

## Chapter III-8 — Curve Fitting

### *Severe Constraint Conflict*

Although the method used for applying the constraints can find a solution even when constraints conflict with each other (are infeasible), it is possible to have a conflict that is so bad that the method fails. This will result in a singular matrix error.

### *Constraint Region is a Poor Fit*

It is possible that the region of coefficient space allowed by the constraints is such a bad fit to the data that a singular matrix error results.

### *Initial Guesses Far Outside the Constraint Region*

Usually if the initial guesses for a fit lie outside the region allowed by the constraints, the fit coefficients will shift into the constraint region on the first iteration. It is possible, however, for initial guesses to be so far from the constraint region that the solution to the constraints fails. This will cause the usual singular matrix error.

### *Constraints Conflict with a Held Parameter*

You cannot hold a parameter and apply a constraint to the same parameter. Thus, this is not allowed:

```
Make/T CWave="K1 > 5"  
FuncFit/H="01" myFunc, myCoefs, myData /C=CWave
```

## NaNs and INFs in Curve Fits

Curve fits ignore NaNs and INFs in the input data. This is a convenient way to eliminate individual data values from a fit. A better way is to use a data mask wave (see **Using a Mask Wave** on page III-198).

## Special Variables for Curve Fitting

There are a number of special variables used for curve fitting input (to provide additional control of the fit) and for output (to provide additional statistics). Knowledgeable users can use the input variables to tweak the fitting process. However, this is usually not needed. Some output variables help users knowledgeable in statistics to evaluate the quality of a curve fit.

To use an input variable interactively, create it from the command line using the Variable operation before performing the fit.

Most of the output variables are automatically created by the CurveFit or FuncFit operations. Some, as indicated below, are not automatically created; you must create them yourself if you want the information they provide.

If you are fitting using a procedure, both the input and output variables can be local or global. It is best to make them local. See **Accessing Variables Used by Igor Operations** on page IV-123 for information on how to use local variables. In procedures, output-only variables are always as local variables.

If you perform a curve fit interactively via the command line or via the Curve Fitting dialog, the variables will be global. If you use multiple data folders (described in Chapter II-8, **Data Folders**), you need to remember that input and output variables are searched for or created in the current data folder.

The following table lists all of the input and output special variables. Some variables are discussed in more detail in sections following the table.

Variable	I/O	Meaning
V_FitOptions	Input	Miscellaneous options for curve fit.
V_FitTol	Input	Normally, an iterative fit terminates when the fractional decrease of chi-square from one iteration to the next is less than 0.001. If you create a global variable named V_FitTol and set it to a value between 1E-10 and 0.1 then that value will be used as the termination tolerance. Values outside that range will have no effect.
V_tol	Input	(poly fit only) The “singular value threshold”. See <b>Special Considerations for Polynomial Fits</b> on page III-265.
V_chisq	Output	A measure of the goodness of fit. It has absolute meaning only if you’ve specified a weighting wave containing the reciprocal of the standard error for each data point.
V_q	Output	(line fit only) A measure of the believability of chi-square. Valid only if you specified a weighting wave.
V_siga, V_sigb	Output	(line fit only) The probable uncertainties of the intercept ( $K_0 = a$ ) and slope ( $K_1 = b$ ) coefficients for a straight-line fit (to $y = a + bx$ ).
V_Rab	Output	(line fit only) The coefficient of correlation between the uncertainty in a (the intercept, $K_0$ ) and the uncertainty in b (the slope, $K_1$ ).
V_Pr	Output	(line fit only) The linear correlation coefficient r (also called Pearson’s r). Values of +1 or -1 indicate complete correlation while values near zero indicate no correlation.
V_r2	Output	(line fit only) The coefficient of determination, usually called simply "r-squared". See <b>Coefficient of Determination or R-Squared</b> on page III-221 for details.
V_npnts	Output	The number of points that were fitted. If you specified a weighting wave then points whose weighting was zero are not included in this count. Also not included are points whose values are NaN or INF.
V_nterms	Output	The number of coefficients in the fit.
V_nheld	Output	The number of coefficients held constant during the fit.
V_numNaNs	Output	The number of NaN values in the fit data. NaNs are ignored during a curve fit.
V_numINFs	Output	The number of INF values in the fit data. INFs are ignored during a curve fit.
V_FitError	Input/ Output	Used from a procedure to attempt to recover from errors during the fit.
V_FitQuitReason	Output	Provides additional information about why a nonlinear fit stopped iterating.  You must create this variable; it is not automatically created.
V_FitIterStart	Output	Use of V_FitIterStart is obsolete; use all-at-once fit functions instead. See <b>All-At-Once Fitting Functions</b> on page III-256 for details.  Set to 1 when an iteration starts. Identifies when the user-defined fitting function is called for the first time for a particular iteration.  You must create this variable; it is not automatically created.