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Least Squares Fitting

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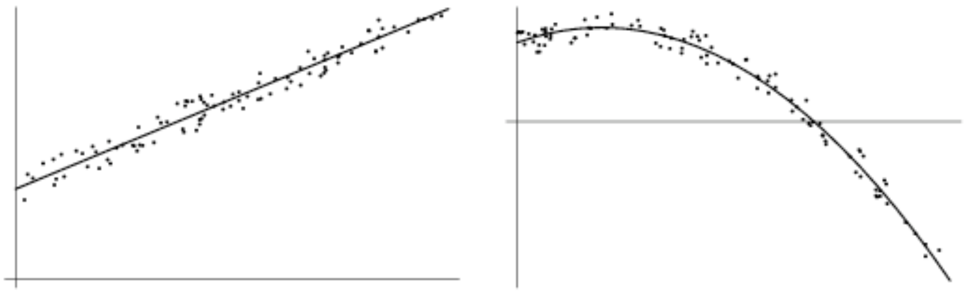
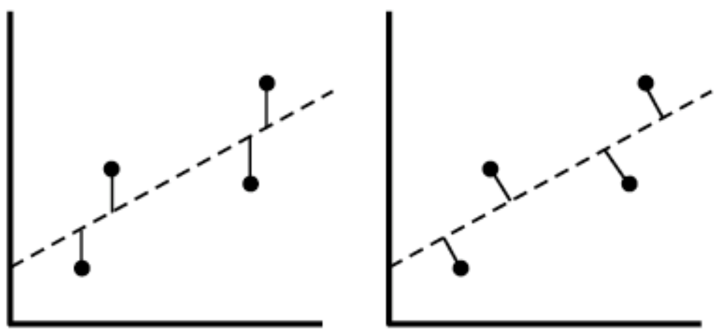


A mathematical procedure for finding the best-fitting curve to a given set of points by minimizing the sum of the squares of the offsets ("the residuals") of the points from the curve. The sum of the *squares* of the offsets is used instead of the offset absolute values because this allows the residuals to be treated as a continuous differentiable quantity. However, because squares of the offsets are used, outlying points can have a disproportionate effect on the fit, a property which may or may not be desirable depending on the problem at hand.



In practice, the *vertical* offsets from a line (polynomial, surface, hyperplane, etc.) are almost always minimized instead of the perpendicular offsets. This provides a fitting function for the independent variable X that estimates y for a given x (most often what an experimenter wants), allows uncertainties of the data points along the x- and y-axes to be incorporated simply, and also provides a much simpler analytic form for the fitting parameters than would be obtained using a fit based on perpendicular offsets. In addition, the fitting technique can be easily generalized from a best-fit *line* to a best-fit *polynomial* when sums of vertical distances are used. In any case, for a reasonable number of noisy data points, the difference between vertical and perpendicular fits is quite small.

The *linear* least squares fitting technique is the simplest and most commonly applied form of linear regression and provides a solution to the problem of finding the best fitting *straight* line through a set of points. In fact, if the functional relationship between the two quantities being graphed is known to within additive or multiplicative constants, it is common practice to transform the data in such a way that the resulting line *is* a straight line, say by plotting T vs. $\sqrt{\ell}$ instead of T vs. ℓ in the case of analyzing the period T of a pendulum as a function of its length l. For this reason, standard forms for exponential, logarithmic, and power laws are often explicitly computed. The formulas for linear least squares fitting were independently derived by Gauss and Legendre.

For nonlinear least squares fitting to a number of unknown parameters, linear least squares fitting may be applied iteratively to a linearized form of the function until convergence is achieved. However, it is often also possible to linearize a nonlinear function at the outset and still use linear methods for determining fit parameters without resorting to iterative procedures. This approach does commonly violate the implicit assumption that the distribution of errors is normal, but often still gives acceptable results using normal equations, a pseudoinverse, etc. Depending on the type of fit and initial parameters chosen, the nonlinear fit may have good or poor convergence properties. If uncertainties (in the most general case, error ellipses) are given for the points, points can be weighted differently in order to give the high-quality points more weight.

Vertical least squares fitting proceeds by finding the sum of the *squares* of the *vertical* deviations R^2 of a set of n data points

$$R^2 \equiv \sum [y_i - f(x_i, a_1, a_2, \ldots, a_n)]^2 \tag{1}$$

from a function f. Note that this procedure does *not* minimize the actual deviations from the line (which would be measured perpendicular to the given function). In addition, although the *unsquared* sum of distances might seem a more appropriate quantity to minimize, use of the absolute value results in discontinuous derivatives which cannot be treated analytically. The square deviations from each point are therefore summed, and the resulting residual is then minimized to find the best fit line. This procedure results in outlying points being given disproportionately large weighting.

The condition for R^2 to be a minimum is that

$$\frac{\partial(R^2)}{\partial a_i} = 0 \tag{2}$$

for $i = 1, \ldots, n$. For a linear fit,

$$f(a, b) = a + b\,x, \tag{3}$$

so

$$R^2(a, b) \equiv \sum_{i=1}^{n} [y_i - (a + b\,x_i)]^2 \tag{4}$$

$$\frac{\partial(R^2)}{\partial a} = -2 \sum_{i=1}^{n} [y_i - (a + b\,x_i)] = 0 \tag{5}$$

$$\frac{\partial(R^2)}{\partial b} = -2 \sum_{i=1}^{n} [y_i - (a + b\,x_i)]\,x_i = 0. \tag{6}$$

These lead to the equations

$$n\,a + b \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i \tag{7}$$

$$a \sum_{i=1}^{n} x_i + b \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i\,y_i. \tag{8}$$

In matrix form,

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i\,y_i \end{bmatrix}, \tag{9}$$

so

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i\, y_i \end{bmatrix}. \tag{10}$$

The 2×2 matrix inverse is

$$\begin{bmatrix} a \\ b \end{bmatrix} = \frac{1}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \begin{bmatrix} \sum_{i=1}^{n} y_i \sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i\, y_i \\ n \sum_{i=1}^{n} x_i\, y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i \end{bmatrix}, \tag{11}$$

so

$$a = \frac{\sum_{i=1}^{n} y_i \sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i\, y_i}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \tag{12}$$

$$= \frac{\bar{y}\left(\sum_{i=1}^{n} x_i^2\right) - \bar{x} \sum_{i=1}^{n} x_i\, y_i}{\sum_{i=1}^{n} x_i^2 - n\, \bar{x}^2} \tag{13}$$

$$b = \frac{n \sum_{i=1}^{n} x_i\, y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \tag{14}$$

$$= \frac{\left(\sum_{i=1}^{n} x_i\, y_i\right) - n\, \bar{x}\, \bar{y}}{\sum_{i=1}^{n} x_i^2 - n\, \bar{x}^2} \tag{15}$$

(Kenney and Keeping 1962). These can be rewritten in a simpler form by defining the sums of squares

$$\mathrm{ss}_{x\,x} = \sum_{i=1}^{n} (x_i - \bar{x})^2 \tag{16}$$

$$= \left(\sum_{i=1}^{n} x_i^2\right) - n\, \bar{x}^2 \tag{17}$$

$$\mathrm{ss}_{y\,y} = \sum_{i=1}^{n} (y_i - \bar{y})^2 \tag{18}$$

$$= \left(\sum_{i=1}^{n} y_i^2\right) - n\, \bar{y}^2 \tag{19}$$

$$\mathrm{ss}_{x\,y} = \sum_{i=1}^{n} (x_i - \bar{x})\, (y_i - \bar{y}) \tag{20}$$

$$= \left(\sum_{i=1}^{n} x_i\, y_i\right) - n\, \bar{x}\, \bar{y}, \tag{21}$$

which are also written as

$$\sigma_x^2 = \frac{\mathrm{ss}_{x\,x}}{n} \tag{22}$$

$$\sigma_y^2 = \frac{\mathrm{ss}_{y\,y}}{n} \tag{23}$$

$$\mathrm{cov}\,(x,\, y) = \frac{\mathrm{ss}_{x\,y}}{n}. \tag{24}$$

Here, $\mathrm{cov}\,(x,\, y)$ is the covariance and σ_x^2 and σ_y^2 are variances. Note that the quantities $\sum_{i=1}^{n} x_i\, y_i$ and $\sum_{i=1}^{n} x_i^2$ can also be interpreted as the dot products

$$\sum_{i=1}^{n} x_i^2 = \mathbf{x} \cdot \mathbf{x} \tag{25}$$

$$\sum_{i=1}^{n} x_i \, y_i = \mathbf{x} \cdot \mathbf{y}. \tag{26}$$

In terms of the sums of squares, the regression coefficient b is given by

$$b = \frac{\operatorname{cov}(x, y)}{\sigma_x^2} = \frac{\mathrm{ss}_{x\,y}}{\mathrm{ss}_{x\,x}}, \tag{27}$$

and a is given in terms of b using (◇) as

$$a = \overline{y} - b\,\overline{x}. \tag{28}$$

The overall quality of the fit is then parameterized in terms of a quantity known as the correlation coefficient, defined by

$$r^2 = \frac{\mathrm{ss}_{x\,y}^2}{\mathrm{ss}_{x\,x}\,\mathrm{ss}_{y\,y}}, \tag{29}$$

which gives the proportion of $\mathrm{ss}_{y\,y}$ which is accounted for by the regression.

Let $\hat{y}_i$ be the vertical coordinate of the best-fit line with x-coordinate x_i, so

$$\hat{y}_i \equiv a + b\,x_i, \tag{30}$$

then the error between the actual vertical point y_i and the fitted point is given by

$$e_i \equiv y_i - \hat{y}_i. \tag{31}$$

Now define s^2 as an estimator for the variance in e_i,

$$s^2 = \sum_{i=1}^{n} \frac{e_i^2}{n-2}. \tag{32}$$

Then s can be given by

$$s = \sqrt{\frac{\mathrm{ss}_{y\,y} - b\,\mathrm{ss}_{x\,y}}{n-2}} = \sqrt{\frac{\mathrm{ss}_{y\,y} - \frac{\mathrm{ss}_{x\,y}^2}{\mathrm{ss}_{x\,x}}}{n-2}} \tag{33}$$

(Acton 1966, pp. 32-35; Gonick and Smith 1993, pp. 202-204).

The standard errors for a and b are

$$\mathrm{SE}(a) = s\sqrt{\frac{1}{n} + \frac{\overline{x}^2}{\mathrm{ss}_{x\,x}}} \tag{34}$$

$$\mathrm{SE}(b) = \frac{s}{\sqrt{\mathrm{ss}_{x\,x}}}. \tag{35}$$

SEE ALSO: ANOVA, Correlation Coefficient, Interpolation, Least Squares Fitting--Exponential, Least Squares Fitting--Logarithmic, Least Squares Fitting--Perpendicular Offsets, Least Squares Fitting--Polynomial, Least Squares Fitting--Power Law, MANOVA, Matrix 1-Inverse, Moore-Penrose Matrix Inverse, Nonlinear Least Squares Fitting, Pseudoinverse, Regression Coefficient, Residual, Spline. [Pages Linking Here]

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