Sortware Review

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SOFTWARE REVIEW

Origin, Version 4 (with 3D, Contour, and Peak Fitting Modules), Microcal Software, Inc., One Roundhouse Plaza, Northampton, MA 01060, USA, $545.

Origin is a software package intended for data analysis and curve plotting. It is aimed at the technical and scientific part of the market. Origin makes it very easy to manipulate columns of numbers (data) and to display these numbers in a useful, graphical manner. Charts are created very easily with Origin. Basic features, such as multiple graphs on a single chart, axis breaks, error bars, log-log and semi-log plots are available, and they work quite well. Applying linear, polynomial and sigmoidal fits is straightforward and the output includes a table with statistical data concerning the goodness of the fit.

The user can plot confidence limits as well as prediction limits of the fitted line. It is a simple manner to add user-defined functions to a data graph. Over and above the standard features, Origin includes analysis tools that make data manipulation easy to perform. For example, data plots can be smoothed (using one of three filters, including FFT). Spectra, chromatograms or any other instrumental output can be imported into Origin, plotted and fitted to several peak shape models; peaks can be located and their areas determined.

Graphs are handled as a collection of objects. The properties of these objects are easily accessible by double-clicking on the objects, so the user can customize the charts according to his specific needs. A chart can include more than one data set, i.e., more than one curve. However, all the plots on a single chart relate to the same axes values. To have two independent graphs on the same chart, the user needs to use the layering system of Origin. Using different layers for different data sets (different columns of data on the same work sheet), the user can control each graph in an independent manner, including plotting in different axes ranges. The graphs can be printed either on a full page or on a part of the page. The user has control on the exact size of the printed plot.

Provided that you have the *3D & Contour* module, both 2D and 3D plots can be obtained. This reviewer found the data entering stage for 3D plots a bit cumbersome. A 3D plot has a large set of tools associated with it; e.g., tilting,

rotation, prospective changes, etc.   As with the 2D plots, all the properties of the objects comprising the chart can be adjusted by the user.   However, this reviewer did find that, after some rotation steps, pressing the RESET ROTATION button in the 3D toolbar does restore the figure to its original position, but one of the axis labels and the tick marks are completely misplaced. The labels can be restored to their rightful place only by manually doing one or two rotation steps.

My only major criticism is the very poor UNDO feature associated with the graphs. Most of the changes which the user can make, such as changing the axis scale and adding a line to connect data points, are not UNDOable. To restore to the original situation the changes have to be corrected manually. The lack of a complete UNDO feature is really unacceptable with present generation software.

The data to be plotted is entered in a spreadsheet-like table called a worksheet. The factory installed default table has two columns. However, the user can increase the number of columns, either temporarily for a given session, or on a permanent basis. The latter is accomplished by saving a worksheet template after adding as many columns as desired.   The columns have properties, such as width, label, and data type that are user-definable. Data types are numerical, time, date, month, and day of week.   The format of numerical entries is, of course adjustable. Column and row statistics are available.

Very rudimentary matrix operations are also available. There is a single level UNDO feature which is accessible only through the Menu bar and not via the Tool bar.   While the user can carry out mathematical manipulation on columns of data. or on ranges of data in a column, there is no back history listing of the changes made.   Since the results of the manipulation are overwritten on the previous data, it is easy to lose track on the action taken after several cycles of manipulation. In such a case, it is difficult to reconstruct the original data.   It is, therefore, a good idea to copy the original data to a new column before beginning to carry out the manipulations.

Scrolling the data with the help of the scroll bar allows you to move continuously through the rows of data in the table. However, scrolling with the cursor down a column in the table is not continuous, but rather proceeds with a complete change of a group of rows or even a complete screen. I found this scroll mode to be annoying, since I did not have a continuous view of my data.

For users who want analyze peaks obtained experimentally, the *Peak Fitting module (PFM)* is well worth having. It allows the user to fit his data to quite a few peak models and to obtain several important characterizing properties such moments, and moments-related quantities (i.e., variance, skew, and excess). Goodness of fit parameters are also available. A report which can be obtained after the fit gives the type of peak which was used in the fit routine, the center of gravity of the peak, its area and width, as well as the width at half the height. The only major shortcoming which I found with the PFM is its inability to handle, in a straight and forward manner, negative peaks.

In summary, Origin is a solid technical and scientific graphics software package. It is flexible enough to handle almost any charting and graphing tasks. If you have been relaying on your spreadsheet for plotting your data, Origin will give you many more degrees of freedom in manipulating your graphs.

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