Version 6

Tutorial Manual

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Tutorial 1: Plotting Your Data

1.1 Introduction

This tutorial will show you how to import ASCII data into a worksheet, plot the data, and then customize some basic elements of the graph.

1.2 Importing Your Data

There are many ways to get your data into Origin. If your data exists in an ASCII file, you can import that file into an Origin worksheet. Origin can import almost any type of ASCII file just by selecting File:Import:Single ASCII or clicking Import ASCII on the Standard toolbar. Origin examines the file, looking for columns of data as well as column header text. With complex ASCII files, Origin may need some help from you. This help is provided in the Import ASCII Options dialog box.

For more information on importing data, including multiple ASCII files, see Chapter 6 in the Origin User's Manual.

To Import the ASCII File:

1) Begin this lesson by clicking New Project on the Standard toolbar.

2) Click Import ASCII on the Standard toolbar.

3) In the Origin 6.0 TUTORIAL folder, select TUTORIAL_1.DAT from the list of files.

4) Click Open. The ASCII file imports into the worksheet.

The worksheet is renamed using the name of the ASCII file you imported. Because the file contains text in the first two rows, the first row of text is used to rename the columns, while the first and second rows of text are used to create column labels. The labels are used for the text in the legend when a graph is created.
1.3 Designating Worksheet Columns as Error Bars

When you import data into a worksheet, the default column designations of X, Y, Y, Y, etc. are used to show data associations. If your data is associated differently, you can manually set the column designations.

In this example, the data has the following associations: X, Y, Err, Y, Err, Y, Err.

To Designate Columns as Error Bars:

1) Click on the Time(X) column heading and drag to the Error3(Y) column heading.

2) Right-click within the highlighted cells to open a shortcut menu.

3) Select Set As: X Y Err Y Err from the shortcut menu. This changes the Error1, Error2, and Error3 columns to error bar columns.

Figure 1.2: Changing Worksheet Column Designations

Note: You may need to resize the worksheet to see all the columns.
1.4 Plotting Your Data

Origin offers a broad range of plotting options. The quickest way to create a graph is to select your worksheet data by highlighting the column(s), and then clicking a graph button on one of the graphing toolbars. When you plot multiple columns using this technique, Origin automatically groups the data plots and increments attributes such as the symbol type and color, so that you can easily distinguish between data plots.

To Plot Your Worksheet Data:

1) With your worksheet data still selected, click Line + Symbol on the 2D Graphs toolbar. The three Y columns are plotted as line and symbol data plots with error bars provided by the error bar columns to the right of the associated Y columns.

Figure 1.3: Plotting the Worksheet Data

Focusing on a Region of Your Graph

You may want to take a closer look at interesting areas of your data, particularly if you have a large number of points. Origin provides a number of tools to accomplish this, including the Enlarger tool. The Enlarger tool automatically rescales the axes of the graph to show only the region of the data plot(s) you select.
To Enlarge a Section of Your Data:

1) Click Enlarger on the Tools toolbar.

2) Click-and-drag with the magnifying glass cursor to draw a box around the large peaks (near X = 1.5) in the graph window. Release the mouse button to complete the operation.

Figure 1.4: Enlarging a Section of Your Data

Figure 1.5: Rescaled Graph
Note: To return the axes to their original scale, double-click on the Enlarger tool.

1.5 Customizing the Graph

Origin allows you to customize every aspect of your graph. The easiest way to customize graphic elements is to double-click on them.

Customizing the Data Plot

Double-clicking on a data plot or the data plot icon in the legend opens the Plot Details dialog box. This dialog box allows you to customize the data plot you selected, as well as all the features of the graph window except for the axes and text labels. The selection on the left side of the dialog box determines the controls available for customizing on the right side of the dialog box. For example, when a line and symbol data plot is selected, you can edit the attributes of the lines and symbols, draw drop-lines to either axis, and select which features are incremented between the grouped data plots.

To Customize the Data Plot:

1) Double-click on the Test1 data plot icon in the legend. The Plot Details dialog box opens with the TUTORIAL1:Time(x), Test1(Y) data plot icon selected on the left side of the dialog box.

2) Select the Symbol tab if it is not currently selected.

3) Select the open circle symbol type from the Preview drop-down list.

4) Click OK.

Note: Because the data plots are grouped, the symbol type of the Test2 and Test3 data plots change to increment from the open circle symbol selected for the Test1 data plot.
Customizing the Axes

Double-clicking on any of the axes in the graph opens the Axis dialog box. Similar to the Plot Details dialog box, you can specify the axis you want to customize by selecting it from the Selection list box on the left side of the dialog box.

To Customize the Axes:

1) Double-click on the X axis.

2) On the Scale tab, type 1.2 in the From text box, 1.8 in the To text box, and .1 in the Increment text box.

Figure 1.6: The X Axis Dialog Box

3) Select the Title & Format tab.

4) Type Time (sec) in the Title text box, overtyping the default text.

5) Select the Left icon from the Selection list box.

6) Type Potential (mV) in the Title text box, overtyping the default text.
7) Select the Scale tab.

8) Type -.001 in the From text box, .014 in the To text box, and .002 in the Increment text box.

9) Click OK.

Figure 1.7: Customizing the Graph

Adding Text to the Graph

To further customize your graph, you can add annotations including text, arrows, lines, and shapes. The tools that let you add these annotations are located on the Tools toolbar. Alternatively, you can right-click anywhere in the graph to add text using a shortcut menu.

To Add Text to the Graph:

1) Click on the Tools toolbar, and then click on the top center position of the graph.

2) In the Text Control dialog box, type Effect of Solvent Loss on Sample Potential.
3) Select 26 from the Size combination box.

Figure 1.8: The Text Control Dialog Box

4) Click OK.

5) Drag the legend so that it is located in the top left corner of the graph, next to the Y axis.

6) Drag the text label you just created so that it is centered at the top of the window.
1.6 Saving Your Project

Your project currently consists of one worksheet and one graph window and the data displayed in both. Both of these windows and the data they contain are saved within an Origin project file when you save the project.

To Save Your Project:

1) Click Save on the Standard toolbar.

2) Type Tutorial_1 in the File Name text box, then click Save. The project is saved as Tutorial_1.OPJ.
This page is left intentionally blank.
Tutorial 2: Exploring Your Data

2.1 Introduction

This tutorial will show you how to mathematically transform data in a worksheet column, sort a worksheet based on primary and secondary columns, plot a range of worksheet data, and mask data from analysis routines.

To begin this tutorial, you will open a new Origin project and import ASCII data.

To Import the Data File:

1) Click New Project on the Standard toolbar.

2) Click Import ASCII then select TUTORIAL_2.DAT from the Origin 6.0 TUTORIAL folder.

3) Click Open.
Figure 2.1: Importing the ASCII File

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>STN</td>
<td>TIME</td>
<td>DEPTH</td>
<td>FLUOR</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>36</td>
<td>845</td>
<td>1</td>
<td>0.35</td>
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<td>9</td>
<td>35</td>
<td>857</td>
<td>2</td>
<td>0.34</td>
</tr>
</tbody>
</table>

Note: There are several columns that are not visible due to the current worksheet size. When there is a reference in this tutorial to a column that is not visible, use the horizontal scroll bar on the bottom of the worksheet to locate it.

### 2.2 Transforming Column Values

You can create or transform datasets using any mathematical expression recognized by Origin in the Set Column Values dialog box. This dialog box provides a text box for you to type a value or mathematical expression to apply to the selected column or range of the column. It also includes a function drop-down list from which you can select a function to add to the text box. In addition, a column drop-down list contains a list of all the columns in the active worksheet. Select the column you want to add to the text box, then click Add Column to add the selected column to the text box.

**To Transform the Column Values:**

1) Right-click on the Depth(Y) column heading.

2) Select Set Column Values from the shortcut menu that opens.

3) Leave col(A)-col(B) highlighted in the text box and select col(DEPTH) from the Add Column drop-down list.

4) Click Add Column. Col(DEPTH) overwrites the highlighted text.
5) Leave the cursor at the current location in the text box and type \( \times 0.3048 \) in the text box.

6) Click OK. The expression you typed in the Set Column Values dialog box is used to update the values in the DEPTH column.

2.3 Sorting Worksheet Data

For more information on sorting, see Chapter 15 in the Origin User's Manual.

Origin can sort individual columns, multiple selected columns, or entire worksheets. Origin offers simple sorting in which specified data is sorted using one "sort by" column and a selected sort order, as well as nested sorting.

To Sort the Worksheet Data:

1) Move the mouse pointer to the upper-left corner of the worksheet to turn the cursor into a downward pointing arrow (see Figure 2.3), then click to select all the columns in the worksheet.
2) Click Sort on the Worksheet Data toolbar to open the Nested Sort dialog box. (To open the Worksheet Data toolbar, select \textit{View: Toolbars}, select the Worksheet Data check box, then click Close.)

3) Select DEPTH from the Selected Columns list box, then click Ascending. The column is added to the Nested Sort Criteria list box. This selection makes DEPTH the primary sort column in ascending order.

4) Select STN from the Selected Columns list box, then click Ascending. This makes STN the secondary sort column in ascending order.

Figure 2.3: Selecting All the Columns in the Worksheet

Figure 2.4: Sorting the Worksheet
5) Click OK.

6) De-select the worksheet by clicking in the upper–left blank space in the worksheet (without the cursor changing to the downward pointing arrow).

The entire worksheet is sorted so that the values in the DEPTH (primary) column are ascending. If there are two cells of equal value in the DEPTH column, then the values in the corresponding rows of the STN (secondary) column are used to determine the worksheet order.

2.4 Plotting a Range of the Worksheet Data

You can set the worksheet display range so that subsequent plotting and analysis are performed only on the data of interest.

To Select a Range of the Worksheet Data:

1) Select View:Go To Row.

2) Type 52 in the dialog box that opens, then click OK.

3) Right-click on the row heading for row number 52.

4) Select Set As Begin from the shortcut menu that opens.
Figure 2.5: Selecting a Range of Worksheet Data

5) Use the vertical scroll bar to move down in the worksheet so that row number 68 is visible.

6) Right-click on the row heading for row number 68.

7) Select **Set As End** from the shortcut menu that opens.

Notice that the data outside the selected range is no longer displayed in the worksheet. The data has not been deleted from the worksheet, only hidden to provide for easier viewing of the selected range. The hidden data can be shown by selecting **Edit: Reset to Full Range**.

**Plotting the Data:**

1) Click the FLUOR column heading to select the column.

2) Drag the horizontal scroll bar on the bottom of the worksheet all the way to the right.

3) CTRL+click on the TEMP column heading. This selects the TEMP column while leaving the FLUOR column selected.
4) Click Double Y Axis on the 2D Graphs Extended toolbar. (To open the 2D Graphs Extended toolbar, select View:Toolbars, select the 2D Graphs Extended check box, then click Close.)

Figure 2.6: Plotting a Range of Worksheet Data

2.5 Masking Data in the Graph

The Mask toolbar is provided for excluding data from Origin's analysis and fitting routines. You can mask individual data points or a range of data. Once data is masked, options become available to change the masked data color, hide or show the masked data, swap the masked and unmasked data, and enable or disable masking.

To Mask a Data Point in the Graph:

1) Click Mask Point Toggle on the Mask toolbar. This activates the Data Reader tool. (To open the Mask toolbar, select View:Toolbars, select the Mask check box, then click Close.)
2) Double-click on the data point in the FLUOR data plot at X = 34, Y = .59. The data point becomes red and the point is masked.
(Tip: With the Data Reader open, click on the FLUOR data plot, then use the LEFT ARROW or RIGHT ARROW keys to read the XY coordinates on the Data Display tool.)

Figure 2.7: Masking Data in the Graph Window

3) Click Change Mask Color on the Mask toolbar. The color changes to green.

4) Click Hide/Show Masked Points on the Mask toolbar to hide the masked data point.

5) Click Hide/Show Masked Points on the Mask toolbar again to show the data point.
2.6 Performing a Linear Fit on the FLUOR Data Plot

Now that a data point is masked in the FLUOR data plot, subsequent analysis and fitting are performed only on the non-masked data. You can, however, disable the mask on the data point, and analyze or fit all the data points in the current selection range.

To Perform a Linear Fit with the Data Point Masked:

1) Select **Analysis: Fit Linear**. A fit line is added to the graph and the Results Log opens displaying the fitting results. You can scroll the Results Log to view the results.

2) Click Refresh on the Standard toolbar and reposition the legend so it fits on the page.

Figure 2.8: Linear Fit of the FLUOR Data Plot with a Masked Data Point
2.6 Performing a Linear Fit on the FLUOR Data Plot

Figure 2.9: The Results Log

By default, the Results Log shows the results for all fitting done in the currently active Project Explorer folder. To change this default behavior, right-click in the Results Log and select a different viewing option.

Each time a new fit is done the results are appended to the Results Log. Each entry in the Results Log includes a date/time stamp, the project file location, the dataset, the type of analysis performed, and the results.

To Perform a Linear Fit with the Mask Disabled:

1) Click Disable/Enable Masking on the Mask toolbar. The masked data point changes from green to black.

2) Select Analysis: Fit Linear. An updated fit line is drawn on the graph.

3) Verify that the mask is disabled by comparing the two fit results in the Results Log.
2.7 Saving the Project

Your Origin project currently consists of your data, worksheets, graph, analysis results and the current folder organization in the Project Explorer.

_To Save the Project:_

1) Select File:Save Project.

2) Type a name in the File Name text box.

3) Click Save.
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Tutorial 3: Creating Multiple Layer Graphs

3.1 Introduction

This tutorial will introduce you to Origin's built-in multiple layer graph templates. It will also show you how to create your own multiple layer graph and then save it as a template.

3.2 Opening the Project File

The data for this tutorial is provided in a project file.

To Open the Project File:

1) Click Open on the Standard toolbar.

2) In the Origin 6.0 TUTORIAL folder, select TUTORIAL_3.OPJ from the list of files.

3) Click Open. A project containing four graph windows and a worksheet opens.

3.3 Viewing Origin's Multiple Layer Graph Templates

Origin contains several built-in, multiple layer graph templates. These templates allow you to select a range of data, then click a button to plot the selected data into multiple layers in a graph window.
The double Y axis graph template is ideal for plotting data that includes two or more dependent datasets and a common independent dataset. A sample double Y axis graph is currently active in your project.

1) Right-click on the double Y axis graph window title bar and select **Hide** from the shortcut menu.

The Project Explorer provides easy access to all the windows in the project. By default, the Project Explorer is docked at the bottom of your workspace. If you cannot see the five icons on the right pane of the Project Explorer, then expand the view by pointing the mouse on the upper edge of the Project Explorer. When the mouse pointer displays $\div$, click-and-drag upward so that you can see all five icons on the right pane. (Note: If your Project Explorer is closed, click on the Standard toolbar.)

**Figure 3.1: The Project Explorer**

<table>
<thead>
<tr>
<th>Name</th>
<th>Type</th>
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<th>Modified</th>
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<th>Link</th>
<th>Label</th>
</tr>
</thead>
<tbody>
<tr>
<td>iPanel</td>
<td>Graph</td>
<td>Miniz.</td>
<td>41K</td>
<td>12/22/...</td>
<td>12/22/ 0</td>
<td></td>
<td></td>
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<tr>
<td>DoubleYaxis</td>
<td>Graph</td>
<td>Normal</td>
<td>22K</td>
<td>12/22/...</td>
<td>12/22/ 0</td>
<td></td>
<td></td>
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<tr>
<td>Horizontal2Panel</td>
<td>Graph</td>
<td>Miniz.</td>
<td>128K</td>
<td>12/22/...</td>
<td>12/22/ 0</td>
<td></td>
<td></td>
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<tr>
<td>UniY</td>
<td>Graph</td>
<td>Miniz.</td>
<td>29K</td>
<td>12/22/...</td>
<td>12/22/ 0</td>
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<td></td>
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<tr>
<td>Vertical2Panel</td>
<td>Graph</td>
<td>Miniz.</td>
<td>22K</td>
<td>12/22/...</td>
<td>12/22/ 0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2) Double-click on the Horizontal2Panel graph icon on the right pane of the Project Explorer.

The horizontal 2 panel graph template is ideal for plotting related data that does not share an independent dataset. You can use the **Edit: Add & Arrange Layers** menu command and the Layer tool to customize the spacing of the layers and to swap the layer arrangement.

3) Right-click on the Horizontal2Panel graph icon on the right pane of the Project Explorer and select **Hide Window** from the shortcut menu.

4) Double-click on the Vertical2Panel graph icon on the right pane of the Project Explorer.
The vertical 2 panel graph template provides the same data presentation as the horizontal 2 panel graph template, but in a one column with two rows configuration.

5) Right-click on the Vertical2Panel graph icon on the right pane of the Project Explorer and select **Hide Window** from the shortcut menu.

6) Double-click on the 4Panel graph icon on the right pane of the Project Explorer.

A 4 panel and a 9 panel (not shown) graph template complete the library of built-in multiple layer graph templates.

### 3.4 Designating Multiple X Columns in the Worksheet

When your worksheet includes multiple X columns, Y columns in the worksheet plot against the nearest X column to the left. Though this default behavior can be disregarded by plotting using the Select Columns for Plotting dialog box and by selecting non-associated columns with CTRL selection, the default plotting behavior allows you to quickly create graphs from associated XY datasets.

**To Designate a Second X Column:**

1) Double-click on the Layers worksheet icon on the right pane of the Project Explorer.

2) Right-click on the Trial2 column heading in the Layers worksheet.

3) Select **Set As:X** from the shortcut menu that opens.

The Trial2 column designation changes to X2 and the columns to the right of it are designated as Y2. In addition, the Trial1 column designation changes to X1 and the columns between Trial1 and Trial2 are designated as Y1. This allows you to quickly determine which column will be providing the X values for the data you are plotting.

### 3.5 Creating a Multiple Layer Graph

Origin cannot possibly contain pre-defined templates for all the different ways in which layers can be arranged, so it lets you to create your own
custom multiple layer graphs. Once you have created a graph, you can save it as a template and then plot to it without having to re-build the same graph every time.

**To Create a Multiple Layer Graph:**

1) Click on the Potential1 column heading to highlight the column.

2) Click Line on the 2D Graphs toolbar.

**Figure 3.2: Line Graph of Potential1 Column**

3) Select **Tools: Layer** to open the Layer tool.

4) With the Add tab selected, click Linked Right Y on the Layer tool. This adds a second layer to the graph displaying only the right Y axis. By default, the X axis of this layer is linked to the X axis of layer 1.

5) Double-click on the layer 2 icon in the upper-left corner of the graph window.
6) Select \texttt{layers\_pressure1} in the Available Data list box.

7) Click \(\rightarrow\) to add the dataset to the Layer Contents list box.

Figure 3.3: Adding Data to Layer 2

8) Click Layer Properties. The Plot Details dialog box opens.

9) Double-click on the Layer2 icon on the left side of the dialog box.

10) Click on the \texttt{LAYERS:\texttt{Trial1(X)}, \texttt{Pressure1(Y)}} data plot icon on the left side of the dialog box. This action opens the Line tab.

Figure 3.4: Graph Tree of Plot Details Dialog Box

11) Select Blue from the Color drop-down list, then click OK.

12) Click OK to close the Layer 2 dialog box.
Figure 3.5: Adding a Right Y Controlling Axis

Origin provides many methods to add layers to your graph. In addition to the Layer tool, you can select menu commands from the Edit menu or from a shortcut menu available outside of the graph page (but within the window).

Arranging Layers in the Graph Window

In this section, you will add and arrange layers to set up a vertical 2 panel graph with left and right Y axes.

To Add and Arrange Layers in the Graph:

1) Select Edit:Add & Arrange Layers.

2) In the Total Number of Layers dialog box, leave the default of 2 Rows and 1 Column.

3) Click OK. Origin asks for permission to create 1 more layer.

4) Click Yes.

5) Click OK in the Spacing dialog box to accept the default settings.
To Add the Right Y Controlling Axis to the Top Layer:

1) With the layer 3 icon selected, right-click in the gray area of the graph window, outside of the page.

2) Select **New Layer (Axes): (Linked): Right Y** from the shortcut menu that opens.
Adding Data to the New Layers

To add the data to layers 3 and 4, you will use the Layer \( n \) dialog box in the same way you added the data to layer 2.

**To Add Data to the New Layers:**

1. Double-click on the layer 3 icon.
2. In the Layer 3 dialog box, select `layers_potential2` in the Available Data list box, then click \( \Rightarrow \) to add it to the Layer Contents list box.
3. Click OK.
4. Double-click on the layer 4 icon.
5. In the Layer 4 dialog box, select `layers_pressure2` in the Available Data list box, then click \( \Rightarrow \) to add it to the Layer Contents list box.
6. Click Layer Properties to open the Plot Details dialog box.
7) Double-click on the Layer4 icon on the left side of the dialog box, then click on the \textit{LAYERS: Trial2(X), Pressure2(Y)} data plot icon.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{graph_tree.png}
\caption{Graph Tree of Plot Details Dialog Box}
\end{figure}

8) Select Red from the Color drop-down list.

9) Click OK to exit the Plot Details dialog box.

10) Click OK.

\section*{Linking Axes}
You can link axes between layers so that when you change the axis scale in one layer the other layer's linked axis updates to the same scale automatically.

\textit{To Link the X Axes:}

\begin{enumerate}
\item Double-click on the layer 3 icon to open the Layer 3 dialog box.
\item Click Layer Properties.
\item Select the Link Axes Scales tab.
\item Select Layer 1 from the Link To drop-down list.
\item Select the Straight (1 to 1) radio button in the X Axis Link group, then click OK.
\item Click OK in the Layer 3 dialog box.
\end{enumerate}
You can test the axis link by double-clicking on the bottom X axis and changing the From or To values on the Scale tab. After clicking OK, the top X axis also reflects your changes.

3.6 Customizing the Legend

By default, Origin creates layer-specific legends. You can, however, alter this default behavior and display the data from all the layers in one legend.

Origin uses the embedded text formatting switch \L( ) to draw the data plot type representations in the legend. To display the correct data plot type representations from different layers, you must specify the layer number followed by a period, then the number of the data plot in that layer.

To Customize the Legend:

1) Click on the text portion of the legend for the bottom layer reading Potential1 (mV), then press DELETE.

2) Double-click on the text portion of the legend for the top layer reading Potential2 (mV).
3) In the Text Control dialog box, type the following text, overwriting \L(1) %1:

\L(1.1) Potential1
\L(2.1) Pressure1
\L(3.1) Potential2
\L(4.1) Pressure2

The preview box on the bottom of the dialog box shows what the text will look like in the legend.

4) Click OK.

5) Drag the legend to a location where it does not overlap with the axes or the data.

The legend now displays the data plot type representations from all the layers in the graph. To prevent Origin from overwriting your custom legend (for example, if you click New Legend on the Standard toolbar) you can rename the legend by right-clicking on the object and selecting **Label Control**.

**To Rename the Legend:**

1) Right-click on the legend.

2) Select **Label Control** from the shortcut menu that opens.

3) Type **Custom Legend** in the Object Name text box.

4) Click OK.
3.7 Saving the Graph as a Template

Template files retain information on how to display the data, but do not actually save the data. The next time you need to create a similar graph, you can select your worksheet data and then select your custom graph template. Your custom template is easily accessed by clicking Template on the 2D Graphs toolbar.

To Save Your Graph as a Template:

1) Right-click on the graph window title bar.

2) Select Save Template As from the shortcut menu that opens.

3) Type Multilayer in the File Name text box.

4) Click Save.
To test your template, you can make the Layers worksheet active, select all the worksheet columns, and then click Template on the 2D Graphs toolbar. Select MULTILAYER.OTP, then click Open.
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4.1 Introduction

Origin offers several methods of fitting functions to your data. These methods vary in speed and complexity to optimize fitting for all users. In this tutorial, you will be introduced to fitting using the menu commands, the tools, and the nonlinear least squares fitter (NLSF). You will then define your own function and fit sample data using the advanced mode of the NLSF.

4.2 Fitting from the Menu

Origin offers access to several fitting functions directly from the Analysis menu. To perform a fit on your data using the menu commands, make sure that the data plot you want to perform the fit on is active, then select the type of fit you want to perform from the Analysis menu. Most of the menu commands require no parameter information from you and will carry out the fit automatically. Some may ask you for some parameter information, but will suggest default values based on your data.

Figure 4.1: Fitting Commands on the Graph Window Analysis Menu

- Fit Linear
- Fit Exponential Decay
- Fit Exponential Growth
- Fit Sigmoidal
- Fit Gaussian
- Fit Lorentzian
- Fit Multiple peaks
- Nonlinear Curve Fit...
4.3 Fitting Using the Tools

For a greater degree of control than the menu commands allow, Origin provides three fitting tools: the Linear Fit tool, the Polynomial Fit tool and the Sigmoidal Fit tool.

Figure 4.2: The Fitting Tools

The fitting tools are available when the worksheet or graph is active. To use the fitting tools, select the dataset or data plot you want to fit, customize the options on the tool, and then click Fit.

4.4 The Nonlinear Least Squares Fitter

The nonlinear least squares fitter (NLSF) is Origin's most powerful and complex method of fitting data. There are two display modes available for the NLSF: basic and advanced. You can switch between modes by clicking the More button in the basic mode or the Basic Mode button in the advanced mode.

The Basic Mode

The basic mode of the curve fitter provides an abbreviated fitting function list and a less complex interface than the advanced mode. Additionally, the basic mode offers less control over the fit and less customization of the reported results.
The Advanced Mode

The advanced mode lets you customize all aspects of the fitting process. It provides access to many more fitting functions than the basic mode and the functions are separated into categories to facilitate searching. The advanced mode also has its own menu and toolbar to provide access to all its features.

To select a function in the advanced mode, select the appropriate category from the Categories list box, then select the desired function from the Functions list box. Once a function is selected, the procedure for fitting is the same as for fitting after you define your own function.
4.5 Fitting a Dataset Using Your Own Function

Opening the Project File

The data for this tutorial is provided in an Origin project file.

To Open the Project File:

1) Click Open on the Standard toolbar.

2) In the Origin 6.0 TUTORIAL folder, select TUTORIAL_4.OPJ from the list of files.

3) Click Open.
The project opens showing a worksheet containing data and a graph window containing a data plot.

**Defining a Function**

You can define your own function in the NLSF and then access that function in future sessions from the fitter’s Functions list box. In the basic mode, you click New to define a function. The following procedure guides you through defining a function in the advanced mode.

**To Define your own Function in the Advanced Mode:**

1) Select **Analysis: Nonlinear Curve Fit**. If the fitter opens in the basic mode, click More.

2) Select **Function: New** from the NLSF menu bar.

3) Type **MyFitFunc** in the Name text box.

4) Select 3 from the Number of Parameters drop-down list.

5) Type **p1*exp(-x^p2/p3)** in the Definition text box.
Figure 4.5: Defining a New Function

6) Click Save.

The function is saved under the name MyFitFunc. The MyFitFunc function will now be available in the list of functions under the currently active category. The currently active category is the selected category in the NLSF Select Function dialog box (Function:Select from the NLSF menu).

Assigning the Function Variables to the Datasets

The next step is to assign the X and Y variables in the function to the corresponding X and Y datasets in the data plot you are fitting.

To Assign the Function Variables to Datasets:

1) Select Action:Dataset from the NLSF menu bar.

2) In the list box at the top of the fitter, click on the Y variable in the list, then click data1_b in the Available Datasets list box.
3) Click Assign.

**Figure 4.6: Assigning Variables to Datasets**

When you assign the Y variable to `data1_b` (the Y dataset), Origin automatically assigns the X variable to `data1_a` (the associated X dataset).

**Simulating Curves to Initialize the Parameter Values**

Origin lets you observe what the function will look like with various parameter values in the Simulate Curves dialog box. This enables you to get an understanding of which parameter values produce curves that look similar to your data. This is important because reasonably good starting parameter values are in most cases a precondition for the success of the fitting process.
To Simulate Curves:

1) Select **Action: Simulate** from the NLSF menu bar.

2) Type 5 in the P1, P2, and P3 text boxes (overwriting the dashes).

3) Click Create Curve.

The parameters you typed in the text boxes are used to create a curve which is plotted in the graph window containing your data plot.
Figure 4.8: Simulated Curve

You can type new parameter values in the text boxes to create a simulated curve which looks more like your data.

4) Type \textbf{10} in the P1 text box (overwriting 5).

5) Click Create Curve.

6) Type \textbf{1} in the P2 and P3 text boxes (overwriting 5).

7) Click Create Curve.
Figure 4.9: Fine-tuning the Simulated Curve

The simulated curve is much more similar to the plotted data with the last set of parameter values. These will be the initial parameter values when Origin fits the data.

**Fitting the Data**

You will now fit the data using the function you defined. The initial parameter values will be used from the Simulate Curves dialog box.

**To Fit the Data:**

1) Select **Action:Fit** from the NLSF menu bar.

2) Click Chi-Sqr. The chi-squared value for the current parameter values displays in the view box.

3) Click 10 Iter.
Origin fits the data, performing a maximum of 10 Levenberg-Marquardt iterations. The fit curve displays in the graph. The chi-squared value and the number of iterations performed are reported in the NLSF view box. The updated parameter values are shown in the Value text boxes.

**Figure 4.10: Fitting Session**

![NonLinear Curve Fitting: Fitting Session](image)

**Creating a Worksheet With the Fitting Results and Exiting the Fitter**

After fitting your data, you can create a worksheet that contains all the results of your fitting session. Additionally, when you close the fitter, Origin displays the parameter fitting results in the Results Log and in a label in the graph window.

**To Create a Worksheet with the Fitting Results**

1) Select **Action: Results** in the NLSF.

2) Click **Param. Worksheet**.
3) Click Close \[\times\] in the upper-right corner of the NLSF to close the NLSF.

4) Click Yes at the Attention prompt.

Figure 4.11: Final Graph (with label repositioned and formatted)

![Graph with parameter results]

After closing the NLSF, a Parameters worksheet displays all the fitting results.

The graph window displays your data plot, the simulated curves, the fit curve, and a text label with the parameter results. To remove the simulated curves from the graph, double-click on the layer 1 icon, then select the `myfitfunc1_b`, `myfitfunc2_b`, and `myfitfunc3_b` datasets in the Layer Contents list box and then click \[\times\]. Click OK to close the Layer 1 dialog box.
The Results Log also displays the parameter results. The Results Log is a dockable, non-editable text window. The results from all the analysis and fitting done in a project are sent to the Results Log for viewing. By default, only the results from analysis performed in the active Project Explorer folder are shown in the Results Log. To change the view mode, right-click in the Results Log and select the desired view mode from the shortcut menu that opens. This shortcut menu also contains options for copying and clearing text from the Results Log.
This page is left intentionally blank.
5.1 Introduction

For more information on 3D graphs, see the plotting chapters in the Origin User’s Manual.

Origin supports 3D graphs from three different data formats: XYY worksheet data, XYZ worksheet data and matrix data. However, 3D surface graphs can only be created from matrix data. This tutorial will focus on converting a worksheet containing XYZ data to a matrix and then creating and customizing a 3D surface graph from the matrix.

5.2 Converting a Worksheet to a Matrix

In this section you will learn how to change a worksheet column’s designation, then convert an XYZ worksheet to a matrix so that it can be plotted as a 3D surface graph.

The data for this lesson is provided in an ASCII file.

To Import the ASCII File:

1) Click New Project on the Standard toolbar.

2) Click Import ASCII on the Standard toolbar.

3) In the Origin 6.0 TUTORIAL folder, select TUTORIAL_5.DAT from the list of files.

4) Click Open.
5.2 Converting a Worksheet to a Matrix

By default, when the file is imported columns are added to the worksheet as Y columns. To convert the worksheet to a matrix it must be in an XYZ format.

To Change the Column Designation:

1) Right-click on the C(Y) column heading.

2) Select Set As: Z from the shortcut menu that opens. Column C is now designated as a Z column.

Selecting the Type of Conversion

Origin provides several methods for converting worksheets to matrices, including direct, expand columns, 2D binning, regular XYZ and random XYZ conversions. The best method to use depends on the type of data in the worksheet.

The data in this lesson is an XYZ worksheet with un-ordered XY data. Thus, the method of conversion you will use is random XYZ.

To Convert the Worksheet to a Matrix:

1) If not still selected, click on the C(Z) column heading to select the column.

2) Select Edit: Convert to Matrix: Random XYZ.
5.3 Creating a 3D Surface Graph

Now that you have your data in a matrix you can create any type of contour or 3D surface graph. For this tutorial you will create a 3D color mapped surface graph.

To Create a 3D Color Mapped Surface Graph:

1) With the matrix active, select Plot 3D:3D Color Map Surface.

The matrix data is plotted as a color map surface graph. The different colors represent different Z-value ranges.
5.4 Customizing the Graph

Origin gives you full control over the color mapping applied to the surface data plot. All the options for customizing the color map are located on the Color Map tab of the Plot Details dialog box.

Changing the Color Map Values

The Color Map tab on the Plot Details dialog box displays the current color map associated with levels of Z values. To edit an individual level or color, click on the value or color in the Level or Fill column. To edit the entire range of levels or colors, click on the Level or Fill column heading. To edit a range of levels, SHIFT + click on the desired values to select a range, then click on the Level or Fill column heading.

To Change the Number of Levels in the Color Map:

1) Right-click on the surface plot.

2) Select Plot Details from the shortcut menu that opens.
3) Click on the Level column heading to open the Set Levels dialog box.

4) Select the Num. of Levels radio button, then type 12 in the associated text box.

Figure 5.4: The Set Levels Dialog Box

<table>
<thead>
<tr>
<th>Set Levels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum</td>
</tr>
<tr>
<td>Maximum</td>
</tr>
<tr>
<td>Num. of Levels</td>
</tr>
<tr>
<td>Log Scale</td>
</tr>
</tbody>
</table>

5) Click OK.

The Color Map tab updates to show twelve levels (plus levels for values above and below the maximum and minimum levels) and associated colors in the list box.

Figure 5.5: Updated Color Map Tab
Changing the Color Map Colors

Customizing the Fill Color Range:

1) Click on the Fill column heading to open the Fill dialog box.

2) Select Red from the From drop-down list.

3) Select Green from the To drop-down list.

Figure 5.6: Editing the Fill Dialog Box

4) Click OK.

5) Click OK in the Plot Details dialog box.
Figure 5.7: The Customized Surface Graph

In addition to editing color ranges, you can edit individual colors. This is especially useful if you have an important section of your data that you want to highlight or make transparent.

*To Edit an Individual Color:*

1) Right-click on the surface plot.

2) Select **Plot Details** from the shortcut menu that opens.

3) On the Color Map tab, click on the color associated with 1.833E -4.
Figure 5.8: Selecting an Individual Color to Edit

![Fill dialog box](image)

The Fill dialog box opens.

4) Select None from the Fill Color drop-down list, then click OK.

5) Click OK in the Plot Details dialog box.

The data plot redraws showing the transparent level.

Figure 5.9: Editing an Individual Color

![Data plot](image)
Adding Contours to the Color Map Surface Graph

To further enhance your graph, you can display contour lines and colors on the top or bottom plane of your surface graph. This is done on the Surface / Projections tab of the Plot Details dialog box.

**To Add Contour Colors to the Bottom Plane of the Surface Graph:**

1) Right-click on the surface graph.

2) Select **Plot Details** from the shortcut menu that opens.

3) Select the Surface / Projections tab.

4) Select the Fill Color check box under the Bottom Contour text.

5) Click OK.

Figure 5.10: The Surface / Projections Tab
5.4 Customizing the Graph

Figure 5.11: Displaying Bottom Contour Colors

With the current Z axis scale range and the current view angle, the surface plot substantially overlaps the bottom contour, blocking it from view. To make more of the contour visible, you can change the Z axis scale to begin from a lower value.

To Change the Z Axis Scale:

1) Select **Format: Axes: Z Axis** to open the Z Axis dialog box.

2) In the From text box, type \(-1E-4\).

3) Click OK.
Figure 5.12: Changing the Z Axis Scale

The Z axis now displays a greater range below the surface graph. This decreases the amount of overlap of the surface plot and the contour, providing for a better visual presentation.

Changing the Perspective of the Graph

When you create a 3D graph, the 3D Rotation toolbar automatically opens. This toolbar contains buttons for controlling the perspective of the 3D graph. By rotating the graph you can further reduce the overlap of the surface plot with the contour, and provide a better perspective for viewing the graph.

Figure 5.13: The 3D Rotation Toolbar

To Rotate the Graph:

1) Click Tilt Up on the 3D Rotation toolbar.

2) Click Rotate Counterclockwise on the 3D Rotation toolbar.
Figure 5.14: Rotating the Graph

This new perspective eliminates the overlap between the surface plot and the contour, and provides better visibility of the transparent section of the surface plot.
Tutorial 6: Creating Presentations with the Layout Page

6.1 Introduction

The layout page is designed to facilitate the creation of graphic presentations. Pictures of any worksheet or graph windows in your project can be displayed and arranged on the layout page. In addition, text and graphic objects can be added to enhance your presentation.

6.2 Adding Graphs, Worksheets and Text to the Layout Page

Pictures of graphs and worksheets are added to the layout page by clicking the buttons on the Layout toolbar, or by selecting associated menu commands. Text can be added with the Text tool, or by pasting from the Clipboard. Shapes, lines and arrows can be added using the drawing tools from the Tools toolbar.

Opening the Project File

The data for this tutorial lesson is provided in an Origin project file.

To Open the Project File:

1) Click Open on the Standard toolbar.

2) In the Origin 6.0 TUTORIAL folder, select TUTORIAL_6.OPJ from the list of files.

3) Click Open.
A project opens, displaying several worksheet and graph windows.

**Creating a New Layout Page**

*To Create a New Layout Page:*


2) If the layout page is displayed in the portrait orientation, right-click on the gray area of the layout page, then select **Rotate Page** from the shortcut menu that opens.

**Adding Pictures and Text to a Layout Page**

When you add a worksheet or graph to the layout page, it is added as a graphic object and the features of the window cannot be edited directly in the layout page. However, all changes made to the original window will be reflected in the layout page.

*To Add Pictures of Graphs and Worksheets to the Layout Page:*

1) Click Add Graph on the Layout toolbar. If the Layout toolbar is not open, select **View:Toolbars**, select the Layout check box, then click Close.

2) Select Graph3 from list box in the Select Graph Object dialog box and click OK.

3) Drag out a box on the lower-left corner of the layout page.
Figure 6.1: Adding a Graph Picture to the Layout Page

When you release the mouse button a picture of the graph window is added to the layout page. When the graph picture is selected, you can drag the picture to a new location, or use the sizing handles to resize it.

4) Right-click on a blank section of the layout page and then select **Add Worksheet** from the shortcut menu that opens.

5) Select Peaks from the list box in the Select Worksheet Object dialog box and click OK.

6) Drag out a box in the lower-right corner of the layout page.
66 • 6.2 Adding Graphs, Worksheets and Text to the Layout Page

Figure 6.2: Adding a Worksheet Picture to the Layout Page

To Add Text to the Layout Page using the Text Tool:

1) Click Text Tool on the Tools toolbar.

2) Click on the upper portion of the layout page, then type **Peaks from Spectroscopy Data** in the Text Control dialog box.

3) Select 36 from the Size combination box.

4) Select Black Line from the Background drop-down list.

5) Click OK.
6.3 Customizing the Appearance of the Layout Page

In this section, you will fine tune the size and position of the graphic objects displayed in the layout page. In addition, you will make changes to the source graph window to change the graph’s appearance in the layout page.

Arranging Pictures on the Layout Page

There are several ways to arrange pictures on the layout page. You can drag the pictures and estimate the position, use the Object Edit toolbar, or view the grid on the layout page and align the pictures using the grid lines as a guide.

To Arrange the Pictures on the Layout Page Using a Grid:

1) Select View:Show Grid.

2) Right-click on the graph picture, then select Keep Aspect Ratio from the shortcut menu that opens. This will preserve the aspect ratio of the source graph window.
3) Resize the graph picture, using the right horizontal sizing handle, to take up the lower-left half of the layout page.

4) Follow the same procedure for the worksheet picture, resizing it to the lower-right half of the layout page.

Note: The grid is only displayed on the layout page within Origin. If the layout page is printed or exported, the grid will not be displayed.

Figure 6.4: Arranging the Objects on the Layout Page

5) Center the text label using the grid lines for alignment.
Editing the Pictures in the Layout Page

Although you cannot edit the worksheets and graphs in the layout page directly, Origin provides a shortcut menu command to go to the source window.

To Edit a Source Window from the Layout Page:

1) Right-click on the graph picture in the layout page.

2) Select **Go To Window** from the shortcut menu that opens. Origin makes the Graph3 window active.

3) Double-click on the gray area of the Graph3 window outside of the page.

4) On the Legends tab of the Plot Details dialog box, select the Full Dataset Name check box.

5) Click next to the Graph 3 icon on the left side of the dialog box, then select the Layer 1 icon from the graph tree.
6) On the Display tab, clear the Clip Data to Frame check box.

7) Click OK.

8) Drag the legend so that it displays within the axes of the graph, then click in a blank section of the graph to de-select the legend.

9) Double-click on the Layout1 icon on the right side of the Project Explorer to re-activate this window. The graph picture reflects your changes.

6.4 Exporting the Layout Page

In addition to customizing your layout page presentation in Origin, you can export the layout page into other applications. Origin provides a number of graphic export filters. In addition, you can copy the layout page to the Clipboard and paste it into other applications.

To Export the Layout Page as a Windows TIFF:

1) Select File:Export Page.

2) Type Presentation1 in the File Name text box.

3) Select Tag Image File (*.TIF) from the Save As Type drop-down list.

4) Click Save.

The layout page is exported as a TIFF and can be inserted into any application that recognizes this file type.
Tutorial 7: Working with Excel in Origin

7.1 Introduction

Origin provides you with the ability to open Excel workbooks from within Origin, provided you have Excel 7 or later installed on your computer. This allows you to combine Excel’s spreadsheet functionality with Origin’s powerful graphing and analysis tools. This tutorial will introduce you to opening an Excel workbook in Origin and plotting the workbook data, and saving workbooks from within Origin.

7.2 Opening an Excel Workbook in Origin

Note: To perform this tutorial, you must have Excel version 7 or later installed on your computer either as a local or network copy. In addition, this tutorial assumes the default settings are selected on the Excel tab of the Options dialog box (Tools:Options).

To Open a Previously Created Excel Workbook:

1) Click New Project on the Standard toolbar.

2) Click Open Excel on the Standard toolbar.

3) In the Origin 6.0 TUTORIAL folder, select TUTORIAL_7.XLS from the list of files.
4) Click Open.

5) Select the Open As Excel Workbook radio button in the Open Excel dialog box, then click OK.

The workbook opens in the Origin workspace. In addition, a combination of Origin and Excel menus and toolbars are now displayed in the workspace.

Figure 7.1: Opening an Excel Workbook in Origin

7.3 Plotting an Excel Workbook in Origin

There are a number of ways to plot Excel workbook data in Origin. These include, but are not limited to, using the Select Data for Plotting dialog box, dragging data to a graph window and using Origin’s default plot assignments.

Creating a Graph Using the Select Data for Plotting Dialog Box

The Select Data for Plotting dialog box lets you select data and then assign plotting designations.
To Create a Graph Using the Select Data for Plotting Dialog Box:

1) Click Column \(\text{Column A}\) on the 2D Graphs toolbar. This opens the Select Data for Plotting dialog box.

2) Reposition the dialog box so that you can see the column headings in the Excel workbook.

3) Click the column A heading in the workbook, then click \(\text{x} \) in the Select Data for Plotting dialog box.

4) Click the column C heading, then CTRL+click the column F heading and then click \(\text{Y} \) in the Select Data for Plotting dialog box.

Figure 7.2: The Select Data for Plotting Dialog Box

The box below the buttons shows the data ranges representing the data types. X:A1:A65536 means that the X data is being represented by column A rows 1 to 65536. The last row number of the column is shown because you selected the whole column.

5) Click Plot in the Select Data for Plotting dialog box, then click Close.

6) Reposition the legend so that the entire legend is on the graph page.
7.3 Plotting an Excel Workbook in Origin

Creating a Data Plot by Dragging Data Into a Graph

When you drag Excel workbook data into a graph, Origin makes assumptions about the plotting designations of the selected data.

- If one column (or a range from one column) is highlighted, then this column supplies the Y values for the data plot. The data is plotted versus row number.
- If more than one column (or a range from more than one column) is highlighted, the leftmost column supplies the X values. All other columns supply the Y values. The data is plotted versus the X values.
- If more than one column (or range from more than one column) is highlighted and the CTRL key is depressed while dragging the data, then all the columns supply the Y values. The data is plotted versus row number.

To Create a Graph Using the Drag-and-Drop Method:

1) Click New Graph on the Standard toolbar. Move the Graph window to the lower-right corner of the workspace, so that when the workbook is active it won’t completely overlap the graph window.
2) Click on the title bar of the workbook to make it the active window.

3) Select the first two columns in the workbook by dragging from the column A heading to the column B heading.

4) Click on the right edge of the selected workbook data, then drag the data to the Graph2 window. When you release the mouse button, column B is plotted against column A as a line plot in the graph window.

5) Click on the graph window to make it the active window.

Figure 7.4: Dragging Data into a Graph Window

Creating a Graph Using Origin’s Default Plot Assignments

For a complete discussion on this feature, see Chapter 4 in the Origin User’s Manual.

This plotting method allows you to select your workbook data and graph type, and then Origin creates the data plots by making assumptions about the plotting assignments of the selected data. This plotting method is not available by default. It must be activated from the Options dialog box.
To Create a Graph Using the Default Plot Assignments:

1) Select **Tools:Options** to open the Options dialog box. (If the workbook is active, then select **Window:Origin Options**.)

2) On the Excel tab, select the Default Plot Assignments check box.

3) Click OK, then click No in the dialog box that opens.

4) Make the Excel workbook active.

5) Click on the column A heading, then CTRL+click on the column D and G headings.

6) Click Area on the 2D Graphs toolbar.

7) Reposition the legend so that the entire legend is on the graph page.

Figure 7.5: Plotting Excel Data Using the Default Plot Assignments
7.4 Saving an Excel Workbook in Origin

There are two ways to save Excel workbooks in Origin projects. You can save the workbook internal or external to the Origin project. When you save a workbook internal to the project, it is saved as part of the Origin project and can only be opened by opening the project. When you save a workbook external to the project, a link to the workbook is saved within the Origin project and the workbook can be opened and edited with Excel.

By default, pre-existing workbooks that are opened in an Origin project are saved external to the project, whereas workbooks that are created from within Origin are saved internal to the project. However, the save option can be changed in the Workbook Properties dialog box.

To Save the Workbook Internal to the Origin Project:

1) Make the Excel workbook active.

2) Right-click on the title bar of the workbook.

3) Select Properties from the shortcut menu that opens.

4) Select the Internal radio button in the Save As group of the Workbook Properties dialog box.

Figure 7.6: The Workbook Properties Dialog Box
4) Click OK.

5) Select **File: Save Project As**.

6) Type **Excel_Tutorial** in the File Name text box.

7) Click Save.

The project is saved and the workbook is saved internal to the project. Any changes that you now make to the Excel workbook located in the TUTORIAL folder will not be reflected in the project file the next time it is opened.
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