Fitting by the Method of Least Squares

When fitting any function to a set of data, one tries to find a model with parameters that can minimize the 'distance' between the data points and the function.

Consider a function $f(x)$ and a set of measurements consisting of x_i and y_i values and an uncertainty δy_i in each measured y_i . The 'distance' between a data point and the function is given by the residual

$$y_i - f(x_i) \ .$$

A measure of how close the function is to the data overall is given by

$$\chi^2 = \frac{1}{N} \sum_i [y_i - f(x_i)]^2 \ .$$

The equation for χ^2 given above is used when the uncertainty in the data points δy_i is unknown. If the uncertainties are known, and especially if they are unequal, a weighted χ^2 is used:

$$\chi^2 = \frac{1}{N} \sum_i \left[\frac{y_i - f(x_i)}{\delta y_i}\right]^2 \ .$$

For either of these options, the method of least squares means finding a function with parameters that minimize χ^2. For instance, if you are fitting a straight line with the form $(x) = mx + b$, you would vary the parameters m and b until you find the minimum χ^2. The fit can be done iteratively, by trial and error, or using more sophisticated minimization techniques.

For the special case of fitting to straight lines, there are analytical solutions for the parameters that can be calculated directly. For instance, if you are fitting $f(x) = mx$ to a set of data, you want to find the value of m that minimizes χ^2. This can be done by taking a derivative and setting it to zero.

$$\frac{\partial}{\partial m} \chi^2 = 0 \ .$$

Using the unweighted version of χ^2, this can be solved as follows.

$$\frac{\partial}{\partial m}\frac{1}{N}\sum_{\mathrm{i}}[\mathrm{y_i} - \mathrm{mx_i}]^2 = 0$$

$$\frac{\partial}{\partial m}\frac{1}{N}\sum_{\mathrm{i}}[\mathrm{y_i^2} - 2\mathrm{mx_iy_i} + \mathrm{m^2x_i^2}] = 0$$

$$\frac{1}{N}\sum_{\mathrm{i}}[-2\mathrm{x_iy_i} + 2\mathrm{mx_i^2}] = 0$$

$$\sum_{\mathrm{i}}\mathrm{x_iy_i} = \sum_{\mathrm{i}}\mathrm{mx_i^2}$$

$$\mathrm{m} = \frac{\sum_{\mathrm{i}}\mathrm{x_iy_i}}{\sum_{\mathrm{i}}\mathrm{x_i^2}}$$

The uncertainty for this special case of an unweighted fit to $f(x) = mx$ is

$$\delta\mathrm{m} = \sqrt{\frac{\frac{1}{N}\sum_i[y_i - f(x_i)]^2}{\sum_{\mathrm{i}}\mathrm{x_i^2}}}$$

The solutions for two other special cases involving weighted fits are given in the next two pages.

Weighted fit to a line with zero intercept (1 parameter fit)

The solution for a weighted fit to the model $y = mx$ is

$$m = \frac{1}{\Delta} \sum_i \frac{x_i y_i}{\delta y_i^2}$$

where

$$\Delta = \sum_i \frac{x_i^2}{\delta y_i^2} \quad .$$

The uncertainty in the slope is given by

$$\delta m = \sqrt{\frac{1}{\Delta}} \quad .$$

Weighted fit to a line with a non-zero intercept (2 parameters)

The solution for a weighted fit to the model $y = mx + b$ is

$$m = \frac{1}{\Delta}\left(\sum_i \frac{1}{\delta y_i^2} \cdot \sum_i \frac{x_i y_i}{\delta y_i^2} - \sum_i \frac{x_i}{\delta y_i^2} \cdot \sum_i \frac{y_i}{\delta y_i^2}\right)$$

and

$$b = \frac{1}{\Delta}\left(\sum_i \frac{x_i^2}{\delta y_i^2} \cdot \sum_i \frac{y_i}{\delta y_i^2} - \sum_i \frac{x_i}{\delta y_i^2} \cdot \sum_i \frac{x_i y_i}{\delta y_i^2}\right)$$

where

$$\Delta = \sum_i \frac{1}{\delta y_i^2} \cdot \sum_i \frac{x_i^2}{\delta y_i^2} - \left(\sum_i \frac{x_i}{\delta y_i^2}\right)^2 .$$

The uncertainties in the fit parameters are given by

$$\delta m = \sqrt{\frac{1}{\Delta} \sum_i \frac{1}{\delta y_i^2}}$$

and

$$\delta b = \sqrt{\frac{1}{\Delta} \sum_i \frac{x_i^2}{\delta y_i^2}} .$$