

Chapter III-8 — Curve Fitting

In the absence of the /XR flag, initial guesses for the adjustments to the independent variable values are set to zero. This is usually appropriate; in areas where the fitting function is largely vertical, you may need nonzero guesses to fit successfully. One example of such a situation would be the region near a singularity.

Holding Independent Variable Adjustments

In some cases you may have reason to believe that you know some input values of the independent variables are exact (or nearly so) and should not be adjusted. To specify which values should not be adjusted, you supply X hold waves, one for each independent variable, via the /XHLD flag. These waves should be filled with zeroes corresponding to values that should be adjusted, or ones for values that should be held.

This is similar to the /H flag to hold fit coefficients at a set value during fitting. However, in the case of ODR fitting and the independent variable values, holds are specified by a wave instead of a string of ones and zeroes. This was done because of the potential for huge numbers of ones and zeroes being required. To save memory, you can use a byte wave for the holds. In the Make Waves dialog, you select Byte 8 Bit from the Type menu. Use the /B flag with the **Make** operation on page V-526.

ODR Fit Results

An ordinary least-squares fit adjusts the fit coefficients and calculates model values for the dependent variable. You can optionally have the fit calculate the residuals — the differences between the model and the dependent variable data.

ODR fitting adjusts both the fit coefficients and the independent variable values when seeking the least orthogonal distance fit. In addition to the residuals in the dependent variable, it can calculate and return to you a wave or waves containing the residuals in the independent variables, as well as a wave containing the adjusted values of the independent variable.

Residuals in the independent variable are returned via waves specified by the /XR flag. Note that the contents of these waves are inputs for initial guesses at the adjustments to the independent variables, so you must be careful — in most cases you will want to set the waves to zero before fitting.

The adjusted independent variable values are placed into waves you specify via the /XD flag.

Note that if you ask for an auto-destination wave (/D flag; see **The Destination Wave** on page III-196) the result is a wave containing model values at a set of evenly-spaced values of the independent variables. This wave will also be generated in response to the /D flag for ODR fitting.

You can also specify a specific wave to receive the model values (/D=wave). The values are calculated at the values of the independent variables that you supply as input to the fit. In the case of ODR fitting, to make a graph of the model, the appropriate X wave would be the output from the /XD flag, not the input X values.

Constraints and ODR Fitting

When fitting with the ordinary least-squares method (/ODR=0) you can provide a text wave containing constraint expressions that will keep the fit coefficients within bounds. These expressions can be used to apply simple bound constraints (keeping the value of a fit coefficient greater than or less than some value) or to apply bounds on linear combinations of the fit coefficients (constrain $a+b>1$, for instance).

When fitting using ODR (/ODR=1 or more) only simple bound constraints are supported.

Error Estimates from ODR Fitting

In a curve fit, the output includes an estimate of the errors in the fit coefficients. These estimates are computed from the linearized quadratic approximation to the chi-square surface at the solution. For a linear fit (line, poly, and poly2D fit functions) done by ordinary least squares, the chi-square surface is actually quadratic and the estimates are exact if the measurement errors are normally distributed with zero mean and constant variance. If the fitting function is nonlinear in the fit coefficients, then the error estimates are an approximation. The quality of the approximation will depend on the nature of the nonlinearity.