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Nonlinear Curve Fitting: Fit Plot

Creating a Fit Plot

Nonlinear least squares data fitting can be performed using Fit Plot. To create a Fit Plot, select your X and Y columns in Table, then select `Table → Create Fit Plot` in main menu, or use the same item in Table context menu, or use `Create Fit Plot` button in the toolbar.
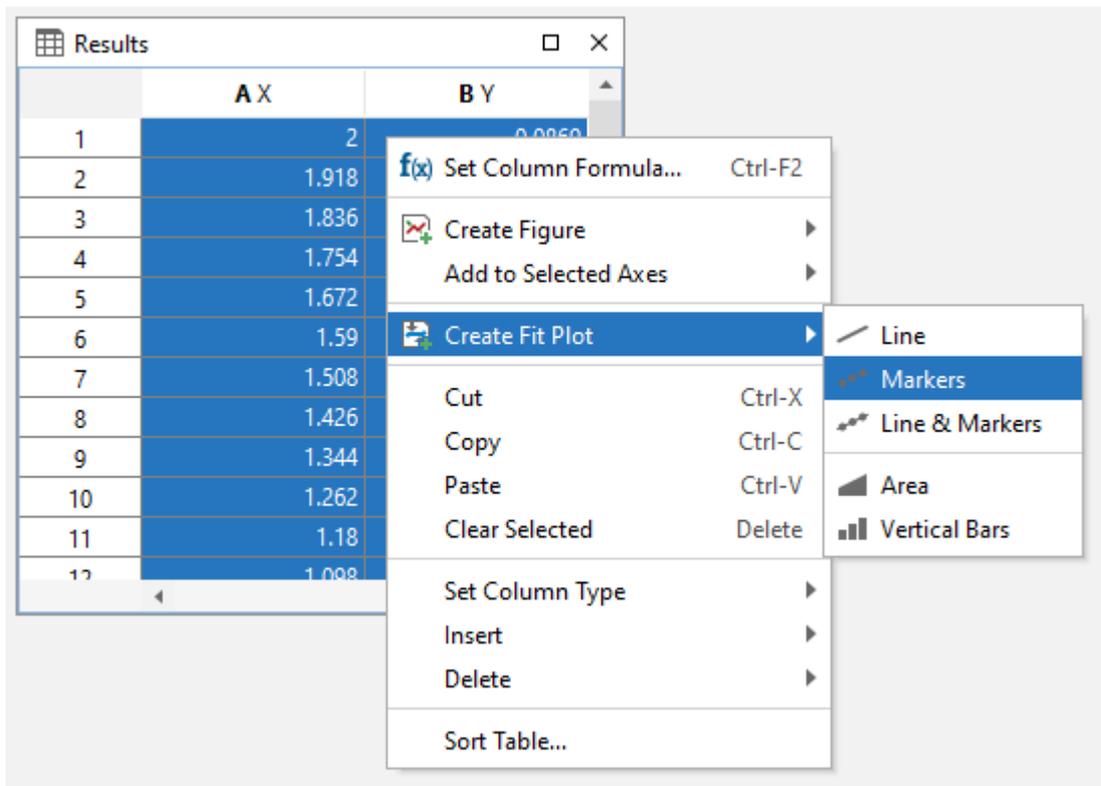
Fitting Methodology

'Nonlinear' means here that analytical fitting function depends nonlinearly on varying parameters (fit parameters). Fit procedure iteratively varies the parameters of fit function to minimize the residual sum of squares. Nonlinear fitting algorithm needs the user to set the initial values of fit parameters.

To fit the data, implement these steps:

1. Create a Fit Plot, specify Y errors in Fit Plot properties, if any
2. Specify fit function by adding Fit Curves
3. Specify initial values of fit parameters (drag curves or enter accurate values)
4. Specify used X data interval
5. Run fitting

Further reading

This manual does not completely cover the complex nonlinear fitting methodology. We recommend you to take a look at this book:

- H. Motulsky and A. Christopoulos, *Fitting Models to Biological Data Using Linear and Nonlinear Regression: A Practical Guide to Curve Fitting.* 2003, GraphPad Software Inc., San Diego CA, graphpad.com. PDF is available for free here.
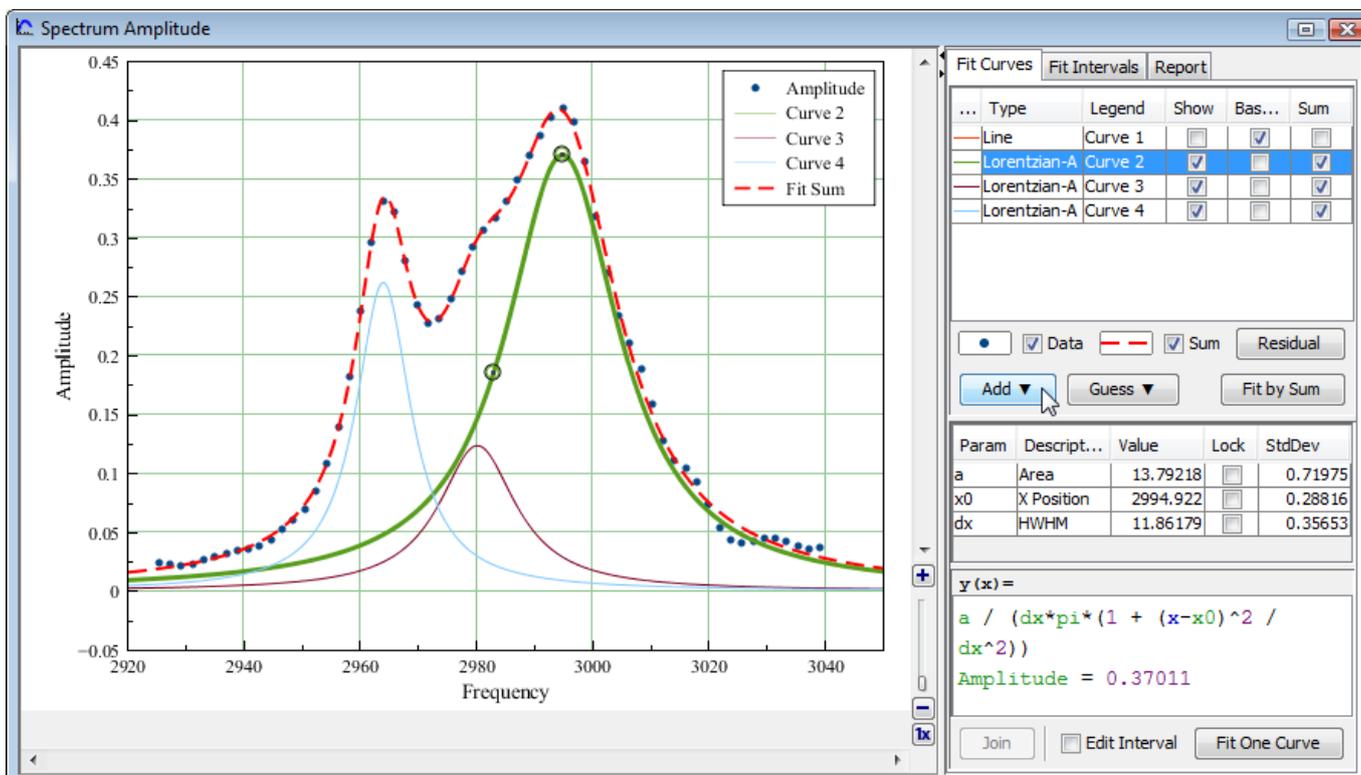
Fit Function is a Sum of Fit Curves

MagicPlot considers fit function as a **sum** of Fit Curves. Ordinarily in peaks fitting each Fit Curve corresponds to one peak in experimental data. Click the Add button to add new Fit Curve to the list. There is a number of predefined Fit Curves types (Line, Parabola, Gauss, Lorentz, etc.) You can also create a Custom Equation Fit Curve and manually enter the formula (Pro edition only). Baseline fitting components may be added to the fitting sum, too.

Fit Plot window contains the list of Fit Curves. Each Fit Curve in the list has three checkboxes:

- Show: Specifies whether to show this Fit Curve on plot. Active only if Baseline checkbox is not set
- `Baseline`: Toggles the subtracting of this Fit Curve from experimental data. You also can use `Residual` button to subtract all Fit Sum from data

- Sum: Specifies whether to use this Fit Curve in sum fit function

Below the Fit Curves list is a parameters table which shows names, values, and descriptions of parameters relating to selected Fit Curve.

Copying and Pasting Fit Curves

You can copy and paste Fit Curves from one Fit Plot to another Fit Plot or Figure. You can also paste the copied Fit Curves to the same Fit Plot to create a copy.

- The copy of Fit Curves with the same parameters and styles will be created if you paste Fit Curves to a Fit Plot.
- A link to the source Fit Curves will be inserted if you paste Fit Curves in a Figure.

Setting Initial Values of Parameters

Nonlinear fitting assumes that certain initial values of parameters are set before fitting. This procedure is very easy if you use Fit Curves of predefined types (not custom equation): you can drag curves on plot. Initial parameters values for each Fit Curve can also be set in parameter table.
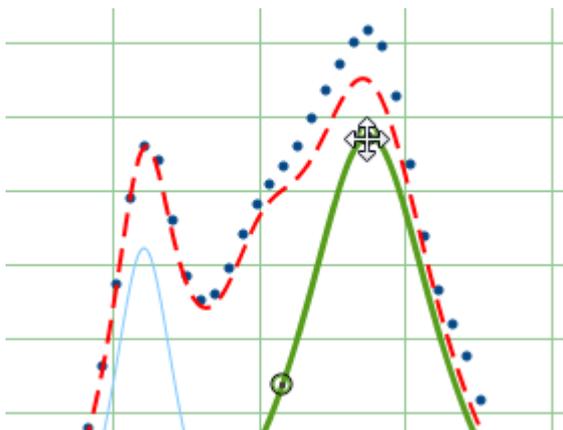
Adjusting Parameters with Mouse Wheel

You can adjust Parameters in table using mouse wheel scrolling when mouse cursor is located under desired parameter: Hold Ctrl key (Cmd key on Mac) and scroll. If Shift key is also pressed the parameter step for one wheel 'click' will be increased.

Parameter Locking

You can lock parameter(s) to prevent varying this parameter during fit and to prevent its changing due to setting initial values by mouse dragging (for built-in functions). Set the checkbox in `Lock` column in parameters list to lock parameter.

Param	Description	Value	Lock	StdDev
a	Area	12.58158	☐	0.71975
x0	X Position	2994.922	☑	0.28816
dx	HWHM	11.86179	☐	0.35653

Joining the Parameters of Fit Curves

MagicPlot allows joining (sometimes referred to as coupling, binding, linking) of fit parameters of different Fit Curves. See Joining the Parameters of Fit Curves for details.

Weighting of Data Points Using Y Errors

MagicPlot allows data point weighting with Y errors. You can specify Y error data in Fit Plot properties dialog. If no Y error data is specified weighting is not used. Weights are calculated as $1 \, / \, Y_{error}^2$ for every point. See Fitting Algorithm and Computational Formulas for details.

Weights must be positive and finite for all points so the Y error values must be positive and non-zero (to prevent infinite weights). MagicPlot checks this condition before fitting and shows an error message if Y errors cannot be used to compute weights.
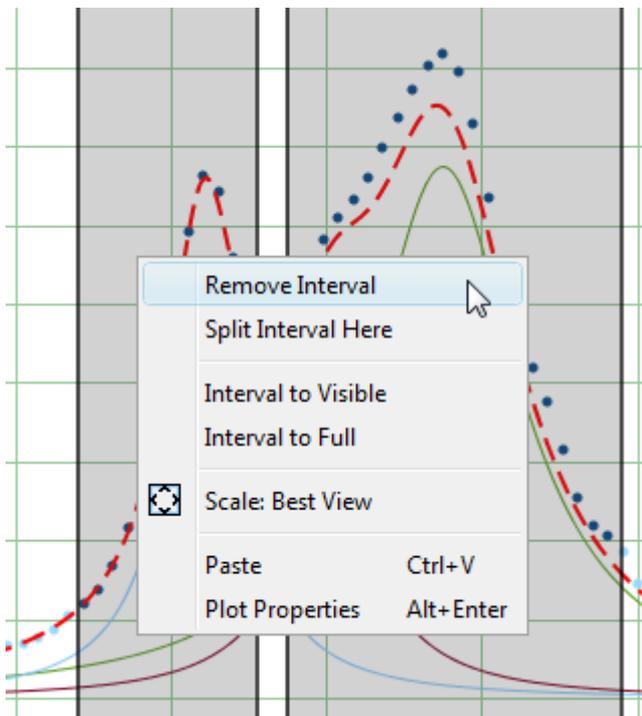
Specifying Fit Intervals

You can set the X intervals of the data which will be used for fitting. Data points outside these intervals are not used to compute the minimizing residual sum of squares. You can use this feature if some data points (especially in the beginning or the end) are inaccurate, e.g. noisy.

Select `Fit Interval` tab to set intervals visually or edit accurate borders values:

- Double click on interval to split it
- Drag the interval border to move it. If intervals intersect, they will be merged
- Use context menu on the plot to create, delete and split intervals

Note: This data intervals are used for fitting Sum only. To set data intervals for the one Curve fitting use `Edit Interval` checkbox.

Baseline Fitting and Extraction

Fit Interval is also usable when baseline fitting. Before baseline fitting you can specify the interval which does not contain any signal points and contains baseline only. Set `Baseline` checkboxes at baseline Fit Curves after baseline fitting to subtract baseline from data. Then specify the whole interval and fit the data.

Note that if you use data processing (integration, FFT, etc.) on Fit Plot, then the difference between the data and baseline curves (which you do see on the plot) will be processed. You can use this behaviour to exclude baseline from data before integrating, see Integration for more information.

'Data-Baseline' Table Column

The 'Data-Baseline' column is appended to the Table with initial (X and Y) data when you create a Fit Plot. The 'Data-Baseline' column contains the difference between initial Y data and baseline approximation (the sum of Fit Curves for which `Baseline` checkbox is set). It is 'Data-Baseline' column that is actually plotted on Fit Plot as data.

Use 'Data-Baseline' column in Table if you want to process the data without baseline. This column is also used as initial data if you use `Processing` menu when Fit Plot is active.

Viewing the Residual Plot

Residual means here the difference between initial data, baseline function and Fit Sum function. MagicPlot offers two different ways to view the residual:

- Press and hold the `Residual` button. The residual will be shown while button is pressed. You can use either mouse or space key (if button is selected) to hold `Residual` button.
- You can either set `Baseline` checkboxes for all summed Fit Curves to subtract them from data and explore the residual plot

Fitting One Curve

You can use MagicPlot to fit the data with single selected Fit Curve by pressing `Fit One Curve` button. In this case a specific data interval for each Fit Curve is used and the main fitting data interval (from `Fit Interval` tab) is ignored. Select `Edit Interval` checkbox in the bottom of the Fit Plot panel to set specific fit intervals for each Fit Curve.

Because of using individual data interval this method is useful for baseline fitting. In order to fit baseline specify the intervals which does not contain signal (peaks) and contain only noise.
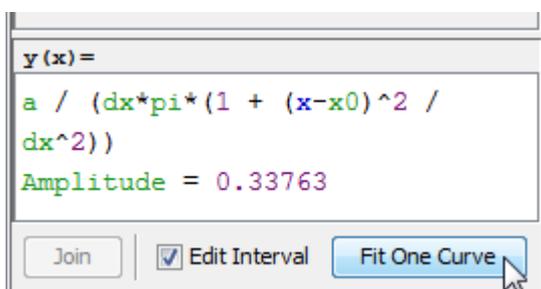
Fit Progress Window

MagicPlot indicates fit process with a special window. Fitting curves are periodically updated on plot while fitting so you can see how fit converges.
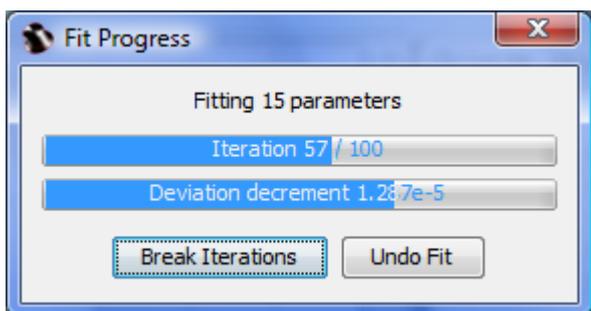
MagicPlot shows current iteration number and deviation decrement with two progress bars while fit is performed. The fit process stops when one of these progress bars reaches the end.

You can see two buttons on fit progress window:

- `Break Iterations`: Breaks iterations after current iteration. Use this button if you suspect that further iterations will not change the result.
- `Undo Fit`: Breaks iterations and reverts fit parameters to their initial (before fit) values. Use this button if you see that fit process converges to wrong result; change initial values of parameters and run fit again.

Undoing Fit

You can undo fit and undo changing initial parameters as usual using Undo function. It is a handy feature when experimenting with different models and initial parameters.

See Also

- Fitting Algorithm and Computational Formulas
- Specifying Custom Fit Equation
- Using Spline for Baseline Subtraction
- Joining the Parameters of Fit Curves
- Guessing Peaks
- Predefined Fit Curves Equations
- transform_xy
- Calculating Integrals and Statistics on Intervals using Fit Plot

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