

```

while(1)
End

```

This function is very limited. It simply does fits to a number of waves in a list. Igor includes a package that adds a great deal of sophistication to batch fitting, and provides a user interface. For a demonstration, choose File→Example Experiments→Curve Fitting→Batch Curve Fitting Demo.

Curve Fitting Examples

The Igor Pro Folder includes a number of example experiments that demonstrate the capabilities of curve fitting. These examples cover fitting with constraints, multivariate fitting, multipeak fitting, global fitting, fitting a line between cursors, and fitting to a user-defined function. All of these experiments can be found in Igor Pro Folder/Examples/Curve Fitting.

Singularities in Curve Fitting

You may occasionally run across a situation where you see a “singular matrix” error. This means that the system of equations being solved to perform the fit has no unique solution. This generally happens when the fitted curve contains degeneracies, such as if all Y values are equal.

In a fit to a user-defined function, a singular matrix results if one or more of the coefficients has no effect on the function’s return value. Your coefficients wave must have the exact same number of points as the number of coefficients that you actually use in your function or else you must hold constant unused coefficients.

Certain functions may have combinations of coefficients that result in one or more of the coefficients having no effect on the fit. Consider the Gaussian function:

$$K_0 + K_1 \exp((x - K_2)/K_3)^2$$

If K_1 is set to zero, then the following exponential has no effect on the function value. The fit will report which coefficients have no effect. In this example, it will report that K_2 and K_3 have no effect on the fit. However, as this example shows, it is often not the reported coefficients that are at fault.

Special Considerations for Polynomial Fits

Polynomial fits use the singular value decomposition technique. If you encounter singular values and some of the coefficients of the fit have been zeroed, you are probably asking for more terms than can be supported by your data. You should use the smallest number of terms that gives a “reasonable” fit. If your data does not support higher-order terms then you can actually get a poorer fit by including them.

If you really think your data should fit with the number of terms you specified, you can try adjusting the singular value threshold. You do this by creating a special variable called V_tol and setting it to a value smaller than the default value of 1e-10. You might try 1e-15.

Another way to run into trouble during polynomial fitting is to use a range of X values that are very much offset from zero. The solution is to temporarily offset your X values, do the fit and then restore the original X values. This is done for you by the poly_XOffset fit function; see **Built-in Curve Fitting Functions** on page III-206 for details.

Errors Due to X Values with Large Offsets

The single and double exponential fits can be thrown off if you try to fit to a range of X values that are very much offset from zero. In general, any function, which, when extrapolated to zero, returns huge or infinite values, can create problems. The solution is to temporarily offset your x values, perform the fit and then restore the original x values. You may need to perform a bit of algebra to fix up the coefficients.