Do not get carried away trying to find good guesses; the initial conditions are just that, guesses. If you are not sure what the guesses should be, keep the initial conditions non-zero, and at the correct order of magnitude that you might expect (be it 0.001, 1, or 1000).

The initial conditions are entered immediately following the curve fit definition. Place a semicolon at the end of the definition and begin entering the initial guesses, separating each with a semicolon. The table below shows the definitions from the previous section with some sample initial guesses.

Curve Fit Definitions with Initial Guesses
m1 * m0 + m2; m1 = 0.5; m2 = 23
m1 + m2 * m0^m3; m1 = –2; m2 = 3; m3 = 2
m1 + m2 * exp(–m3 * m0); m1 = 5; m2 = 1; m3 = 0.5
m1 * exp(–m2 * m0) * cos(m3 * m0 + m4); m1 = 4; m2 = 0.7; m3 = 2.2; m4 = 15

9.4.3 Curve Fit Definition Dialog

The Curve Fit Definition dialog is used to enter the equation, initial guesses, and allowable error to be used in the curve fit. You can also choose to specify partial derivatives or to weight the data.

This dialog can be displayed using either of the following methods:

- Choose a curve fit from the **General** submenu (**Curve Fit** menu). In the dialog that is displayed, click **Define.**
- Choose **Curve Fit > Edit General.** In the dialog that is displayed, select the name of a curve fit and click **Edit.**

The various features of the Curve Fit Definition dialog are discussed below.

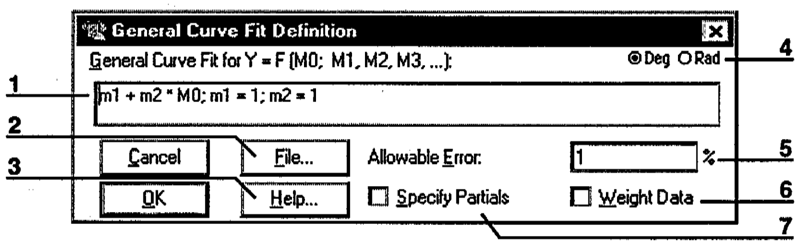

Figure 9-10 Curve Fit Definition dialog

1. **Text Field**
   Curve fit definitions and initial guesses are entered in this area of the dialog.
2. **File...**
   Clicking this button displays a text editor that can be used to create, open, or save a curve fit definition. The definition appears on the first line and any partial derivatives appear on the lines below it.
3. **Help...**
   Click this button to display the Help dialog.

4. **Degrees/Radians Buttons**
   These buttons determine whether the results of trigonometric functions are in degrees or radians.
5. **Allowable Error:**
   The value entered in this field helps KaleidaGraph determine when to stop iterating. Iterations stop if either of the following occurs:
   - Chi Square does not change for a certain number of iterations.
   - The percent change in the normalized Chi Square is less than the Allowable Error.
6. **Weight Data**
   When selected, you can specify a data column that contains weights for the variable you are fitting. These weights should represent the individual errors of the data values. Each weight is used internally as: 1/(weight^2). The smaller the error value, the larger the internal weight. If this check box is not selected, a weight value of 1.0 is used for all data points.
7. **Specify Partials**
   The algorithm that KaleidaGraph uses in calculating each iteration of the General curve fit requires evaluating the partial derivative of the function with respect to each parameter. If **Specify Partials** is not selected, KaleidaGraph numerically approximates the derivative. If this option is selected, the dialog expands, as shown in Figure 9-11.

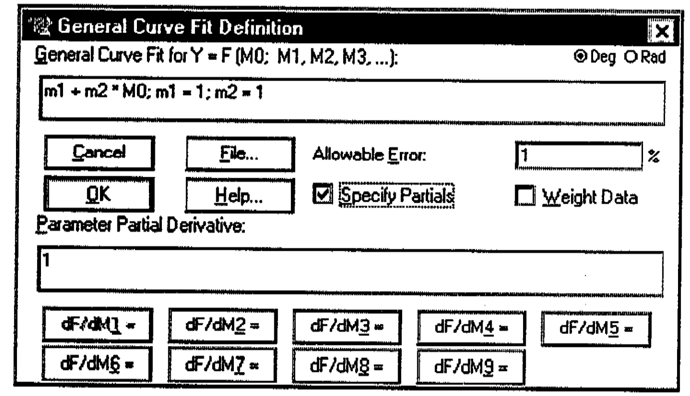

Figure 9-11 Expanded Curve Fit Definition dialog

The nine buttons at the bottom of the dialog allow each partial derivative to be entered in the text field above the buttons. The biggest advantage of specifying the partial derivatives is accuracy. The curve fit algorithm uses these partial derivatives to direct itself where to move after each iteration to find the best solution. In general, sharp deviations in the surface may not be accurately approximated, so the actual partial derivatives are preferred.

You can choose to specify only some of the partial derivatives, but not all of them. It is better to let KaleidaGraph approximate the partial instead of specifying the wrong derivative. If a partial derivative is missing, KaleidaGraph numerically approximates that partial derivative.

D.2 Statistics Equations

n = number of data points
x_i = current data value (from 1 to n)
$\bar{x}$ = mean of the data

Mean

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

RMS (Root Mean Square)

$$\left[\frac{1}{n}\sum_{i=1}^{n} x_i^2\right]^{1/2}$$

Standard Deviation

$$\sqrt{\frac{\sum_{i=1}^{n} x_i^2 - n(\bar{x})^2}{n-1}}$$

Standard Error

$$\frac{\text{Standard Deviation}}{\sqrt{n}}$$

Variance

$$\frac{\sum_{i=1}^{n} x_i^2 - n(\bar{x})^2}{n-1}$$

Skewness

$$\frac{\frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^3}{\left(\frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^2\right)^{3/2}}$$

Kurtosis

$$\frac{\frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^4}{\left(\frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^2\right)^2} - 3$$

D.3 Student t-Test Equations

$\bar{x}$ = mean of the data N = number of data points x_i and y_i = current data value (from 1 to N)

t value (single sample)

$$t = \frac{\bar{x} - \text{Test Value}}{\text{Standard Error}(x)}$$

t value (paired data)

$$t = \frac{\overline{x_A} - \overline{x_B}}{s_D}$$

$$s_D = \sqrt{\frac{Var(x_A) + Var(x_B) - 2Cov(x_A, x_B)}{N}}$$

$$Cov(x_A, x_B) \equiv \frac{1}{N-1}\sum_{i=1}^{N}(x_{A_i} - \overline{x_A})(x_{B_i} - \overline{x_B})$$

t value (unpaired data with equal variance)

$$t = \frac{\overline{x_A} - \overline{x_B}}{s_D}$$

$$s_D = \sqrt{\frac{\sum_{i\in A}(x_i - \overline{x_A})^2 + \sum_{i\in B}(x_i - \overline{x_B})^2}{N_A + N_B - 2}\left(\frac{1}{N_A} + \frac{1}{N_B}\right)}$$

t value (unpaired data with unequal variance)

$$t = \frac{\overline{x_A} - \overline{x_B}}{\sqrt{Var(x_A)/N_A + Var(x_B)/N_B}}$$

Correlation

$$\frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_i (x_i - \bar{x})^2}\sqrt{\sum_i (y_i - \bar{y})^2}}$$

F value

$$\frac{\text{Larger Variance}}{\text{Smaller Variance}}$$

D.4 Curve Fit References

General Curve Fit

Press, W. H., Flannery, B. P., Teukolsky, S. A., and Vetterling, W. T. *Numerical Recipes in C*. Cambridge University Press, New York (1988).

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Beyer, W. H. *Standard Mathematical Tables*. CRC Press, Cleveland (1976).

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Stineman, R. W. A consistently well-behaved method of interpolation. *Creative Computing*, July (1980).

Weighted Curve Fit

Chambers, J. M., Cleveland, W. S., Kleiner, B., and Tukey, P. A. *Graphical Methods for Data Analysis*. Duxbury Press, Boston (1983).