CurveExpert 1.2

CurveExpert 1.2 is a comprehensive curve fitting system for Windows.   It employs a large number of regression models (both linear and nonlinear) as well as various interpolation schemes to represent your data in the most precise and convenient way.   In addition, the user may define any customized model desired for use in a regression analysis.

If you intend to keep this program, please register it so that I can continue development and support of this program.   Registration is quick, easy, and inexpensive -- the fee is only $35.00 for the 16-bit (Windows 3.1) version, and $40.00 for the 32-bit (Windows 95/Windows NT) version.   See Available Versions for more information on the platforms supported by CurveExpert.   High school or college students can subtract $15.00 off of the above prices for a student discount; simply include a copy of your university or high school ID.   Send your registration today!   You may also read over the benefits of registering section for extra information on registering.

If you have already registered, I extend a warm welcome and thank-you.

If you have any suggestions, or there is any regression model that you would like to see added to the repertoire, please send me mail or e-mail right away.   I will gladly to listen to your comments.

Help Topics for CurveExpert 1.2:

Features
Procedures
Data Modeling with CurveExpert
Graphing with CurveExpert
Working with Data
Using CurveFinder
Performance Issues
Frequently Asked Questions (FAQ)
Bugs and Feedback
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Registration Form

Features

- Over 35 built-in regression <u>models</u> to choose from, along with over 15 additional models provided as user-defined models
- <u>User-defined models</u> allow you to input, design, and manage your own regression functions with up to 19 parameters
- Toolbox of fitting techniques includes linear/nonlinear regression and many types of interpolation/spline fitting.
- Uses the Levenberg-Marquardt algorithm for quick and robust nonlinear regression performance.
- Unlimited number of data points.
- As curve fits are applied, a ranking chart keeps track of the best to the worst models
- <u>CurveFinder</u> examines every possible regression model for your data set and returns the best one
- Full-featured <u>graphing capability</u> with customizable, dynamic graphs gives immediate feedback on curve fit quality
- User has the ability to terminate a computation at any time
- Customizable plots can be copied directly to the clipboard for use in another Windows application
- Easy to use point-and-click interface
- Reads simple ASCII data files and can ignore comments or text in the file
- Data set can be scaled, translated, sorted, the outliers removed,   or edited by hand similarly to a spreadsheet
- Analysis tools allow the location of exact points on the curve fit as well as differentiation and integration of any model.
- Full featured <u>toolbar</u> and <u>status bar</u> increase your productivity

Procedures

The CurveExpert main window is divided into five main parts: the data window, ranking chart, the toolbar, menu bar, and the status bar.   A sample CurveExpert window is shown below:

CurveExpert 1.2 -- UNREGISTERED COPY   NUM   Beanroot.dat

Menu Bar

Like all Windows applications, you can select items off of the menu bar to accomplish certain tasks. To find out what each menu item does, click here.

Tool Bar

The toolbar gives access to frequently used commands.   Watch the status bar (at the bottom of the main window) as you move the mouse across each button to find the function of each one of these buttons.

Status Bar

The status bar shows you the current status of CurveExpert and gives you help on the function of the toolbar buttons.

Data Window

This window is the spreadsheet-like interface that occupies the left side of the CurveExpert main window.   The data window holds all of the data that is to be modelled.   The first column of data is the x data, while the second column holds the y data.   As of this version of CurveExpert, the third column is not used.   To edit a data point, simply click the cell that it is in and type in the new value.

Ranking Chart

The ranking chart ranks all of the valid regression models from best to worst.   The standard error and correlation coefficient (described in detail in the Data Modeling section)   are used to determine these rankings.   Note that each curvefit in the chart "lights up" as you move the mouse over it -- clicking on any one of the models listed in this chart will open a graphing window of that model. Note that interpolations are *not* included on this list.

Menu Commands

Below, you will find all of the menu choices in CurveExpert 1.2.   Choose any of them to obtain a description of what they do.

File

   New
   Open
   Save
   Save As
   Export
   Preferences
   AutoGuess Enabled
   Print
   Print Setup
   Exit

Edit

   Undo
   Cut
   Copy
   Paste
   Clear
   Select All
   Cut Last Row

Data

   Plot
   Manipulate
   Reexamine
   Clear CurveFits
   Information
   Calculate Groups
   CurveFinder

Interpolate

   Lagrangian Interpolation
   Linear Spline
   Quadratic Spline
   Cubic Spline
   Tension Spline

Apply Fit

   Linear Regression Fits
   Nonlinear Regression Fits
   User Model

Window

   Tile
   Cascade
   Refresh All
   Restore All
   Minimize All

[Close All](#)

Extras

[History File](#)
[Edit Current File](#)

Help

[Help](#)
[How to Use Help](#)
[About](#)

Setting your Preferences

The **Preferences** dialog allows you to set important parameters that CurveExpert will use during operation.   Two separate sets of user preferences are maintained for the single and double precision versions (registered users only).   The user preferences are divided into three main categories:

> Application
> Regression
> Printing

Preferences Property Control Buttons

OK: Press OK to apply all of your changes to the current CurveExpert preferences and quit the dialog.

Cancel: Press Cancel to discard any changes that you have made to the preferences and quit the dialog.

Help: Press Help to get help on the currently selected tab of the Preferences dialog.

Comments

If an invalid entry has been entered in any of the tabbed pages, then the offending entry will be selected, and the computer's speaker will sound.

Application Preferences

The application preferences tabbed page sets user preferences that control the overall behavior of CurveExpert in the Windows environment.

Data Files

Data File Location: The directory in which you store your data files can be input in this edit field. For convenience, each time CurveExpert is started, the directory will be automatically changed to this working directory.   By default, this directory is set to be the CurveExpert home directory.

Default Data File Extension: If a file extension is not supplied in the File|Open or File|Save dialog box, then this extension is automatically added.   Default: DAT

Automatic Data Sorting: Selecting this checkbox will automatically sort any data file as it is read into CurveExpert.   Default: Off

Graph Rendering

The graph rendering radio buttons may be set to Slow, Medium, or Fast.   Each setting has advantages and disadvantages.

The "Slow" setting requires no extra memory, but all graphs are drawn from scratch when their window is resized or uncovered.

The "Medium" setting requires a small amount of extra memory and behaves like the "Slow" setting, with the exception that any user-model graphs will be drawn using "Fast" rendering.   See below; this is the default.

The "Fast" setting requires a large amount of extra memory, because the contents of every graph window are cached for quick redraws.   The graph is only drawn the first time it is opened, and each

time it is resized.   Any other graph viewing will take a minimal amount of time to redraw, since the image is stored in memory.   This option is most useful for users who have extremely large data sets that take a long time to draw.

<u>Switches</u>

Enable Background Processing: When CurveExpert is iterating, it can take complete control over Windows (faster), or do its processing in the background (slower).   Checking this checkbox will force CurveExpert to do its calculations in the background.   This is recommended, since certain windows processes need attention often.   On the other hand, if CurveExpert is the only application running, then the best performance will be obtained by leaving this box unchecked.   Default: Enabled

No graphs, only information: CurveExpert gives you the option of viewing the graph first, or the fit information first.   If this checkbox is selected, the model information (coefficients, etc.) will be shown directly, instead of a graph.   Default: Disabled

3D Dialog Effects: Attractive (in the opinion of the author) gray dialogs with 3D effects are the default in CurveExpert.   If you prefer the white dialogs with no 3D effects, deselect this checkbox. Default: Enabled.

Save Main Window Position: CurveExpert saves the position of the main window when the application is exited, so that when it is opened again, it assumes the same position.   If this behavior is undesirable, deselect this checkbox.   Default: Enabled.

Regression Preferences

The regression preferences tabbed page sets user preferences that control the regression and mathematical operation of CurveExpert.

Linear Regression Defaults

Maximum Polynomial Degree: Enter the maximum degree of a polynomial allowed by CurveExpert in this field.   This setting determines the number of polynomials examined by <u>CurveFinder</u> in a search sweep, and it also prevents choosing a wildly oscillating polynomial by accident.   This number may not exceed 19.   Default: 10

Default Polynomial Degree: Enter the default degree of polynomials used in CurveExpert in this field.   The default polynomial degree is the polynomial that will be calculated by the <u>Calculate Groups</u> command, and the degree that will appear by default when you select a polynomial from the Apply Fit menu.   Default: 4

Nonlinear Regression Parameters

Regression Tolerance: Enter the desired tolerance for nonlinear regression convergence in this field.   The nonlinear algorithm uses this number to determine whether or not it has converged on the correct model parameters.   Mathematically speaking, the difference between the standard errors in two consecutive iterations must be smaller than this tolerance for the computation to terminate.   The smaller the tolerance, the more accurate the parameters will be, but the algorithm will take much more time to converge.   Default: 1e-6

Diverging Iterations: Enter the number of iterations that the standard error (mentioned above) must increase for the algorithm to declare divergence.   Default: 10

Maximum Iterations: Enter the maximum number of iterations for the nonlinear algorithm to perform before it is forced to terminate.   Default: 100

Regression Options

Weighting: CurveExpert can either perform no weighting for each point, or weight each point by $1/y^2$ as the nonlinear regression progresses.   Using no weighting is most appropriate when no known relationship exists between the variances of the data around the fitted curve and the y values of the points.   However, it is often the case in experiments that it is known that the uncertainty is a certain percentage of the y value; in this case, weighting the points by $1/y^2$ can prevent the larger scatter at higher y from adversely affecting the regression model.   Default: No Weighting

Automatic Initial Guesses: Enabling this checkbox will let CurveExpert generate initial guesses for built-in nonlinear regressions for you.   This option, in effect, enables AutoGuess upon startup. Default: Enabled

Quick Derivatives: The partial derivatives of the model with respect with each of its parameters is required in the Levenberg-Marquardt algorithm for nonlinear regression.   CurveExpert uses central differencing to approximate these partial derivatives; however, more precise approximations can be accomplished using Richardson's extrapolation.   Checking the "Quick Derivatives" checkbox uses simple central differencing; leaving this checkbox unselected forces CurveExpert to use Richarson's extrapolation for the numerical derivatives.   The latter is more accurate, but much slower than using central differences.   Default: Enabled

Printing Preferences

The printing preferences tabbed page sets user preferences that control printing settings and margins that CurveExpert will use for graph hardcopies and data tables.

Current Printer Info

This section shows all information for the currently selected printer.   The name, driver version, orientation, paper size, and resolution are shown.

Default Print Type

The default print type determines whether the "Black and White" or "Color" printing selection will be automatically selected when a graph is printed.   Of course, the user may change the selection at print-time.   This option is included for the convenience of color printer users.   Default: Black and White.

Print Margins

The top, left, bottom, and right margins (in inches) can be set in each of these edit fields.   Note that no margin can be less than 0 inches, and no corresponding margins can add to higher than the paper extent plus the unprintable margin.

Print Setup

Press the Print Setup button to change the current printer and/or the printer configuration.

File|Save

Choose this menu item to save any changes that you have made to the data set.

File|New

Choose the New menu item to clear all curvefits, clear all data, and restart from scratch

Status Bar

The statusbar shows a QuickHelp line on any currently selected menu item.   A key item to look for (when scanning over data models) is the equation form that will appear in the status bar.   While in normal operation, the status bar shows, in order from left to right:

- QuickHelp line, caps lock status, num lock status, filename

While a calculation is progressing (see <u>While CurveExpert is Working</u>), the status bar shows:

- Model being processed, calculation flag, iteration count, current value of chi square.

Toolbar

The toolbar gives quick access to the most frequently used menu commands.   A picture of the toolbar is shown below:

The buttons are (from left to right):

File|New
File|Open
File|Save
File|Print
Edit|Cut
Edit|Copy
Edit|Paste
Apply Fit|Linear
Apply Fit|Quadratic
Apply Fit|Polynomial
Apply Fit|User Model
Data|CurveFinder
File|Enable Autoguess
Help|Help

While a calculation is progressing, the normal toolbar buttons are disabled, and the toolbar shows two extra buttons that you can use to abort calculations.   See While CurveExpert is Working for details.

Data Window

The data window shows all of the data either entered or read in from a file.   To edit an entry, simply click on it and enter the new number.

File|Save As

Choose this menu item to save the current data set into a file that you specify.   Note that all data files saved by CurveExpert will be stored in a tab delimited format.

Manual Editing

At any time, you can click on the numbers in the data window and edit them, just as you can in a spreadsheet.

File|Exit
Exit CurveExpert 1.1 by choosing this menu choice, double clicking in the system box in the upper left corner, or by pressing Alt-F4.

Help|About

Choosing to view the About box will give you version information, owner information, memory usage, and whether or not a math coprocessor is detected.

Data|Calculate Groups

Calculate groups of curve fits (that you specify), and open a graphing window for each one of them.

Graphing Menu|Find Main Window

If the main CurveExpert window becomes obscured by graphing windows, use this menu item to pop it to the top.

Edit|Cut

Remove the selection in the data window and put it in the clipboard

Edit|Copy

Copy the selection in the data window to the clipboard

Edit|Paste

Paste the contents of the clipboard at the caret

Edit|Undo
Undo the last edit in the data window

Edit|Cut Last Row

Remove the last (x,y) pair from the data set

Edit|Clear

Remove the selection in the data window

Data|Plot Data

Plot only the current data in a new graphing window.   See <u>Graphing in CurveExpert</u> for more details.

File|Print

Choose "Print" from the main menu to generate a hardcopy of the data set.   The data set will be printed in two columns of x and y data, and each point is labeled sequentially.

If the printer is not set as desired, press the Setup button and configure the printer.   Pressing OK will commence printing, and pressing the Cancel button will return you to the CurveExpert main window.

File|Print Setup

Choose "Print Setup" to manipulate your printer settings before you do any printing.   The changes made in this dialog will affect both printouts of data and hardcopies of plots.

Data|Reexamine

Choosing this menu item will recalculate the mean, standard deviation, etc. of your data set.   Also, some curve fits cannot be performed if your data set has zeros or negatives -- the appropriate curve fits will be deactivated if CurveExpert detects the presence of zeros and/or negative numbers in your x/y data.

Window|Tile

Places all graphing windows "tiled" on the desktop surface.   For a large number of graphing windows, this may produce undesirable visual effects.   However, this allows an easy comparison of curve fits for a small number of graphing windows.

Window|Cascade

Places all graphing windows "cascaded" on the desktop surface.   This way, you can find the graphing window that you want quickly and easily.

Window|Close All

Closes all open graphing windows.

Window|Refresh All

In the case that a plot is not updated properly, choose this menu item to redraw all graphing windows.

Window|Minimize All

Minimize all open graphing windows to the bottom of the desktop.

Window|Restore All

Restore all minimized graphing windows to their previous location on the desktop.

Help|Help

Choosing "Help" from the Help menu activates this online documentation, which allows you to learn how to use CurveExpert.

Graphing Menu|Close

Close the current graphing window.

Graphing Menu|Help

Open the CurveExpert online documentation on how to use graphing windows.

File|AutoGuess Enabled

If this menu item is checked, then CurveExpert will automatically calculate initial guesses for the nonlinear regression algorithm, for built-in regression models.   If left unchecked, you must specify initial guesses for built-in models.   Note that AutoGuess does not affect user-defined models -- you must always provide initial guesses for these.

Recommended: Enabled

Data|Clear Curvefits

CurveExpert caches the results of past curve fits that you have performed, so that if you choose the same one again, the fit does not have to be recalculated. To clear the cache so that everything is calculated anew, select this menu item. Note that the cache is cleared automatically every time the data is edited, so the only time this item might be useful is if a regression happened to converge to a local minimum, and you would like to clear that result and use new initial guesses.

Extras|View History

Viewing the history file will show you the iteration history of the last regression model that was performed. The first column is the iteration number, the next columns are the values of the parameters (a, b, c...), and the last column is the value of the standard error of the estimate at that iteration. Note that at iteration 0, the parameters are equal to the inital guesses. You can view this file to gain insight into the workings of the nonlinear regression algorithm.

Extras|Edit Current File

You may use the notepad to edit the current data file or view it as necessary.   Note that changes that you make there will NOT be reflected in the data set.   To affect the changes, the data file must be reread by using File|Open.

Edit|Select All

Choose this menu item to select all of the text in the current spreadsheet cell.

Help|How to Use Help
Choose this menu item to obtain directions from Windows on how to use the help system.

Graphing in CurveExpert

CurveExpert has extensive graphing capability.   This capability gives you immediate feedback on the performance of a particular data model.

Graphing Window Overview

CurveExpert allows you to open many graphing windows at one time so that you may compare different curve fits.   Note that changes that you might make to a particular graphing window will affect only that window.   See the Graph Properties dialog to see how to apply your changes to all plots, as well as saving your customizations for future use.

Each graph has a consistent user interface.   Press the right mouse button to obtain the graphing menu, which gives you access to all of the functions available for plots, such as customizing the plot, obtaining model information, analyzing the model, or printing the plot.   Zooming and panning are controlled by dragging a rectangle across the graph pane and/or pressing the arrow keys.   Any plot can be autoscaled by pressing Shift+A.

The most vital piece of information that you might want to access are the values of the model parameters.   Press the <u>Info</u> button, select "Information" from the graphing menu (by clicking the right mouse button), or press Ctrl-I to access this (as well as other) information.   Note that if the graph title is displayed, the Info button is not available; choose "Information" from the graphing menu or press Ctrl-I to access the curve fit information.

Graphs can be customized by selecting "<u>Graph Properties</u>" from the graphing menu.

It is possible that CurveExpert will not be able to properly draw your graph.   For example, the y-extents might be negative on a graph that is being drawn with log axes.   Or, the extents might be set such that a singularity in the model exists somewhere in the domain.   CurveExpert will notify you of these occurrences with a error message printed on the graphing surface.   In these cases, reset the graphing extents using the <u>XY Axis Properties</u> section of the Graph Properties dialog (accessed via the popup menu described below).

Graphing Controls

Zoom: You may zoom in on a region on the graph by holding down the left mouse button, dragging over the area of interest from top left to bottom right, and then releasing the button.   Likewise, zoom out by holding down the left mouse button, dragging from bottom right to top left, and then releasing the button.   Zooming out will cause the entire graphing area to be enclosed in the rectangle that was made by dragging "backwards."

Note: Zooming is not available on log or semilog plots.   Also note that any zoom that starts or ends outside of the graphing pane will be ignored.

Pan: To pan the graph in any direction, press the arrow keys.   This will pan the graph in the direction that you choose by a magnitude of the major tick length.   Holding SHIFT while pressing the arrow keys gives you finer control by only panning one minor tick length.   Note: panning in the direction of a log scaled axis is not supported.

AutoScale: Press SHIFT-A to autoscale the graph.   Autoscaling guarantees that every data point on the plot will be shown, which is the default for a newly opened graphing window.

Graphing Menu

By pressing the right mouse button or by pressing Ctrl-M in any graphing window, you can pick from the graphing menu (keyboard equivaluents are listed also):

[Ctrl-W]	<u>Find Main Window</u>
[Ctrl-G]	<u>Graph Properties</u>
[Ctrl-I]	<u>Information</u>
[Ctrl-T]	<u>Generate Table</u>
[Ctrl-L]	<u>Analyze</u>

[Ctrl-C]	<u>Copy</u>
[Ctrl-P]	<u>Print</u>
[Ctrl-X]	<u>Close/Exit</u>
F1	<u>Help</u>

Graph Properties

The Graph Properties dialog allows you to modify all of the scaling and characteristics of the current graph   This dialog is divided into four major sections:

- X Axis
- Y Axis
- Point/Line
- Overall

Graph Property Control Buttons

OK: Press OK to apply all of your changes to the current CurveExpert graph and quit the dialog.

Apply: Press Apply to "try out" your graph property changes.   The graph will be updated immediately, but you may still press Cancel to discard your changes.

Apply to All: Press Apply to All to immediately apply all of the current graph properties to the current plot and all open plots.   All attributes as well as the scaling for the current plot are copied to all other plots; hence, all graphs will have exactly the same view, colors, line thicknesses, etc.   *This action CANNOT be undone by pressing the "Cancel" button*.

Save as Default: If you would like to save your graph attribute and scaling setup permanently, click this button.   This information will then be used on every plot that is drawn by CurveExpert.

Cancel: Press Cancel to discard any changes that you have made to the graph properties and quit the dialog.

Help: Press Help to get help on the currently selected tab of the Graph Properties dialog.

Autoscale: Press this button to have CurveExpert automatically set the graph axes and tick mark increments.   This is the default view for a newly opened graphing window, and ensures that all data points will be shown on the graphing window.   This button is only available on the X and Y axis tabs.

Comments

If an invalid entry has been entered in any of the tabbed pages (for example, entering 0 for the Resolution parameter on the Overall page), then the offending entry will be selected, and the computer's speaker will sound.

X axis and Y Axis Properties

The X axis and Y axis property sheets modify all graph properties that are associated with the x/y axes, such as the scaling, tick marks, and axis labels.

Scaling

Axis scaling is determined by the settings in the **High** and **Low** edit fields.   As the names imply, the graph will be displayed over the range set by the Low value and the High value.   Major tick marks will be placed at increments specified in the **Increment** edit field.   Also, if the corresponding **Show Grid Lines** box is checked, grid lines will be displayed at each major tick.   The number of minor ticks displayed between the major ticks is specified in the **No. of Minors** field.

Scale Type

The Scale Type section allows you to specify whether the axis should be scaled on a normal (linear) scale or a logarithmic scale.   To use normal (linear) axes, select the Normal radio button.   Likewise,

to use logarithmic axes, select the Log radio button.

Using logarithmic scales has limitations -- a plot showing zero or negative numbers on the axis in question cannot be scaled logarithmically.   Of course, you can always reset the **High** and **Low** values to positive values to be able to scale the axis logarithmically.   Note that the **High**, **Low**, and **Increment** fields are not represented exactly when using logarithmic scaling -- the closest multiple of ten is chosen for the High and Low entered, and multiples of the next lower major tick are used for the minor increments.

Tick Labels

The tick labels for both axes can be customized by using the Tick Labels section of the Graph Properties dialog.   The following options are available:

Fixed Point: Select this radio button if you would like the numbers at every major tick to have fixed point format.   The number of decimal places displayed is set in the "Precision" edit box below this radio button.

Scientific: Select this radio button if you would like the numbers at every major tick to have a scientific/engineering format.   The number of decimal places displayed is set in the "Precision" edit box below this radio button.

Precision: The number in this field indicates the number of decimal places that will be displayed on the tick labels along the axes.

Rotation: The tick labels can be rotated from 0 to 360 degrees.   Enter the desired number of degrees to rotate these labels in the Rotation field.

Font: The font used for the tick labels can be modified by clicking this button.   Any Truetype font and any color can be chosen; refer to the Changing Graph Fonts section for details.

Miscellaneous

Axis properties that do not fall under one of the above categories are documented below.

Label: Type in the axis label that is desired for the axis in question.

Font: The font used for the axis label can be modified by clicking this button.   Any Truetype font and any color can be chosen; refer to the Changing Graph Fonts section for details.

Show Label: Select this checkbox if the axis label should be displayed.   If this box is not checked, then the axis label will not be drawn.

Show Grid Lines: Select this checkbox if grid lines (associated with the axis in question) should be shown at every major tick mark. If this box is not checked, then the grid lines will not be drawn.

Grid Lines at Minors: Normally, grid lines are drawn only at the major ticks.   Checking this button will cause the grid lines to be drawn at every minor tick also.

Ticks Inside: Select this checkbox if all major and minor ticks should be drawn inside of the graph pane.   If this box is not selected, all ticks will be drawn outside of the graph pane.

Point and Line Properties

The Point/Line property sheet modifies all graph properties associated with the appearance of the data point markers and the curve representing the model prediction.

Data Point Properties

Show points: This checkbox will determine whether data points are drawn on the plot or not.

For residual plots, this choice will read 'Show Residuals as Points.'   When this checkbox is selected, all residuals will appear as points on the graph.   When left unselected, the residuals will be drawn as bars.   Note that the properties of the residual points and/or bars can be controlled by the following properties, just as normal data points can.

Fill points: This   checkbox determines whether the points will be drawn as a solid color or an

outline.   For example, if the 'circle' symbol is chosen and the 'Fill points' options is checked, a solid disk will be drawn at each data point.   The color used to fill the point is the same as the color used to draw the outline.

Point size: Enter the size of the symbol that will denote the data points, in pixels.   This size may not be negative.   The up/down buttons beside the edit control may also be used to change the size.

Point color: The current point color is displayed beside this button.   To change this color, press this button and choose a new color.

Symbol: Press the 'Symbol' button to obtain a list of possible markers that can be used for each data point.   The currently selected symbol will have a checkmark beside it on the symbol menu.   Currently, the supported symbols are the circle, square, triangle, inverted triangle, hourglass, plus, and cross.

Line Properties

Line Width: Enter the width, in pixels, of the curve that will be drawn as the curve fit.   This size may not be negative.   You may also use the up/down buttons beside the edit control to change the size. Note that the 'Line Width' setting is only valid for solid lines;   if any other style of line is chosen, then the width of the line will be one.

Resolution: Enter the stepsize, in pixels, that the curve will be updated.   The curve is made of of straight line segments that appear as a curve when the resolution is small enough; however, the finer the resolution (lower number) the slower the curve will be drawn.   For optimum performance, set the resolution to the highest number possible without degradation of plot quality.

Line Color: The current line color is displayed beside this button.   The line color is used to draw the curve fit line.   To change this color, press this button and select a new color.

Line Style: Press this button to display a menu with the available line types.   Note that the 'Line Width' setting is only valid for solid lines;   if any other style of line is chosen, then the width of the line will be one.

Sample

This area of the Point/Line property dialog shows a sample of the currently selected point and line combination.   Note that the background color is the currently selected 'Fill Color' from the 'Overall' tab.   Also note that this sample is dynamically updated as you change the settings on this tabbed page.

Overall Graph Properties

The Overall property sheet modifies all properties associated with the plot as a whole, such as the title, graph pane, graph box, and graph coloring.

Show Header Instead of Title

Selecting this checkbox will display the header instead of the graph title.   The header consists of the information button (which you can press to invoke the Information Dialog), directions concerning how to invoke the graphing menu, and the value of the standard error and the correlation coefficient for the current model.   If this checkbox is left unselected, the title that is defined by the user in the 'Graph Title' field will be centered in the window/page in the title font.

Graph Title

Enter the text for the graph title in this field.   The string may be up to 255 characters long; if the title is too long for one line, then room will be made for it on the plot and it will broken up into multiple lines.   Note that the title will not be displayed unless the 'Show Header Instead of Title' checkbox (above) is left unselected.

Graph Title Font

Press this button to select a font for the title.   See also <u>Changing Graph Fonts</u> for further details concerning how to use the font selection dialog.

Graph Pane

Border Buttons: Select or deselect the pane border checkboxes to show or hide the lines around the graph pane.

Lock Frame Color: If this button is checked, then all text drawn on the graph will automatically follow the selected Frame Color (see below).   When this button is unchecked, the text colors can be individually selected through the "Font" selections in the Graph Properties dialog.   Note that the text colors selected through the font dialogs *will not be used* unless this checkbox is unselected.

Fill Color: The current fill color is displayed beside this button.   The fill color is the color that will be used to shade in the background of the graph.   To change this color, press this button and choose a new color.

Grid Color: The current grid color is displayed beside this button.   The grid color will be used to draw the dotted grid lines that are drawn at every major tick.   To change this color, press this button and choose a new color.

Frame Color: The current frame color is displayed beside this button.   The frame color is used to draw the border around the graph as well as the tick marks.   To change this color, press this button and choose a new color.

Outside Fill: The current outside fill color is displayed beside this button.   The outside fill color is the color that is painted outside of the graphing frame.   Since the axes labels and various other printed items are drawn in this area, this color should not be the same as the Frame color. Remember that if the font color for the title, axes labels, etc. are the same color as the Outside Fill color, then they will be invisible!   See the *Lock Frame Color* switch above for more information concerning this.

Graph Box

Show Graph Box: To show or hide the graph box, select or deselect this checkbox, respectively. The graph box is the box that encloses the entire graph.   This box is not very visible for on-screen plots; therefore, this option is most relevent for printed or copied plots.

Box Width: Enter the line width, in pixels, that the graph box will be drawn with. Click the corresponding up/down arrows to increase or decrease this line width.

Box Color: Click this button to select the color with which the graph box will be drawn.

Rectangular Corners: Selecting this radio button will draw the graph box as a simple rectangle.

Rounded Corners: Selecting this radio button will draw the graph box as a rectangle with rounded corners.

Changing Graph Fonts

All of the fonts that CurveExpert uses for the graph title, x and y labels, and the x and y axes can be customized.   Since this type will possibly undergo rotation and a wide range of scaling, the fonts that can be used are limited to the TrueType family.   Screen and/or raster fonts are not likely to rotate or scale properly.

To specify a font, select the font family (such as "Arial" or "Courier New") to determine what the appearance of the font will be.   The font style can be changed to give the font its normal look, an italic flavor, or the heavier bold style.   Often, the bold and italic styles can be combined.   The point size controls the size of your font.   A point, roughly 1/72 of an inch, will be used to determine the font size both on the screen and on the printer.   The Strikethrough and Underline checkboxes will draw a line through or under the text, respectively.   Finally, the color of the text can be changed simply by selecting a different color from the Color listbox.

As you choose the family, style, size, and color of the font, a sample display will be updated in the bottom right area of the font dialog.   Note that this sample will contain the current Window Fill color (used in coloring the area outside of the graphing pane) as the background, since all of the text in the plots is drawn in this area.   The sample box will also contain the text applicable to the font that you are modifying.

Note that the text colors selected through the font dialogs *will not be used* unless the **Lock Frame Color** checkbox in the <u>Graph Properties Dialog</u> is left unselected.   By default, the text colors are forced to follow the graph frame color, so the color settings in the font dialogs will have no effect.

Limitations: When running the 32-bit version under Win32s, the sample display of the font does not work.   This is a bug in Win32s (version 1.30).   The font will still be properly selected and display correctly on your plot, however.

Model Information

The Model Information dialog gives all of the information needed to apply a curve fit and some supplemental information about the performance of the given model. The most important information contained in this panel are the values of the parameters of the model. This dialog is divided into four major sections:

- Coefficients
- Covariance
- Residuals
- Comments

Information Control Buttons

OK: Press OK to close this window.

Help: Press Help to get CurveExpert help on how to interpret the items in the this dialog.

Copy: Press the copy button to copy the current information to the clipboard. See the individual sections below for the specific data that will be copied.

Coefficients

The Coefficients page gives the most vital information about the model in the current graph. The values of the coefficients are given here as well as the model equation, so that meaning of the parameters is clear.

Model

The **Model** section gives the data modeling equation so that the interpretation of the coefficients is clear. The coefficients a,b,c, etc. in the **Coefficients** section match the corresponding parameters shown in the model.

Coefficients

The **Coefficients** section gives the values of the relevant parameters for the current model -- these coefficients are always expressed as a, b, c, d, and so on. These coefficients match the model shown in the **Model** section. If the list of coefficients exceeds the extent of the window that they are shown in, a scrollbar will appear to allow you to scroll through the parameters.

Copy

If the Copy button is pressed when the coefficient tab is active, the list of coefficients is copied to the clipboard.

Covariance Matrix

The covariance matrix gives further information about the relation between the model parameters and their uncertainties. The entries along the diagonal are directly related to the uncertainty in each parameter -- for example, the entry in matrix position (2,2) corresponds to the uncertainty in the second parameter (which is b). The off-diagonal components are the covariances between parameters. For

example, the entry in matrix position (3,4) is the covariance between parameters 3 and 4 (which are c and d). The covariance matrix can be used in further statistical analysis of the regression model and its goodness-of-fit. At this time, CurveExpert offers this matrix as additional information to the user, and does not draw any conclusions based on its entries. Note also that the inverse of the covariance matrix is the curvature matrix.

Copy

If the Copy button is pushed when the covariance tab is active, the entire covariance matrix, in nxn format, is copied to the clipboard.

Residuals

The residual plot graphically depicts the difference between the data points and the model evaulated at the data points. The residual at point *i* is defined by

$$residual = y_i - f(x_i)$$

where y_i is the measured value at x_i, and $f(x_i)$ is the predicted value at x_i. These distances are shown as bars or points on the residual plot; the magnitudes of the data points are simply replaced by the residual defined above. If the residual is positive, then the data point is above the model's prediction; likewise, if the residual is negative, then the data point is below the model's prediction. The residuals can provide an indication of a particular model's performance. If there are runs of like-signed residuals, then a better model for the data is likely to exist.

Optimally, the residuals should exhibit a random scatter around zero, which indicates that the data points are randomly distributed around the curve. A "run" is a sequence of like-signed residuals, which stand out on the residual plot. A large number of runs indicates that data systematically deviates from the curve.

Open/Close Plot

Press this button to open or close a large residual plot. Opening the plot simply shows the residual plot in its own window in which you may resize, zoom, print, and alter the properties just as with any other graph. While the residual plot window is open, this button will change to read "Close Plot." Clicking this button will then close the large residual graph.

Copy

If the Copy button is pushed when the residual tab is active, a table of residuals is copied to the clipboard. This table is in a two-column format separated by a tab character. The first column is simply the x data, and the second column is the difference between the data point and the model evaluated at that point (y_i -- $f(x_i)$).

If a copy of the plot is desired, simply open a plot window of the residuals (by clicking the 'Open Plot>>' button and then select 'Copy' from the graphing menu of that plot.

Comments

The comments page is meant to give additional information on the error involved in the curve fit, and also gives other miscellaneous information that could apply to your particular model.

Errors

The **Error** section gives you information on the curve fit performance.   Two quantities are used to express the "goodness" of a particular curve fit -- the correlation coefficient and the standard error of the estimate.   In general, the correlation coefficient will range from 0 to 1, with a correlation coefficient of 1 being the best.   In some peculiar circumstances, CurveExpert will report a correlation coefficient greater than one; this is indicative of a very poor data model.   The standard error will be strictly positive, with a smaller standard error representing the better curve fit.   For more information, refer to the Data Modeling with CurveExpert section.

Comments

The **Comments** section gives you important information about the current model, such as information regarding the characteristics of interpolation, or the performance of a nonlinear regression.   For nonlinear regression, the message will inform you if the fit converged, the number of iterations required for convergence, and the tolerance imposed to determine convergence.   Note that information in this field is not available ofter a graphing window has been closed or reopened, or after a model search by CurveFinder.

Copy

If the Copy button is pushed when the comments page is active, the error information and the comments section is copied to the clipboard.

Analyze Fit

The Analyze Fit feature allows easy location of x/y points, differentiation, and integration of a curve fit that has been performed.   Since this feature may only be used from the graphing window (by choosing Analyze from the graphing menu or pressing Ctrl-L), all calculations will be based on the model from the invoking window.   The following analyses are supported by this tool:

- Find a Y Value
- Find an X Value
- Differentiation
- Integration

Analyze Fit Control Buttons

Calculate: Press calculate to compute the information on the active page.   The item calculated could be the location of an x point, location of a y point, a derivative, or an integral (depending on the active page).

Close: Press Close to indicate that you are through analyzing the current model.   The dialog box will be closed.

Help: Press Help to get CurveExpert help on how to use the Analyze Fit feature to locate discrete points, differentiate, and integrate the model function.

Find a Y Value, y=f(x)

CurveExpert can evaluate the curve fit at a given x to give you the projected y value by the current curve fit.   Just type in the point at which you want to evaluate the curve fit (the x value) in the "**At X=**" field and press Apply or <Enter> on your keyboard. The calculator will then show the corresponding y value.   If CurveExpert cannot evaluate the curve fit at the point that you specified, then the word ERR is printed in the result field.

Find an X Value x=f(y)

CurveExpert can evaluate the curve fit at the given y to give you the projected x value.   Just type in the point at which you want the corresponding x in the "**At Y=**" field and press OK or <Enter> on your keyboard. The calculator will then show the corresponding x value.   If CurveExpert cannot find the corresponding x value, then the word ERR is printed in the result field.

NOTE that the results obtained for the x value should be, at the least, visually checked with the graph. There is a chance the the root (x-value) returned matches a y value on the graph at a location other than what was intended.   This occurs simply because functions may have multiple roots, and CurveExpert may locate any one of them (since all of them are just as valid as the other) without assistance from the user.   Consider a simple quadratic y=x^2:   if you want the x value corresponding to y=4, there are two valid answers to this question (2 and -2).   So, although this search facility in CurveExpert is very powerful, it should be used with care.   The optional **Initial Guess for X** field should be used wisely so that the correct root is located.

Most of the time, the initial guess field is not needed; however, as mentioned above, the desired x-value may not be returned.   In this case, you must set the **Initial Guess for X** to a value reasonably close to the root (x-value) that you are trying to find.   This greatly assists CurveExpert in finding the correct root. Note that the number shown in this field when the Analyze Tool is invoked is the initial guess generated by CurveExpert, which will subsequently be used in the computation of the x-value.

Differentiating at a point

Simply fill in the point at which you want to take a derivative into the "At X=" edit field.   Then press the "Calculate" button, and the result will be displayed beside the "dY/dX=" entry.   The default value at which the derivative will be computed is the current midpoint of the graphing window.   If a derivative calculation fails, the word ERR will appear in place of the result.

The derivatives are taken using a central difference combined with Richardson extrapolation to refine the derivative.   This refinement is terminated when successive refinements yield less than 0.01% difference in the derivative.

Integrating over an interval

To integrate a function on the interval [a,b], Fill in the value of **a** in the "From X=" field, and the value of **b** in the "to X=" field.   Then press the "Calculate" button, and the result will be displayed beside the "I(ydx)=" entry.   The default interval over which the integral will be taken is the current extent of the invoking graphing window.   If an integral calculation fails, the word ERR will appear in place of the integral result.

The integral of the model function is taken using Simpson's 1/3 rule coupled with the Romberg integration method.   The interval is divided into successively finer subintervals which are integrated with Simpson's rule and summed, and these results are refined with the Romberg method.   Refinement is terminated when when successive iterations yield less than 0.01% difference in the integral or when the interval has been divided into over 32767 subsegments.   If the integral did not converge before the maximum number of segments is exceeded, a note will appear informing you of this occurance.   Use the result of an unconverged integral with due caution.

Graphing Menu|Copy Plot

Selecting this menu item copies the current plot to the clipboard so that you can paste it into another application.   Best results when copying are obtained by resizing the graphing window to the actual size that you want to paste into the other application, and then selecting "Copy Plot."

Limitations:

None.   In previous versions of CurveExpert (1.21 and older), due to an limitation in the Windows interface, a copied plot will not be able to accept a two-line plot title.   The version of the plot that is copied to the clipboard will have the entire title, but it will all be printed on one line.   This limitation has been removed as of CurveExpert 1.22.

Graphing Menu|Print

Selecting this menu item prints a hardcopy of the the current plot.   A print dialog will be shown that will allow you to select printers and change the print setup. If the printer is not set as desired, press the Setup button and configure the printer.   Pressing OK will commence printing, and pressing the Cancel button will return you to the CurveExpert graph window.

Note that you may select whether the printout will be in color or black and white by selecting the **Black and White** and **Color** radio buttons at the bottom of the dialog.   If you have a black and white printer and select a color plot, then the plot will be grayscaled before it is sent to the printer.

Creating a Table

The CurveExpert table generation mechanism generates a data table based on the current data model. This table will contain the calculated model values(y) corresponding to the range of x data points that you specify.   To create a table, CurveExpert must know the following information:

1) **The starting x value**
2) **The ending x value**
3) **The resolution (increment,step size) of the table**

Simply fill this information into the provided spaces on this dialog box, enter a filename, and press the 'OK' button.   By default, the tables generated by CurveExpert have the extension '.TAB.' The generated table will simply be two columns of data: the first column is the x data, and the second column is the calculated y data from the model that you specified.

Table Control Buttons

OK: Press OK after you have entered all of the necessary information and you are ready to save your table.

Cancel: Press Cancel to abort this operation and not create a table.

Delimiter: Press this button to specify the type of delimiter, or separator, to use in the table.   You may choose a space, tab, or comma to separate the x and y columns.   The default delimiter is a tab.

Help: Press Help to learn on how to generate a table from a given data model.

Table X Range

This region of the dialog box is where you can specify the starting and ending x value and the resolution of the table, as discussed above.

Minimum: Enter the starting x value of the table in this edit field.

Maximum: Enter the ending x value of the table in this edit field.

Increment: Enter the interval in x that you want the data model to be calculated.   Note that this number must be the same sign as (maximum-minimum).   By specifying a negative Increment and a minimum greater than the maximum, it is possible to generate reverse-order tables.

Example

For example, suppose that you wanted to generate a table file named "mydata.tab" for a range of

$$x=0.0, 0.5, 1.0, 1.5...10.0$$

with comma separators between columns.   You would specify **0.0** in the 'Minimum' field, **10.0** in the 'Maximum' field, and **0.5** in the 'Increment' field.   Then press the 'Delimiter' button and choose 'Comma' from the delimiter menu.   Finally, you would enter the filename mydata.tab in the File Name field and press the 'OK' button.

Setting the Polynomial Degree

For a polynomial regression, you must supply what degree of polynomial that you would like. Polynomials usually tend to give decent curvefits to almost any data set, but higher order polynomials (as a rule of thumb, over 9) tend to oscillate badly.   Also, polynomials offer no insight into the model that governs the data.

Note that you may not choose a polynomial degree greater than or equal to the number of points in the data set minus one.   A polynomial degree equal to the number of points in the data set minus one is simply interpolation, and that type of curve fitting can be obtained via the **Interpolation** menu.   Degrees greater than the number of data points cause an overconstrained problem, to which the solution is undefined.   Note also that you may not choose a polynomial degree of one or two; use the built-in linear and quadratic curvefits instead.   In short, the polynomial degree that you can enter in this dialog box is limited to

$$2 < \text{degree} < n\text{-}2$$

Using CurveFinder

Using the built-in CurveFinder essentially does all of the hard work for you.   You provide the data file, and the CurveFinder does the rest.   It sifts through every possible curvefit, ranks the fits from best to worst, and presents you with the best one.   Choosing CurveFinder from the Data menu will invoke a dialog box that will ask you for input on which families of of regression models to search. Also, you may use the "all on" and "all off" buttons to check or uncheck all of the families at once.   See Regression Models and Linear Regression for details on each built-in model.

If the polynomial family is included for consideration, you must specify the maximum degree of the polynomial that CurveFinder will consider in the "Polynomial Constraint" area.   Of course, if the polynomial family is not included, the polynomial contraint will simply be ignored.

Once you are finished selecting which model families CurveFinder should search, press the OK button. The calculation will then proceed, and each curvefit is ranked according to its standard error and correlation coefficient (see the Data Modeling with CurveExpert section for the appropriate equations), and the best fit is then displayed in the graphing window.   That's all there is to it!

Note that CurveFinder considers ONLY regressions (linear and nonlinear) in its search for the best fit. Further, as described above, you can select only certain families to be considered in the search for the best curvefit.   See Regression Models for a description of the model families.   Interpolations are guaranteed to pass through each of the data point, so an evaluation of their performance relative to a regression-type curvefit is rather difficult.   Therefore, interpolations are excluded from the CurveFinder's search; however, you may still decide to try these curvefits manually when CurveFinder is done.

This dialog will automatically generate initial guesses for the nonlinear regression models, whether AutoGuess is enabled or not.   If a particular curvefit diverges or generates a floating point exception, it is excluded from the calculation process.   In the case that an important curvefit in the group is not calculated, you must select that curvefit manually from the Apply Fit menu and adjust the initial guesses, if necessary.

The CurveFinder dialog is shown below:

All On
Press this button to select all of the families listed in this dialog for consideration in the CurveFinder's search.

All Off
Press this button to deselect all of the families listed in this dialog.

Model Families
Checking the checkbox beside a model family will cause every curvefit in that family to be considered in the CurveFinder's evaluation.   Families that are not marked by an 'X' will not be included.

Polynomial Constraint
If the polynomial family is included for consideration, you must specify the maximum degree of the polynomial that CurveFinder will consider in the "Polynomial Constraint" area.   Of course, if the polynomial family is not included, the polynomial contraint will simply be ignored.

CurveFinder Control Buttons

OK: Click the OK button to signify that you are finished choosing regression families, and that CurveExpert should begin calculating the families that you selected.

Cancel: Click the Cancel button to abort and not calculate any curvefits with CurveFinder.

Help: Click the Help button to find out how to use the CurveFinder dialog.

Calculate Groups

The **Calculate Groups** dialog allows you to automate the process of finding the right data model.   This option is most helpful when you have data that follows a certain trend that matches a particular model family or families.   Using **Calculate Groups**, you can select those families that you would like to see, and CurveExpert will automatically calculate all of the curvefits in that group, rank them on the main window's ranking chart, and open a graphing window for each of the curvefits.   See Regression Models for a description of the model families.

This dialog will automatically generate initial guesses for the nonlinear regression models, whether AutoGuess is enabled or not.   If a particular curvefit diverges or generates a floating point exception, it is excluded from the calculation process.   In the case that an important curvefit in the group is not calculated, you must select that curvefit manually from the Apply Fit menu and adjust the initial guesses, if necessary.

The **Calculate Groups** dialog is shown below:

All On

Press this button to select all of the families listed in this dialog.

All Off

Press this button to deselect all of the families listed in this dialog.

Model Families

Click the checkbuttons beside each model family to include them in the calculation.   Families that are not marked by an 'X' will not be included.

Calculate Groups Control Buttons

OK: Click the OK button to signify that you are finished choosing regression families, and that CurveExpert should begin calculating the families that you selected.

Cancel: Click the Cancel button to abort and not calculate any curvefits.

Help: Click the Help button to find out how to use the Calculate Groups dialog.
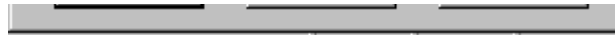
Setting Initial Guesses

All nonlinear regression algorithms require initial guesses to commence the search for the optimum regression parameters.   As long as <u>AutoGuess</u>is enabled, CurveExpert normally will calculate initial guesses for all built-in nonlinear regressions (linear regressions do not require initial guesses) for you automatically.   However, in the case of a poorly performing curvefit, you might want to set these initial guesses manually.   Also, you must set these initial guesses manually if you are using a user-defined nonlinear regression model.

In many cases, the physical interpretation of the individual parameters in a regression model may not be clear; hence, an inordinate amount of time can be spent simply trying to obtain appropriate initial guesses.   To facilitate this process, CurveExpert provides a **dynamic view plot** which adjusts itself every time you adjust the initial parameters.   This allows you to see the behavior of the curve, and adjust the parameters by hand in such a way that the curve is fairly close to the data points.   To display this plot, simply click the **Show Plot** button.   Subsequently, any changes you make to the initial guesses will be shown immediately on the dynamic view plot.

Hint: The plot drawing speed is increased automatically by CurveExpert; it increases the "Resolution" parameter.   To increase speed even more, right click on the plot window, choose "Attributes" off of the popup menu, and increase the "Resolution" parameter further.

The initial guess window is shown below:

Initial Guess Control Buttons

> **OK:**   Press OK to accept the initial guesses entered in the Parameter Guesses section and let CurveExpert perform the nonlinear regression.
> **Cancel:**   Press Cancel to abort the regression and return to the main CurveExpert window.
> **Help:**   Press Help to get CurveExpert help on setting initial guesses for a nonlinear regression.

Model Display

> To ensure that the meaning of the parameters is clear, this display shows you the equation for the model that you are providing initial guesses for.

Parameter Guesses

> **Guess Listbox/Edit Control:**   Enter an initial guess for each parameter in the corresponding field. Refer to the Model Display for the use of each of the parameters in your nonlinear regression model. The number of parameters required for you to enter will match the number of parameters that are in the model, and you may scroll up or down as necessary.
> **Show Plot:**   Click this button to dynamically view the changes that you make to the regression parameters.   This will greatly assist you in obtaining good initial estimates for the parameters.

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16-bit version:

CURXPT.EXE
CURXPTS.EXE (registered only)
CURXPT.HLP
CURVLIB.DLL
CURVRES.DLL
DIAGEXT.DLL
HKLIB.DLL
INSTLIB.DLL
CURVES.INI
README.TXT
VENDOR.TXT
HISTORY.TXT
FILE_ID.DIZ

32-bit version:

CVXPT32.EXE
CVXPTS32.EXE (registered only)
CURXPT4.HLP
CURXPT4.CNT
CURVLIB3.DLL
CURVRES3.DLL
DIAGEXT3.DLL
INSTLIB3.DLL
HKLIB3.DLL
CURVES.INI
README.TXT
VENDOR.TXT
HISTORY.TXT
FILE_ID.DIZ

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The DIAGEXT.DLL tab-control extensions were modified from original source by Freeman-Teresa Software and Mr. Edward McCreary:

TabCtrl v1.0

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Support, Bugs, and Feedback

If you have any questions at all about the use of CurveExpert, or need technical support, feel free to contact the author at the contact points listed below. Also, suggestions for the improvement of this program are always welcome!   Also, be sure to read over the Benefits of Registering.

Care has been taken to test CurveExpert 1.2 thoroughly, but as we know, bugs may still slip through this process. If you have a problem using this program, experience a bug in the program, or have any suggestions for improvement, please contact me at the address below.   For a bug report, the resolution of the problem will be facilitated greatly by sending me a debug report from CurveExpert.

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About the author...

About the Author

Hello, my name is Daniel Hyams.   I intend to give you the best support possible for this software, so rest assured that I will do my best to take care of any problem that you encounter, or answer any questions that you might have.

I would like to thank several people.   First, Charles Petzold for writing such a fantastic book (Programming Windows 3.1) that was worth more than gold throughout this project.   Next, the beta testers that provided excellent feedback on the performance of this software, potential uses, and potential problems.   A very special thank-you to my wife Michelle, who patiently put up with my endless work hours on this project throughout its two-year development.   Last and most of all, I would like to thank the Lord; without His blessing this project would have never materialized.

The Lord is my shepherd, I shall not want.   He makes me lie down in green pastures; He leads me beside quiet waters.   He restores my soul.   He guides me in the paths of righteousness for His name's sake.   Even though I walk through the valley of the shadow of death, I fear no evil, for Thou art with me. Thy rod and Thy staff, they comfort me.   Thou dost prepare a table before me in the presence of my enemies.   Thou hast anointed my head with oil;   my cup overflows.   Surely goodness and lovingkindness will follow me all the days of my life, and I will dwell in the house of the Lord forever.

--- Psalm 23, NAS ---

Data Information

The data information dialog gives you statistical information about the current data set in CurveExpert. First, the number of data points in set is given, along with the memory requirement of storing that data. Note that the "memory allocated" statistic shows the total amount of memory allocated for data, curvefits, and open graphing windows.

Other statistics given by this dialog are the average, minimum, maximum, and standard deviation from the mean of both the x and y data.   The average is a simple arithmetic average, which is defined as

The standard deviation from the mean describes the scatter of the data set around the average (higher standard deviation means more scatter).

$$N - 1$$

A sample of the data information dialog is shown below:

Data Manipulation

CurveExpert supports a flexible text file format for easy data import and supports four types of data manipulation after the file has been read. Manipulating your data using the built-in features of CurveExpert can be very beneficial to curve fit performance.   Please review the <u>Avoiding Floating Point Exceptions</u> section.   All data manipulation options are organized into a folder that is obtained via the Data|Manipulate menu.

<u>Working with Data Files</u>
<u>Manual Editing</u>
<u>Scaling</u>
<u>Translation</u>
<u>Clipping</u>
<u>Sorting</u>

Working with Data Files

CurveExpert reads a plain ASCII text file, which has two columns: one column for x data, and one column for y data.   You can produce these text files by hand, by spreadsheet, or any other method that can produce two columns of data.   Note that the type of delimiter in the data file is irrelevent -- the columns need only be separated by a nonnumeric character.   Therefore, the data file may have tab, space, or comma delimited data.

Comments may be interspersed freely within the data files, with the only restriction being that comments must either be placed on a line by themselves or after any data on that line.   Note again that there must be two numbers on a line for the data to be read correctly, and that if a line starts with a number, it is assumed to be a data line.   If it starts with a nonnumeric character, the line is assumed to be a comment.   Here are two examples, where the user wants all of the numeric data in the file to be read into CurveExpert:

<u>INCORRECT</u>		<u>CORRECT</u>	
1.0	2.5	1.0	2.5
2.0	2.7	2.0	2.7
2.5	2.9	2.5	2.9
this is text 2.9	3.1	2.9	3.1 this is text
3.1	3.2	3.1	3.2

When CurveExpert reads the first example, it assumes that the line with 'this is text' is a comment, and that line is discarded.   In the second example, the line with the comment starts with a number and is read correctly.

Scaling

To obtain the best curve fitting performance, you should scale your data to order one if the data is extremely large or small.   Review the   <u>Floating Point Exceptions</u> and <u>Performance Issues</u> sections for reasons why you might want to scale your data.

The **Data Manipulation** dialog box is the control that you use to multiply your data set by a scaling factor.   After opening this box via the Data|Manipulate menu choice, press the "Scale" tab.

To scale your data set, type in the desired scale factor into the scaling fields, and select the "Enable" buttons if you want a scale factor to be applied to the indicated column of data.   Leaving the "Enable" checkboxes unselected means that CurveExpert will ignore the factor in the corresponding field.   Finally, click the "Apply" button; the results of the scaling will immediately be apparent in the main window's spreadsheet.

Note that after scaling the data, CurveExpert does not automatically get rid of the current curve fits (to

prevent work that you have done from being lost).   If you wish to clear the curvefit cache, then select Data|Clear Curvefits.

Translation

Translating your data by a fixed additive factor can remove a known bias from the data set, as well as allow a better choice of a function to model the data.   The **Data Manipulation** dialog box is the control that you use to add a factor to your data set.   After opening this box via the Data|Manipulate menu choice, press the "Translate" tab.

To translate your data set, type in the desired translation factor into the scaling fields, and select the "Enable" buttons if you want translation to be applied to the indicated column of data.   Leaving the "Enable" checkboxes unselected means that CurveExpert will ignore the factor in the corresponding field.   Finally, click the "Apply" button; the results of the translation will immediately be apparent in the main window's spreadsheet.

Note that after translating the data, CurveExpert does not automatically get rid of the current curve fits (to prevent work that you have done from being lost).   If you wish to clear the curvefit cache, then select Data|Clear Curvefits.

Clipping

Clipping (or pruning) your data means to remove any outliers that might contaminate a curve fit which is applied to your data set.   This operation clips the data at a given x/y maximum and minimum. The **Data Manipulation** dialog box is the control that you use to clip outliers from the data set.   After opening this box via the Data|Manipulate menu choice, press the "Clip" tab.

Fill in the desired maximum and minimum for the x/y data, and press the Apply button.   The results of the data clipping operation will be immediately apparent in the main window's spreadsheet.

Note that after clipping the data, CurveExpert does not automatically get rid of the current curve fits (to prevent work that you have done from being lost).   If you wish to clear the curvefit cache, then select Data|Clear Curvefits.

Sorting

CurveExpert can sort the entire data set, using the either the independent variable (x) or the dependent variable (y) as the key.   When this operation finishes, all of your data will be in order of the key that was chosen.   This operation is crucial for interpolation-type data fits. The **Data Manipulation** dialog box is the control that you use to sort the data set.   After opening this box via the Data|Manipulate menu choice, press the "Sort" tab.

To sort the data set, choose the appropriate sort key (x or y) and press the Apply button. The results of the sorting operation will be immediately apparent in the main window's spreadsheet.   If the independent variable (x) is used as the key, the result of the sorting will be a data set that is in order with increasing x.   Conversely, if the dependent variable (y) is used, the data set will be in order with increasing y.   Note again that sorting the data set on x is crucial for interpolation type curve fits.

Opening and Saving Data Files

Data files in CurveExpert are simply two-column text files with the first column for the x data, and the second column for the y data.   See Working with Data Files for more information on the format of a CurveExpert data file.

Opening Data Files:

Simply choose the file that you want to use, and CurveExpert will read that file, examine it, and display the data in the main window for manipulation.   If necessary, you may manually edit the data or use the data manipulation features included in the **Data** menu (see the Working with Data section).   You are now ready to perform some curve fits on the data using the Apply Fit or Interpolate menu.

Note that you may select the **Read Only** checkbox to prevent the file that you have opened from being written to at any time during a CurveExpert session.   This keeps accidental saves from overwriting possibly valuable comments and data in the file that was initially opened.   A protected/read-only file's name will appear in the status bar in red.

Saving Data Files:

Data files will be written in two column form with no headers or footers.   A tab separates the first and second columns.   Note that if a data file that contains comments is read into CurveExpert and subsequently saved over the same file, the original comments are lost.

File Export

Exporting a file allows you to easily transfer data out of CurveExpert, most often to a spreadsheet.   The exported file will contain the data points along with the specified curvefit's approximation to the data evaluated at every data point.   Also, if you desire, the exported file can contain the specified model's coefficients (a,b,c,d...) and statistics describing your data set such as the mean and standard deviation.

The filename for the exported file is entered in the File Name field as usual.   The extra buttons on the right hand side of the Export dialog are special settings for the exporting operation.

Delimiters:

The **Delimiter** button allows you to choose what type of delimiter you would like to use to separate the data columns.   The default is a tab delimiter, but you may also use a single space or a comma.

Specifying Curve fit Type:

The curvefit that you will export is, by default, set to the last curve fit that was performed.   Its name is shown in the **Export Options** group.   If you wish to change this curve fit, click the **Change Curvefit Type>>** button -- a list of curve fits that have already been calculated will appear, and you may select from that list.   Note that a curve fit must already be calculated to be valid for exporting. If the curvefit you desire is not on the list, cancel the **Export** dialog, calculate the curvefit via the Apply Fit or Interpolation menus, and then reopen the **Export** dialog.

Include Coefficients:

The checkbutton **Include Coefficients** signifies whether you would like the curvefit coefficients to be present in the exported file.   Note that for spline interpolations, the coefficients are given as the coefficients of EACH piecewise polynomial used betwen each knot/data point.   The default is ON.

Include Statistics:

Lastly, the checkbutton **Include Statistics** signifies whether you would like relevant statistics to be present in the exported file.   The statistics that will be included are: X and Y data minimum, X and Y data maximum, X and Y data mean, and the X and Y data standard deviation. The default is ON.

Frequently Asked Questions

1) Why does CurveExpert suddenly erase my curve fits off of the ranking chart?

Any time that CurveExpert detects that the data set has changed, all curve fits are marked as invalid. The ranking chart shows only those fits that are valid, so the ranking chart is erased. The data set can change by manual editing or using the built-in data manipulation tools in the Data menu.

2) How can I increase the speed at which the graphs are updated?

Particularly if one has a large number of data points, the graphing windows are sometimes updated very slowly, as the data point marker must be drawn for every point. However, CurveExpert has a setting in its application defaults, called the Render Level, that can be used to 'ease the pain' of slow redraws. The tradeoff is that a large chunk of precious GDI memory will be used for each graph is open.

Choose File|Preferences, and select "Fast Rendering."

Note that when drawing the plot for the first time, or when resizing the window, it will take just as long for the graph to be drawn. The advantage comes about because once this drawing is done, it is saved. Now every time the window is covered/uncovered by another window, or moved to a different location, it does not have to be redrawn from scratch.

3) Why is there a huge number for standard error and correlation coefficient sometimes? Is this a bug?

No, this is not a bug. This is CurveExpert's way of telling you that your data set is badly out of scale -- in the course of computing the standard error of the estimate and correlation coefficient, an accumulation of differences between the curvefit and data points and the mean and the data points takes place. If this calculation overflows, which is quite likely when the magnitudes of the x or y data sets are very large, then CurveExpert does the best it can by setting this sum to the maximum allowed by the data representation (single precision or double precision). This usually leads to unrealistic values for the standard error and correlation coefficient. The solution to this problem is to rescale your data to a magnitude of one.

4) As nonlinear regression progresses, the indicator for standard error (S) sometimes freezes, although the iteration counter keeps on ticking. What is going on?

Without getting into the internals of the Marquardt-Levenberg method for nonlinear regression (see the <u>Theory</u> section), suffice it to say that everything is still functioning correctly. If the algorithm detects that the standard error (chi square) increases during an iteration, then the new parameters are discarded. This naturally forces the chi square for the current iteration will be the same as the last. However, all is not lost -- if this situation occurs, the algorithm makes adjustments to some internal parameters and performs another iteration. It is searching for an 'optimum' value of these internal parameters so that it can reduce the chi square and therefore find better parameters. If the chi square only adjusts itself every other iteration, then the internal parameters are 'on the edge' of optimum and the calculated regression parameters are being discarded every other time.

5) A spline fit never matches my data at the points like it is supposed to, and sometimes has spikes and/or wildly oscillating tendencies. Is there something amiss?

Two items will definitely cause this behavior -- [1] fitting splines to unsorted data or [2] fitting splines to data with replicate values, i.e., two or more x data points are the same. The solution to problem #1 is easy; simply sort the data using CurveExpert's built-in <u>sort</u> feature. Reapply the spline fit, and everything should work as planned. If problem #2 is the issue, then I have to question the use of a spline to fit your data. I would recommend that one or more of the replicate values be removed, or you will be forced to use a regression-type model.

Other reasons that splines might fail is because of the sheer number of data points.   Round-off errors in the computations can accumulate, causing incorrect splines to be shown.   Be careful when applying splines to very large data sets.   Again, splines are usually used on small to moderate size data sets.

And as always, as yet another reminder, make sure that your data set is scaled to reasonable numbers (preferably on the order of one).   High or low values may be causing excessive round-off error, overflow, or underflow in the computations.

6)   Lagrangian interpolation sometimes bombs with a floating point exception. What gives?

Check in your data set for a replicate value, i.e., two or more x data points are the same.   If this is an issue, then I have to question the use of interpolation to fit your data.   I would recommend that one or more of the replicate values be removed, or you will be forced to use a regression-type model.

And as always, as yet another reminder, make sure that your data set is scaled to reasonable numbers (preferably on the order of one).   High or low values may be causing excessing round-off error, overflow, or underflow in the computations.

7)   I am using a Postscript printer driver, and my plots will simply not print in the orientation (portrait or landscape) that I tell it to.   Is there anything that I can do?

There is a bug in the Postscript printer driver (perhaps it is fixed by now) that causes it to always print in the orientation specified in the Control Panel.   Unfortunately, this means that you cannot adjust the orientation in CurveExpert.   However, you may open the Control Panel, select Printers, select the Postscript printer, and click the Setup button.   Here, you may adjust the orientation.   Now plots from CurveExpert will print in the orientation that you have specified through the Control Panel.

8)   CurveExpert saves the previous window position, and I don't want it to. How do I turn this behavior off?

From the File menu, choose Preferences.   Deselect the checkbox that says "Save Window Position."

9)   How do I obtain a debugging report to send to the author?

The key is running CurveExpert with the '-d' parameter.   From the Program Manager or File Manager, choose 'Run'.   Use the Browse command to look in the CurveExpert directory and find the executable, which is CURXPT.EXE.   Double click on this file.   You should then see the 'Run...' dialog again with the full path to CURXPT.EXE in the 'Command Line' field.   Add a ' -d' to the string already in the dialog, and press OK.   CurveExpert will now record information information both onscreen and in a file called CXPTxxxx.REC, where xxxx is a unique number.   If multiple debug files are saved, they will be numbered consecutively.

If you are having a problem with CurveExpert, the best way to solve the problem is to contact me, describe the problem, and send the debug file mentioned above.   Obviously, the problem should be reproduced while the debug file is being made.

10)   Why are grid lines drawn as solid lines (instead of dotted) on some computers?

I wish that it was a bug in CurveExpert; if it were, I could fix it.   However, this happens because of a bug in the display driver installed on your computer.   Contact your video card vendor or Microsoft for the latest driver.   If your driver is the latest version, then you may report the bug to the author of the driver (usually the company that manufactured the video card).

11)   When I paste a column from Excel or Quattro Pro into CurveExpert, only the first number in the column gets put into the cell that I am pointing to.   Is this a

bug?

No, CurveExpert does not yet support a full column paste into the built-in spreadsheet.   This functionality is planned in the near future, perhaps in the next release of CurveExpert.

For now, the fastest way to move data between a spreadsheet and CurveExpert is to use the 'Extract' or 'Export' command in your spreadsheet to write the desired columns into an ASCII text file.   Then, read this text file into CurveExpert.   You might find that this operation is *almost* as fast as a copy/paste operation, after it has been streamlined.   However, the author realized that the cut/paste solution is more intuitive and faster, so this functionality will be implemented soon!

Computational Performance

The computational performance is divided into three sections.   The first described the operations that you can perform while CurveExpert is working on a computation of some sort.   The second gives useful tips on improving the performance of CurveExpert, and the third gives some sample data on the relative speed of CurveExpert's different flavors.

- While CurveExpert is Working
- Tips
- Sample Speed Tests

While CurveExpert is Working

While the calculation proceeds, you can watch the status bar to see what regression is being calculated, the iteration number, and (most importantly) the standard error (chi square) of the model as the nonlinear regression algorithm progresses.   The chi square lets you know how well the model is currently fitting the data, and it should be steadily decreasing, in an optimum situation.

When CurveExpert is working, the toolbar andmenus are disabled except for two new buttons on the far right hand side of the toolbar. Note that for interpolations and linear regressions, each button has the same meaning.   They will both terminate the calculation immediately and no results will be shown. Also note that if background processing is disabled, these buttons will also be disabled; in effect, the ability to stop the calculation (in a graceful manner) is lost if background processing is disabled.

Yellow Check: (Keyboard Equivalent: ESCAPE)

Press this button to stop the computation for a particular curvefit.   The parameters are accepted as they are; this button is handy when the standard error has dropped to a stable value, but CurveExpert is continually "tweaking" the values of the parameters to arrive within the tolerance bounds set in the File|Preferences dialog.   Selecting this button will accept the current parameters as they are.   The same operation can be accomplished by pressing Esc on the keyboard.

Red Stop Sign: (Keyboard Equivalent: SHIFT+ESCAPE)

Press this button to abort all calculations immediately.   The same operation can be accomplished by pressing Shift+Esc on the keyboard.

Tips to Increase Computational Performance

CurveExpert has been optimized to perform regressions and interpolations as quickly as possible. Additional speed gains are sure to some in later versions; however, you can greatly speed up the operation and reliability of CurveExpert by carefully following certain guidelines:

Tip #1:

Always, always, always scale your data sets to the order of one.   You may do this prior to reading in your data file, or after your data file has been imported using the scaling feature in CurveExpert. This point cannot be overemphasized!   If you contact me with a problem concerning a situation where CurveExpert will not fit a certain set of data, this is the first questions that I will ask.

Imagine a data set with x values ranging from 1000 to 10000 and a regression model where the term exp(a*x) is involved.   Unless a very good initial guess for a is given, chances are that an exponential to a very large power (eg. exp(1000)) will be taken in the course of the nonlinear regression algorithm.   The calculation will overflow, and the regression will fail as a result.   Even if the regression happens not to fail, the regression algorithm will have an exceedingly tough time finding the correct parameters, since a small change in the free parameters will cause a tremendous change in the size of the term.   The moral of the story: always scale your data!

Note that CurveExpert is able to perform correctly on data in any scale, as long as the calculations do not overflow or underflow.   So, if a data set is giving problems, scaling it should be the first action to take.

Tip #2:

Enabling background processing (in the File|Preferences dialog) slows down computation considerably, since the calculation must pause for Windows to process pending messages for all running programs.   If you are running CurveExpert by itself, or you don't care if another program is ignored when CurveExpert is calculating, then turn this option off!   Calculations speed will increase greatly.   The CALC flag in the status bar will be written in red when background processing is disabled to remind you that every other program is halted while CurveExpert works.

Tip #3:

Don't set the tolerance parameter (in the File|Preferences dialog) too low.   In regression modelling, not much advantage is to be gained by setting a very strict tolerance.   Its main purpose in life is to prevent the nonlinear regression algorithm from converging on local minima.

Tip #4:

CurveExpert uses double-precision floating point numbers to do all calculations. The registered version of CurveExpert comes with two executables: one version using single-precision calculations (seven sig figs), and the second using double-precision (15 sig figs).   Using a single-precision (theoretically) greatly speeds up performance, at the cost of accuracy. Especially with extremely large data sets, the single-precision version should provide a speed and memory advantage.   By registering, you can make the choice yourself.   See the sample speed test data below for an indication of the performance of the different packages.

You may check what type of data representation is being used by CurveExpert by selecting Help| About.

CurveExpert Speed Tests

CurveExpert has become faster as the version number has increased; this section is meant to demonstrate this fact, as well as compare the speed of the double and single precision versions (registered users only).   All data was taken on a 486 DX-266 Intel computer, with the 'Background Processing' flag turned off, QuickDerivatives turned off, and the nonlinear regression tolerance set at 1e-

6. The table below demonstrates the time, in seconds, required for the following tests to be performed.

Test 1: data set -- ONION.DAT, run CurveFinder with all options checked, polynomial max of 4.
Test 2: data set -- BEANROOT.DAT, run CurveFinder with all options checked, polynomial max of 4.
Test 3: data set -- BEANROOT.DAT, User Model for Truncated Fourier Series, initial guesses all at 1.0.

	Test 1	Test 2	Test 3
CurveExpert 1.14 (double)	96	37	55
CurveExpert 1.20 (double)	72	27	35
CurveExpert 1.14 (single)	51	17	29
CurveExpert 1.20 (single)	36	14	20

Floating Point Exceptions

CurveExpert takes every precaution to avoid math errors, a.k.a. floating point exceptions.   Here are some ways that you can avoid these errors:

Tip #1:

Take care to scale both x and y data to a magnitude of one.   For example, if you have data that describes atmospheric pressure at different elevations, you might have (in metric units) a data set that looks like:

```
x=[-100, 0, 100, 500, 1000, 4000] meters
y=[102000,101325,101000,100500,100000,99900] Pascals
```

Using the scaling feature in the **Data** menu of CurveExpert, you can scale this data using a scale factor of 0.001 on the x data, and 0.00001 on the y data.   So, you would then have the following data set:

```
x=[-0.1, 0, 0.1, 0.500, 1, 4] kilometers
y=[1.02,1.01325,1.01,1.005,1.0,0.999] bars
```

The second example is much more likely to allow nonlinear regressions to converge, and also will allow higher order polynomial fits to be performed with more accuracy.   If you have a data set that seems particularly ill-behaved, scaling can help solve this problem.

Tip #2:

Make sure that the data is appropriate to the model.   Especially look out for using logarithmic or exponential families of models with data that contains zeros or negatives.   For example, it is not possible, in any shape or form, to obtain a negative or zero with the basic exponential model (y=ae^(bx), assuming a is nonzero).   So, it is not wise to use a model that cannot reflect the trends in the data.   CurveExpert should disallow the use of certain regression models with data that is negative or zero; however, in the case that one should slip through or you are using a user-defined model, you should be aware of the characteristics of the data modeling equations so that choices of an incorrect model can be avoided.

Tip #3:

If you are using an interpolation-type curvefit, the data points MUST BE SORTED!   Use the Data| Manipulate feature in CurveExpert to sort your data points correctly.   It is quick and painless!

Tip #4:

Some curvefits are simply ill-behaved, i.e. prone to divergence.   For some data sets, it may not be possible to converge certain nonlinear regression models.

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Data Modeling with CurveExpert

Given a set of data points, often called "observations," a common need is to condense the data by fitting it to a model in the form of a parametric equation.   This "model equation" can be anything that the user desires -- it can range from a simple polynomial to an extremely complex model with many parameters. One important consideration in selecting an appropriate model is the underlying law that the data represents.   Optimally, the curvefit model should be chosen to reflect that law so that the parameters in the curvefit have physical interpretation and meaning.

Data modeling may be performed by several techniques: interpolation, regression, or data smoothing. Interpolation and regression are the types supported by CurveExpert.   Interpolation guarantees that the fitted curve will pass through each and every data point.   Regression simply ensures that the "merit function", which is an arbritrary function that measures the disagreement between the data and the model, is minimized.   In this approach, the model parameters are adjusted until the merit function becomes as small as possible.   One of the features of CurveExpert is the large number of nonlinear regression models that are available. This type of model is the most commonly used in real-world applications.

Interpolation
   <u>Lagrangian Interpolation</u>
   <u>Splines</u>

Regression
   <u>Linear Regression</u>
   <u>Nonlinear Regression</u>

For regression curve fits, error is assessed using the standard error and correlation coefficient.   These tools are not perfect, but they do give helpful evaluation of the performance of the curve fit.   The *standard error of the estimate* is defined as follows:

$$\sqrt{\frac{\sum}{n_{points} - n_{param}}}$$

where **y** denotes the value calculated from the regression model, **y$_i$** denotes the data points, and n$_{param}$ is the number of parameters in the particular model (so that the denominator is the number of degrees of freedom).   Note that this error function doubles as the merit function for nonlinear regression as discussed in the <u>Theory</u> section.   The standard error of the estimate quantifies the spread of the data points around the regression curve.   As the quality of the data model increases, the standard error approaches zero.

Another measure of the "goodness of fit" is the *correlation coefficient*.   To explain the meaning of this measure, we must return to the data points and define the standard deviation, which quantifies the spread of the data around the mean:

$$\sqrt{\frac{}{n_{points} - 1}}$$

where the average of the data points (ybar) is simply given by

$$\frac{}{n_{points}} \sum_{i=1}$$

Note that the standard deviation (i.e., standard error of the mean) operates in exactly the same fashion as the standard error of the estimate defined above; however, it considers the spread around a constant line (the mean) as opposed to the spread around the regression model.   This is the uncertainty of the dependent variable prior to regression.   Thus, the improvement (or error reduction) due to describing the data in terms of a regression model can be quantified by subtracting the two quantities.   Because the magnitude of the quantity is dependent on the scale of the data, this difference is normalized by the standard deviation around the mean to yield

$$S_t$$

where **r** is defined as the correlation coefficient.   As the regression model better describes the data, the correlation coefficient will approach unity.   Note that CurveExpert will sometimes compute a correlation

coefficient that is above one; this is indicative of a very poor fit.

For a perfect fit, the standard error of the estimate will approach $S_r=0$ and the correlation coefficient will approach r=1.

Lagrangian Interpolation

Lagrangian interpolation is simply interpolating the data set with a polynomial. The order of the polynomial is determined by the number of points in the data set -- the polynomial must have enough degrees of freedom to fit the data set at every point. Therefore, in a data set with n points, the interpolating polynomial will be of n-1 degree.

Lagrangian polynomials are particularly well suited for data sets with a low number of data points (8 or less). Preferably, the data points should not have too much scatter. Like all polynomials, the Lagrangian interpolating polynomial exhibits more oscillatory behavior as the degree increases. Therefore, the use of Lagrangian interpolations should be avoided if the number of data points is large. Currently, CurveExpert limits the use of this type of interpolations to data sets with 13 points or less.

As the name implies, extrapolating beyond the scope of the data points with an interpolating polynomial can be very detrimental. Interpolations only provide accuracy *between* the data points -- using them to obtain y data outside of the range of the data points must be done very carefully.

Spline Interpolation

CurveExpert implements four types of spline interpolation:
<u>Linear Spline</u>
<u>Quadratic Spline</u>
<u>Cubic Spline</u>
<u>Tension Spline</u>

Linear Splines

Linear splines are the simplest form of spline -- they simply approximate the range between data points by a straight line.   The purest definition of a linear spline is that is simply ensures that each discrete spline matches the data points.   These splines are simply a "connect-the-dot" approach that can be useful in increasing the resolution of a given table of values by using linear interpolation between each point.   However, if this is the application, cubic splines provide a much more accurate representation between the data points.

Quadratic Splines

Quadratic splines interpolate the range between data points by a 2_{nd} order polynomial (quadratic). Quadratic spline curve fitting ensures that each spline is equal to the data points, and that the 1_{st} derivative of the splines are continuous, even at the knots.   Quadratic splines perform better than simple linear splines, but are often characterized by "swinging" too high or too low past the data points.

Quadratic splines must have one free condition specified for the first spline.   CurveExpert follows common practice, which is to specify that the 2_{nd} derivative of the first spline is zero -- this has the effect of connecting the first and second points with a straight line.

The implementation of quadratic splines used in CurveExpert requires a good deal of memory and crunching time (even more than that of the cubic spline).   Do not use this curvefit on an excessive number of data points!   Use caution when applying this class of splines.

Cubic Splines

Cubic splines interpolate the range between data points by 3_{rd} order polynomials (cubics).   Cubic spline curve fitting ensures that each spline is equal to the data points, the 1_{st} derivatives are continuous at the knots, and the 2_{nd} derivatives are continuous at the knots.   Since discontinuities in 3_{rd} and higher derivatives cannot be visually detected, cubic splines have an "aesthetically pleasing" appearance.   In fact, cubic splines mimic the behavior of drafting splines used in olden days.

Various end conditions can be used for cubic splines.   Common practice is to use "natural" end conditions by specifying that the 2_{nd} derivative of the end splines are zero at the endpoints.   This gives the visual appearance of "straightening out" at the ends, which is the behavior of a physical drafting spline.   This behavior is the type implemented in this version of CurveExpert.

Tension Splines

Tension splines behave similarly to cubic splines, with the addition of a parameter (the tension) which specifies how "tightly" the spline forms to each knot.   A low tension parameter will yield a spline similar to a cubic spline; whereas at high tension, the spline will approach a linear spline.

The **Set Tension** dialog box allows you to set this parameter before the tension spline curvefit is performed.   You can experiment with the tension to obtain the visual quality that you want in your spline.

Note that there is no easy way to specify a tension spline, except by creating a table of its values.   It is also very ill-behaved -- expect a few complaints from CurveExpert about floating point errors.   To alleviate this type of error, make sure that your data is scaled to an order of one, and give intermediate

tension parameters (0.1 to 20).

Linear Regression

Models which consist of a linear combination of a particular set of functions X_k are called linear models, and linear regression can be used to minimize the difference between the model and data. The general form of this kind of model is

$$y(x) = \sum a_i X_i(x$$

where $X_k(x)$ are fixed functions of **x** that are called the *basis functions*, and a_k are the free parameters. Note that "linear" refers only to dependence of the model on the parameters a_k; the functions $X_k(x)$ may be nonlinear.

Minimization of the above linear model is performed with respect to the merit function

The minimum of the above equation occurs where the derivative of **S** with respect to the parameters disappears. Substituting the linear model into this function, taking the first derivative, and setting this equal to zero gives the normal equations that can be solved directly for the parameters a_k.

Linear Regression Models

In CurveExpert, all of the linear models implemented are linear combinations of x_n. These models are listed below:

Linear Fit:	y = a+bx
Quadratic Fit:	y = a+bx+cx^2
Polynomial Fit:	y = a+bx+cx^2+dx^3+....

Nonlinear Regression

This help topic has two subsections:

Theory

This program uses the Levenberg-Marquardt method to solve nonlinear regressions.   This method combines the steepest-descent method and a Taylor series based method to obtain a fast, reliable technique for nonlinear optimization.   This statement will be repeated later, but can bear stating at the beginning of this discussion: neither of the above optimization methods are ideal all of the time; the steepest descent method works best far away from the minimum, and the Taylor series method works best close to the minimum.   The Levenberg-Marquardt (LM) algorithm allows for a smooth transition between these two methods as the iteration proceeds.

In general, the data modeling equation (with one independent variable) can be written as follows:

$$y = y(x; a)$$

The above expression simply states that the dependent variable **y** can be expressed as a function of the independent variable **x** and vector of parameters **a** of arbitrary length.   Note that using the ML method, any nonlinear equation with an arbitrary number of parameters can be used as the data modelling equation.   Then, the function we are trying to minimize (sometimes called the "chi square" or the "merit function") is

$$\chi^2(a) = \sum_{i=1}^{N} \left(y_i - y(x_i, a) \right)$$

where **N** is the number of data points, x_i denotes the x data points, y_i denotes the y data points, and $y(x_i, a)$ is an arbitrary nonlinear model evaluated at data point i.   This merit function simply measures the agreement between the data points and the parametric model; a smaller value for the merit function denotes better agreement.

Now, we will take a step back to provide a framework of optimization methods.   From the area of pure optimization, which will not be explained here, two basic ways of finding a function minimum are a Taylor series based method and the steepest-descent method.   The Taylor series method states that sufficiently close to the minimum, the function can be approximated as a quadratic.   Without detailed explanation of that method, a step from the current parameters **a** to the best parameters a_{min} can be written as

$$a_{min} = a_{cur} + H^{-1} \cdot \left[-\nabla \chi (a_{cur}) \right]$$

where **H** is the Hessian matrix (a matrix of second derivatives).   If the approximation of the function as a quadratic is a poor one, then we might instead use the steepest-descent method, where a step to the best parameters from the current parameters is

$$a_{min} = a_{cur} - c \nabla \chi (a_{cur})$$

This equation simply states that the next guess for the parameters is a step down the gradient of the merit function.   The constant **c** is forced to be small enough that a small step is taken and the gradient is accurate in the region that the step is taken.

Since we know the chi square function, we can directly differentiate to obtain the gradient vector and the Hessian matrix.   Taking the partial derivatives of the merit function with respect to **a** gives

$$\frac{\partial \chi^2}{\partial a_k} = -2 \sum_{i=1}^{L} \frac{1}{\sigma_i^2} \frac{\partial}{\partial a_k}$$

To obtain the Hessian matrix, take the gradient of the gradient above (so that we have a matrix of partial second derivatives):

$$\frac{\partial \chi^2}{\partial a_k \partial a_l} = 2 \sum_{i=1}^{L} \frac{1}{\sigma_i^2} \frac{\partial}{\partial a_k} \frac{\partial}{\partial a_l} - (y_i - y(x_i, a)) \frac{\partial}{\partial a_k \partial a_l}$$

Now, for convenience, define the curvature matrix and the gradient vectors as

$$\frac{1}{2} \frac{\partial}{\partial a_k} \frac{1}{\sigma_i^2} \frac{\partial}{\partial a_k} \qquad \frac{1}{2} \frac{\partial}{\partial a_k \partial a_l} \frac{\partial}{\partial a_k} \frac{\partial}{\partial a_l}$$

[Note that the second derivative term in **C** will be ignored because of two reasons: it tends to be small

because it is multiplied by (y-y_i), and it tends to destabilize the algorithm for badly fitting models or data sets contaminated with outliers.   This action in no way affects the minimum found by the algorithm; it only affects the route in getting there.]   So, the Taylor series method (inverse Hessian method) can be written as the following set of linear equations:

$$\sum_{i=1}$$

[1]

This linear matrix will be our workhorse for this method after some modification; it can be solved for the increments δa that, when added to the current approximation for the parameters, gives the next approximation.   Likewise, we can substitute our "convenient" definitions into the steepest descent formula to obtain

$$\delta a_i = c \upsilon_i$$

[2]

Neither of the aforementioned optimization methods are ideal all of the time; the steepest descent method works best far away from the minimum, and the Taylor series method works best close to the minimum.   The Levenberg-Marquardt (LM) algorithm allows for a smooth transition between these two methods as the iteration proceeds.

The first issue in deriving the LM method is to attach some sort of scale to the constant **c** in the steepest-gradient method (equation 2).   Typically, there is no obvious way to determine this number, even within an order of magnitude.   However, in this case, we have access to the Hessian matrix; examining its members, we see that the scale on this constant must be $1/C_{ll}$.   But, that still may be too large, so let's divide that scale by a nondimensional factor (λ) and plan on setting this much larger than one so that the step will be reduced (for safety and stability).

The second issue to formulate the LM method is noting that the steepest-descent and Taylor series methods may be combined if we define a new matrix M_{ij} by the following:

$$\left[\; M_{ij} = C_{ij} , \; i \neq j \right.$$

This matrix combines equations [1] and [2] into a convenient and compact form.   So finally, we have a means of calculating the step δa in the parameters by the following system of linear equations:

$$\sum_{l=1}$$

[3]

Note that when λ is large, the matrix **M** is forced to be diagonally dominant; consequently, the above equation is equivalent to the steepest descent method (equation 2).   Conversely, when the parameter λ goes to zero, the above equation is equivalent to the Taylor series method (equation 1).   So, we vary λ to switch between the two methods, continually calculating a parameter correction δa that we apply to our most recent guess for the parameter vector.   The steps that are taken in the LM algorithm are as follows:

[1] Compute S(a)
[2] Pick a conservative value for λ (0.001 in CurveExpert)
[3] Solve the linear equations (equation 3) for δa
[4] Evaluate S(a+δa)
[5] If S(a+δa) >= S(a), increase λ by a factor (10 in CurveExpert) and go back to step [3].
[6] If S(a+δa) < S(a), decrease λ by a factor (10 in CurveExpert), correct the parameter vector by a=a+δa, and go back to step [3].

Iteration is stopped when |S(a+δa) - S(a)| < tolerance.   This tolerance is the value specified in the File| Preferences dialog.

Nonlinear Regression Models

Nonlinear regression models come in all shapes and sizes -- in CurveExpert, an attempt has been made to include as many models as possible, while at the same time providing relevent models to a wide range of applications.   Also, keep in mind that if the model that you desire is not built-in to CurveExpert, you may define your own using the Define User Models facility.

In CurveExpert, the nonlinear models has been divided into families based on their characteristic behavior.   These families and their members are enumerated below:

Exponential Family

Exponential models have the exponential or logarithmic functions involved.   They are generally convex or concave curves, but some models in this group are able to have an inflection point and a maximum or minimum.

Exponential:	$y = a*exp(b*x)$
Modified Exponential:	$y = a*exp(b/x)$
Logarithm:	$y = a+b*ln(x)$
Reciprocal Logarithm:	$y = 1/(a+b*ln(x))$
Vapor Pressure Model:	$y = exp(a+b/x+c*ln(x))$

Power Family

The Power Family involves raising one or more parameters to the power of the independent variable, or raising the dependent variable to the power of a given parameter.   This family is generally a set of convex or concave curves with no inflection points or maxima/minima.

Power Fit:	$y = a*x^b$
Modified Power:	$y = a*b^x$
Shifted Power:	$y = a*(x-b)^c$
Geometric:	$y = a*x^{(b*x)}$
Modified Geometric:	$y = a*x^{(b/x)}$
Root Fit:	$y = a^{(1/x)}$
Hoerl Model:	$y = a*(b^x)*(x^c)$
Modified Hoerl Model:	$y = a*b^{(1/x)}*(x^c)$

Yield-Density Models:

The yield-density models are widely used, especially in agricultural applications.   These models historically have been used to model the relationship between the yield of a crop and the spacing or density or planting.   Essentially two types of response are observed in practice: the "asymptotic" and "parabolic" yield-density relations.   If the response is such that as density (x) increases, but the yield (y) approaches a fixed value, the relationship is asymptotic.   If the response is such that there is a distinct optimum as the density increases, the relationship is parabolic.   Of course, these types of relationships occur commonly in other scientific areas; therefore, this family of models is very useful.

Reciprocal Model:	$y = 1 / (a + bx)$
Reciprocal Quadratic:	$y = 1 / (a + bx + cx^2)$

Bleasdale Model: $y = (a + bx)^{(-1/c)}$

Harris Model: $y = 1 / (a + bx^c)$

Growth Family

Growth models are characterized by a monotonic growth from some fixed value to an asymptote. These models are most common the engineering sciences.

Exponential Assoc (2): $y = a*(1-exp(-bx))$

Exponential Assoc (3): $y = a*(b-exp(-cx))$

Saturation Growth: $y = ax / (b + x)$

Sigmoidal Family

Processes producing sigmoidal or "S-shaped" growth curves are common in a wide variety of applications such as biology, engineering, agriculture, and economics.   These curves start at a fixed point and increase their growth rate monotonically to reach an inflection point.   After this, the growth rate approaches a final value asymptotically.   This family is actually a subset of the Growth Family, but are separated in CurveExpert because of their distinctive behavior.

Gompertz Model: $y = a * exp (-exp(b - cx))$

Logistic Model: $y = a / (1 + exp (b - cx))$

Richards Model: $y = a / (1 + exp(b - cx))^{(1/d)}$

MMF Model: $y = (ab + cx^d)/(b + x^d)$

Weibull Model: $y = a - b*exp(-cx^d)$

Miscellaneous Family

As with many things in life, some things just don't fit into nice categories.   The miscellaneous family is the one in which these "different" nonlinear regression models live.

Sinusoidal Fit: $y = a + b*cos(c*x + d)$

Gaussian Model: $y = a*exp((-(x - b)^2)/(2*c^2))$

Hyperbolic Fit: $y = a + b/x$

Heat-Capacity Model: $y = a + bx + c/x^2$

Rational Function: $y = (a + bx) / (1 + cx + dx^2)$

Defining Custom Regression Models

CurveExpert allows you to define your own nonlinear regression models.   All you have to do is type in the equation!   When you choose Define User Model from the Apply Fit menu, you will be presented with a dialog in which you can type or choose your model.   Type your model into the edit field provided, or choose a model from the scrolling list.   You may use <u>operators</u> and <u>functions</u> in your model that are defined at the end of this help page.

Parameters should start at letter 'a' and continue sequentially.   CurveExpert allows you to use up to 19 parameters, lettered a..s.   All arithmetic operations are valid, as well as the symbol ^ to raise a number to a power.   Here is an example of what you could enter in the User Defined Model dialog box:

<p align="center">a*x*log(b+x)+c^x</p>

Note that there is no need to enter the 'y=' before the function -- only the right hand side of the model is entered.

Logical operators are also supported in your user-defined regression models.   The operators that are less than (<), greater than (>), less than or equal to (<=), or greater than or equal to (>=).   Each of these expressions evaluate to one if the expression is TRUE, or zero if the operation is FALSE.   In this way, you can implement logical expression into your model.   For example, if you would like to construct a model of two separate lines to where one line is applicable to the region of x<=5, and one line is applicable to x>5, then you might construct the following four-parameter model:

<p align="center">(a+b*x)*(x<=5)+(c+d*x)*(x>5)</p>

These logical operators can be combined in any way to create your user defined model.   See below for a complete list of the supported arithmetic and logical operators.

A picture of the User Model dialog is shown below, with a description of the controls/operations following:

User Model Control Buttons

OK: Press OK to use the model that you have entered to fit the data set.   The nonlinear regression calculation will begin.   If there is a syntax error with your model, you will be notified at this time.

Cancel: Press Cancel to abort this operation and return to the main window.

Help: Press Help to learn how to apply custom regression models.

Model Edit Field

Type your custom regression model into this field, using a...s for the model parameters. Parameters should start at letter 'a' and continue sequentially. CurveExpert allows you to use up to 19 parameters, lettered a..s.   All arithmetic operations are valid, as well as the symbol ^ to raise a number to a power.   Note that there is no need to enter the 'y=' before the function -- only the right hand side of the model is entered.   Also, you may edit the text in this box at any time, even after you have selected a model from the Model List.

The normal cut, copy, and paste keys can be used in this edit field; i.e., Ctrl+X for cut, Ctrl+C for copy, and Ctrl+V for paste.

Model List

User models that have been saved will be listed in this box.   Scroll up or down to see them all.   Selecting an item from this box will simply copy its formula to the **Model Edit Field** so that you can either click OK to calculate that model, or modify it as necessary.   Double-clicking a model in this list will select that model for a regression immediately.

Add Model

Clicking on this button will add the model that is in the **Model Edit Field** to the **Model List**.   This operation permanently saves a model that you have typed in.   You will be asked what to call the model so that a name (not a formula) will be added to the list.

Remove Model

Clicking on this button will remove the highlighted model from the **Model List** *permanently*.   A dialog will ask you to verify this operation.

The following operators are supported by CurveExpert to be used in your regression model:

+	addition
-	subtraction
-	unary minus
*	multiplication
/	division
^	power
<	less than
>	greater than
<=	less than or equal to
>=	greater than or equal to
!=	not equal
==	equal

The following functions and variables are supported by CurveExpert to be used in your regression model:

abs	absolute value
fact	factorial
sqrt	square root
exp	exponential
log	natural logarithm
ln	natural logarithm
log10	base-10 logarithm
sin	sine
cos	cosine
tan	tangent
asin	arcsine
acos	arccosine
atan	arctangent
sinh	hyperbolic sine
cosh	hyperbolic cosine
tanh	hyperbolic tangent
pi	the constant 3.14159....
avgx	average of the x column
avgy	average of the y column
stdx	standard deviation of the x column
stdy	standard deviation of the y column
minx	minimum of the x column

miny	minimum of the y column
maxx	maximum of the x column
maxy	maximum of the y column

Available Versions of CurveExpert

CurveExpert is available as a 16-bit or 32-bit package.   The chart below summarizes the platforms that are supported by both of these versions.

	16-bit	32-bit
Windows 3.1	x	
Windows 3.1 + Win32s 1.30 or later		x
Windows 95	x	x
Windows NT 3.51 or later	x	x

You can order either version; see the <u>registration form</u> for details.   The 16-bit version is recommended if you run Windows 3.1 exclusively.   However, if you have Windows 95, Windows+Win32s, or Windows NT, the 32-bit version offers more enhanced features; also, the computations are significantly faster in the 32-bit version.   In addition, running a 32-bit version in its native environment (Win95 or WinNT) allows the operating system to manage multitasking properly and in the most transparent manner.

Win32s is an extension to Windows 3.1 that allows you to run most 32-bit programs in the Windows 3.1 16-bit environment.   If you would like to obtain Win32s, you can do so for free at the following Internet ftp site:

ftp://ftp.microsoft.com/softlib/mslfiles/pw1118.exe

Download this file to your computer and follow the enclosed directions.   Note that *most* 32-bit programs will run using Win32s; however, multithreaded 32-bit programs will not.

Development Information

CurveExpert has been developed under the Windows 3.1 and Windows 95 operating systems.   The 16-bit version was built with Borland C++ 4.00, while the 32-bit version was built with Microsoft Visual C++ 4.1.   The first 16-bit version was released on October 18, 1995 as version 1.0; the first 32-bit version was released on May 12, 1996 as version 1.23 (to be synchronized with the the 16-bit version).

An Ultra 486DX266 with 24MB of RAM is used to develop CurveExpert.   Storage equipment includes a 800MB Maxtor hard drive and a 120MB 1/4" tape drive.   Multimedia extensions are a 4X Sony CSD-760E CDROM and Turtle Beach Monte Carlo 16-bit sound card.

Registration Form

Of course, as all shareware emphasizes, this is not free software.   If you would like to continue to use CurveExpert, please register!   Be sure to read over the benefits of registering to find out extra items that are available for registered users.   If you are interested in a site license, please contact the author directly for pricing information. Press **Print** to obtain a hardcopy of this order form.

For information on how to order by credit card, click HERE!

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Note for Students:

Unfortunately, things will get too complex if I allow students to register at the reduced price through PsL. So, if you are a student and want to register at the reduced rate, you will have to fill out the order form and mail it directly to the address shown on the registration form.   You will not be able to register using a credit card.   This is the only difference in support between reduced-price and full-price customers.

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Benefits of Registering

If you like this program and find it useful, please support it by registering this software. This will entitle you to several benefits:

Support

Registration will entitle you to telephone, FAX, and email support.   As I have stated several times, I am committed to giving the best support possible -- but at the same time, I can't afford to spend hours on the phone or answering email from everyone who even looks at this package.   So, for support, please register !

If you want to see additional features in CurveExpert, please register your software. I will be glad to try to implement features that are suggested; however, this obviously can't be done for every idea that comes across the table.   If you are registered, I will definitely give more time and thought to your needs and/or wants.   Also, this project will likely take the back burner to more important things if it is not supported by the user base.

Extra Features

This one is obvious, but the registered version will have your name on the opening screen and in the About box instead of the disconcerting "UNREGISTERED EVALUATION COPY."   See the **It's Just the Right Thing to Do** section below.

CurveExpert uses double-precision floating point numbers to do all calculations. The registered version of CurveExpert comes with two executables: one version using single-precision calculations (seven sig figs), and the second using double-precision (15 sig figs).   Using a single-precision (theoretically) greatly speeds up performance at the cost of accuracy. Tests of the two versions have shown that, in practice, the single-precision package is actually slower than the double-precision package for moderate data sets.   This difference can be attributed to the fact that more precise calculations can improve computational algorithm performance (i.e., fewer iterations to convergence).   Note, however, that with extremely large data sets, the single-precision version should provide a speed and memory advantage.   That also brings up a valid point: using the single-precision representation slices memory usage in half.   By registering, you can make the choice of which version to use yourself.   You may check what type of data representation is being used by CurveExpert by selecting Help|About.

Upgrades

All minor upgrades will be provided free; only a shipping and handling charge will be assessed.   In addition, major upgrades will be priced at the difference between the price you paid for the original version and the new price of the software.   For example, if you register this software now for $35 and CurveExpert 2.0 is priced at $40, an upgrade for you will cost $5 plus shipping and handling. So, register!

[Definition: minor upgrades are an increment in the minor version number, i.e. 1.1 -> 1.2.   Minor upgrades consist of bug fixes, interface modifications, and small feature additions. Major upgrades are increments in the major version number, i.e. 1.5->2.0.   Major upgrades will contain major new enhancements and features over the previous version.]

It's Just the Right Thing to Do

More to the point, though, registration will make you feel good and ease the conscience. I have not infested the program with nagging registration notices or crippled it in any way, so that you get a true indicator of the ability of this package. I trust you to support CurveExpert and the shareware concept if you use this package.

I can definitely see a pattern here...follow the colored words!