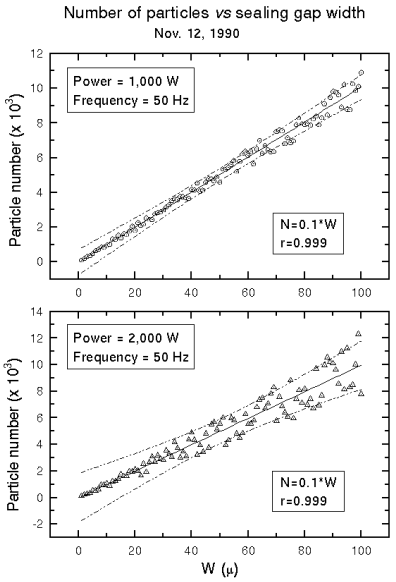


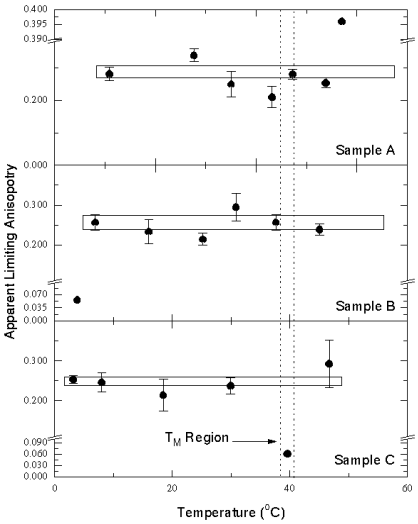


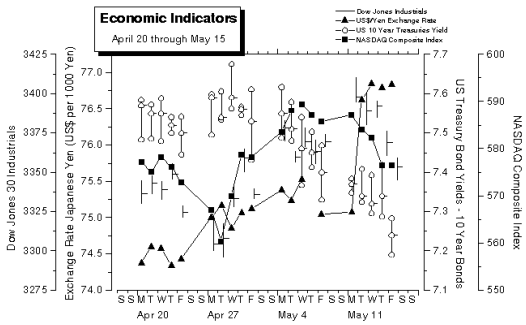



Injection Number
Residues
µCal/Mole
Data: RNAHHH_DH
Model: 1SITES
ChiÂ² = 0.0048
n 1.02 0
K 55926.671 908.429
ΔH -13546 26
K - 30
K + 30
Raw Data
K + 120
mCal/Mole
Subtract Baseline
and reference
and Integrate
Time (sec)


Absolute Temperature (K)
apo-N + apo-C
apo-N + Fe-C
Fe-N + apo-C
Fe-N + Fe-C
ΔH of Binding (kcal/mole)
and with Ca+
pH=3.2
Mg added
Cntrl
Fe-N+apo-C
Fe-N+Fe-C
apo-N+apo-C
apo-N+Fe-C
R lnK
Temperature °C


Number of particles vs sealing gap width
Nov. 12, 1990
Power = 1,000 W
Frequency = 50 Hz
N=0.1*W
r=0.999
Particle number (x 10³)
Power = 2,000 W
Frequency = 50 Hz
N=0.1*W
r=0.999
Particle number (x 10³)
W (µ)


Sample A
Sample B
Sample C
T_M Region
Apparent Limiting Anisopotry
Temperature (°C)


Economic Indicators
April 20 through May 15
Dow Jones Industrials
US$/Yen Exchange Rate
US 10 Year Treasuries Yield
NASDAQ Composite Index
Dow Jones 30 Industrials
Exchange Rate Japanese Yen (US$ per 1000 Yen)
US Treasury Bond Yields - 10 Year Bonds
NASDAQ Composite Index
Apr 20
Apr 27
May 4
May 11