Straight-line fit

The following is a recipe for fitting a straight-line to data *analytically*, i.e. without an iterative fitting procedure. The references are P. Bevington ”Data Reduction and Error Analysis for the Physical Sciences”and Particle Data Book 2000.

1 Straight line fit - unweighted

Fitting data to a straight-line, $y(x) = \alpha_1 + \alpha_2 x$, for independent measurements y_i with *equal variance* σ_y^2, one obtains the following estimates of α_1 and α_2:

$$\hat{\alpha_1} = (g_1\Lambda_{22} - g_2\Lambda_{12})/\Delta, \tag{1}$$

$$\hat{\alpha_2} = (g_2\Lambda_{11} - g_1\Lambda_{12})/\Delta, \tag{2}$$

where

$$(\Lambda_{11}, \Lambda_{12}, \Lambda_{22}) = \sum(1, x_i, x_i^2), \tag{3}$$

$$(g_1, g_2) = \sum(1, x_i)y_i, \tag{4}$$

respectively, and

$$\Delta = \Lambda_{11}\Lambda_{22} - \Lambda_{12}^2. \tag{5}$$

The covariance matrix of the fitted parameters is:

$$\begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} = \frac{\sigma_y^2}{\Delta}\begin{pmatrix} \Lambda_{22} & -\Lambda_{12} \\ -\Lambda_{21} & \Lambda_{11} \end{pmatrix} \tag{6}$$

The estimated variance of an interpolated or extrapolated value of y at point x is:

$$(y - y_{\mathrm{true}})^2 = \frac{1}{\Lambda_{11}} + \frac{\Lambda_{11}}{\Delta}\left(x - \frac{\Lambda_{12}}{\Lambda_{11}}\right)^2. \tag{7}$$

2 Straight line fit - weighted

If the independent measurements y_i have individual variances $\sigma_{y_i}^2$, a weighted straight-line fit is represented by the following estimates of α_1 and α_2,

$$\hat{\alpha_1} = (g_1\Lambda_{22} - g_2\Lambda_{12})/\Delta, \tag{8}$$

$$\hat{\alpha_2} = (g_2\Lambda_{11} - g_1\Lambda_{12})/\Delta, \tag{9}$$

where

$$(\Lambda_{11}, \Lambda_{12}, \Lambda_{22}) = \sum(1, x_i, x_i^2)/\sigma_i^2, \tag{10}$$

$$(g_1, g_2) = \sum(1, x_i)y_i/\sigma_i^2, \tag{11}$$

respectively, and

$$\Delta = \Lambda_{11}\Lambda_{22} - \Lambda_{12}^2. \tag{12}$$

The covariance matrix of the fitted parameters is:

$$\begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} = \frac{1}{\Delta} \begin{pmatrix} \Lambda_{22} & -\Lambda_{12} \\ -\Lambda_{21} & \Lambda_{11} \end{pmatrix} \tag{13}$$

The estimated variance of an interpolated or extrapolated value of y at point x is:

$$(y - y_{\text{true}})^2 = \frac{1}{\Lambda_{11}} + \frac{\Lambda_{11}}{\Delta} \left(x - \frac{\Lambda_{12}}{\Lambda_{11}} \right)^2 . \tag{14}$$