

Chapter III-8 — Curve Fitting

If the fit has gone far enough and you are satisfied, you can click the Quit button, which finishes the iteration currently under way and then puts the results in the history area as if the fit had completed on its own.

Sometimes you can see that the fit is not working, e.g., when chi-square is not decreasing or when some of the coefficients take on very large nonsense values. You can abort it by pressing the **User Abort Key Combinations**, which discards the results of the fit. You will need to adjust the fitting coefficients and try again.

Initial Guesses

The Levenberg-Marquardt algorithm is used to search for the minimum value of chi-square. Chi-square defines a surface in a multidimensional error space. The search process involves starting with an initial guess at the coefficient values. Starting from the initial guesses, the fit searches for the minimum value by travelling down hill from the starting point on the chi-square surface.

We want to find the deepest valley in the chi-square surface. This is a point on the surface where the coefficient values of the fitting function minimize, in the least-squares sense, the difference between the experimental data and fit data. Some fitting functions may have only one valley. In this case, when the bottom of the valley is found, the best fit has been found. Some functions, however, may have multiple valleys, places where the fit is better than surrounding values, but it may not be the best fit possible.

When the fit finds the bottom of a valley it concludes that the fit is complete even though there may be a deeper valley elsewhere on the surface. Which valley is found first depends on the initial guesses.

For built-in fitting functions, you can automatically set the initial guesses. If this produces unsatisfactory results, you can try manual guesses. For fitting to user-defined functions you must supply manual guesses.

Termination Criteria

A curve fit will terminate after 40 passes in searching for the best fit, but will quit if 9 passes in a row produce no decrease in chi-square. This can happen if the initial guesses are so good that the fit starts at the minimum chi-square. It can also happen if the initial guesses are way off or if the function does not fit the data at all.

You can change the 40-pass limit. See the discussion of `V_FitMaxIters` under **Special Variables for Curve Fitting** on page III-232. Usually needing more than 40 passes is a sign of trouble with the fit. See **Identifiability Problems** on page III-226.

Unless you know a great deal about the fitting function and the data, it is unwise to assume that a solution is a good one. In almost all cases you will want to see a graph of the solution to compare the solution with the data. You may also want to look at a graph of the residuals, the differences between the fitted model and the data. Igor makes it easy to do both in most cases.

Errors in Curve Fitting

In certain cases you may encounter a situation in which it is not possible to decide where to go next in searching for the minimum chi-square. This results in a “singular matrix” error. This is discussed under **Singularities in Curve Fitting** on page III-265. **Curve Fitting Troubleshooting** on page III-266 can help you find the solution to the problem.

Data for Curve Fitting

You must have measured values of both the dependent variable (usually called “y”) and the independent variables (usually called “x” especially if there is just one). These are sometimes called the “response variable” and “explanatory variables.” You can do a curve fit to waveform data or to XY data. That is, you can fit data contained in a single wave, with the data values in the wave representing the Y data and the wave’s X scaling representing equally-spaced X data. Or you can fit data from two (or more) waves in which the data values in one wave represent the Y values and the data values in another wave represent the X data. In this case, the data do not need to be equally spaced. In fact, the X data can be in random order.

You can read more about waveform and XY data in Chapter II-5, **Waves**.