Linear Least Squares Fitting

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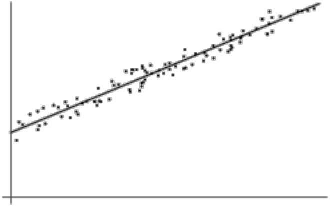
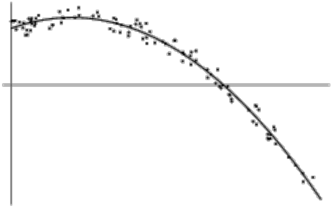
What is Least Squares Fit?

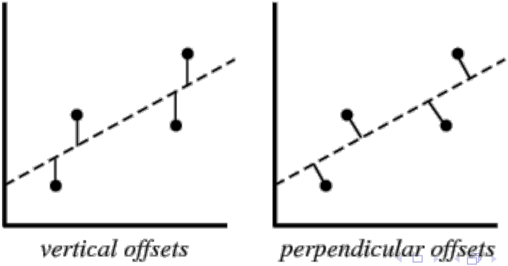
- A procedure for finding the best-fitting curve to a given set of points by minimizing the sum of the squares of the offsets (called residuals) of the points from the curve.
- The sum of the squares of the offsets is used instead of the offset absolute values, to permit the residuals to be treated as a continuous differentiable quantity.
- However, this may cause outlying points to have a disproportionate effect on the fit.





What is Least Squares Fit?

- In practice, vertical offsets from a curve (or surface!) are minimized instead of perpendicular offsets.
- This provides a simpler analytic form for the fitting parameters and when noisy data points are few in number, the difference between vertical and perpendicular fits is quite small.
- Accommodates uncertainties of the data in x and y
- The fitting technique can be easily generalized from a best-fit line to a best-fit polynomial when sums of vertical distances are used.



Linear least Squares Fitting

- The linear least squares fitting technique is the simplest and most commonly applied form of linear regression (finding the best fitting straight line through a set of points.)
- The fitting is linear in the parameters to be determined, it need not be linear in the independent variable x.
- If the functional relationship between the two quantities being graphed is known, the data can often be transformed to obtain a straight line.
- Some cases appropriate for a linear least squares fit:

$$v = u + at, \quad T \propto \sqrt{\ell}, \quad F = a/r^2, \quad V = U \exp(-t/\tau)$$

Non-linear least squares

- For non-linear 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.
- Some examples where non-linear least squares fit is needed to determine the function parameters:

$$\psi = A\sin(\omega t + \phi)$$

$$f_N(x, \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right]$$

The Procedure

- Find the residual (sum of the squares of the vertical deviations) of a set of data points from a function with m (linear) parameters

$$R^2 = \sum_i \left[y_i - f(x_i, a_1, \ldots, a_m)\right]^2$$

- The resulting residual is then minimized to find the best fit

$$\frac{\partial (R^2)}{\partial a_i} = 0 \quad \forall\ i,\ (1 \ldots N)$$

- A statistically more appropriate measure is

$$\chi^2 = \frac{1}{N-m} \sum_i \frac{\left[y_i - f(x_i, a_1, \ldots, a_m)\right]^2}{\sigma_{y_i}^2 + \sum_j a_j^2 \sigma_{x_i}^2}$$

- For a linear fit $f(x, a, b) = a + bx$ with errors in y

$$\chi^2 = \frac{1}{N-2} \sum_i \frac{\left[y_i - a - bx_i\right]^2}{\sigma_{y_i}^2}$$

The Procedure

So we get the equations

$$\chi^2(a,b) = \sum \frac{[y_i - a - bx]^2}{\sigma_{y_i}^2}$$

$$\frac{\partial(\chi^2)}{\partial a} = -2\sum \frac{[y_i - a - bx_i]}{\sigma_{y_i}^2} = 0$$

$$\frac{\partial(\chi^2)}{\partial b} = -2\sum \frac{[y_i - a - bx_i]\,x_i}{\sigma_{y_i}^2} = 0$$

Which leads to

$$a\sum \frac{1}{\sigma_{y_i}^2} + b\sum \frac{x_i}{\sigma_{y_i}^2} = \sum \frac{y_i}{\sigma_{y_i}^2}$$

$$a\sum \frac{x_i}{\sigma_{y_i}^2} + b\sum \frac{x_i^2}{\sigma_{y_i}^2} = \sum \frac{x_i y_i}{\sigma_{y_i}^2}$$

The Procedure

If y-errors are undefined, then we set them all to 1 (i.e. equal weights to all points), and the simultaneous equations for a and b are

$$na + b\sum x_i = \sum y_i$$

$$a\sum x_i + b\sum x_i^2 = \sum x_i y_i$$

The Fit Parameters

Define sums of squares:

$$S_{xx} = \sum \frac{(x_i - \bar{x})^2}{\sigma_i^2}$$

$$S_{yy} = \sum \frac{(y_i - \bar{y})^2}{\sigma_i^2}$$

$$S_{xy} = \sum \frac{(x_i - \bar{x})(y_i - \bar{y})}{\sigma_i^2}$$

Which leads to

$b = S_{xy}/S_{xx}$ the regression coefficient *and* $a = \bar{y} - b\bar{x}$

The quality of fit is parametrized by

$R^2 = \frac{S_{xy}^2}{S_{xx}S_{yy}}$ the correlation coefficient

Fitting error

The fitting error at each point is

$$e_i = y_i - (a - bx_i)$$

The estimator of the variance of e_i would be

$$s^2 = \sum \frac{e_i^2}{n-2}$$

or

$$s = \left[\frac{S_{yy} - bS_{xy}}{n-2} \right]^{1/2} .$$

The standard error in the fitted parameters is

$$SE(a) = s \left[\frac{1}{n} + \frac{(\bar{x})^2}{S_{xx}} \right]^{1/2}$$

$$SE(b) = \frac{s}{S_{xx}^{1/2}}$$

Examples

- Physical Pendulum

$$T(\theta_0) = T_0 \left(1 + \frac{1}{4}\sin^2\frac{\theta_0}{2} + \cdots\right)$$

  Plot T *versus* $\frac{1}{4}\sin^2\frac{\theta_0}{2}$
  or T *versus* $\sin\,\theta_0$

- Young's modulus

$$Y = \frac{MgL^3}{4BW^3\delta}$$

  Plot δ *versus* M

Examples

- Euler's Method (Friction)

$$T_1 = T_2 \exp(\mu\,\theta)$$

Plot T_1 *versus* $\exp(\mu\,\theta)$
or $\ln T_1$ *versus* $\mu\,\theta$ or $\ln T_1$ *versus* $\ln T_2$

- Viscosity

$$\eta = \frac{2a^2\,(\rho_{sphere} - \rho_{fluid})\,g}{9\,V_T}$$

Plot V_T *versus* $a^2\,(\rho_{sphere} - \rho_{fluid})$

Examples

- Helmholtz Coil

$$B = \mu_0 N I \frac{a^2}{2} \frac{1}{\left(z^2 + a^2\right)^{3/2}}$$

  Plot B *versus* z or B *versus* $\left(z^2 + a^2\right)^{3/2}$

- Faraday's Law
  Plot V *versus* θ_{max}
- Galvanometer constant
  Plot θ *versus* $1/R$

Examples

- Magnet Repulsion

$$F = \left(\frac{\pi\mu_0}{4}\right) M^2 R^4 \left[\frac{1}{z^2} + \frac{1}{(z+2h)^2} - \frac{2}{(z+h)^2}\right]$$

  Plot mg *versus* z
  or mg *versus* $\left[\frac{1}{z^2} + \frac{1}{(z+2h)^2} - \frac{2}{(z+h)^2}\right]$

- Intensity of light

$$I = \frac{a}{r^2} + c$$

  Plot I *versus* $1/r^2$
  or I *versus* r
  or Plot $\sqrt{I}$ *versus* $1/r$

Inference on derived quantities

- The standard error on the linear fit parameters a and b have a bearing on the physical quantity (which is the aim of the experiment) that you derive based on the fit.
- Use standard error propagation method to find the error in the final quantity.
- As an example, in the Young's Modulus experiment, the slope b of the best fit line to the graph of δ *versus* M is related to Y through

$$Y = \frac{gL^3}{4BW^3}\frac{1}{b}$$

- The error in the fitted value of b propagates to an error in Y:

$$Y = \frac{gL^3}{4BW^3}\left[\frac{1}{b} \pm \frac{-SE(b)}{b^2}\right]$$

Points to note

A few points are extremely important in this context

- There has to be a physical basis for choosing a function.
- A good fit (small chi-square) for a particular function does not imply a cause–effect relationship or the correctness of the function.
- A small chi-square alone is not adequate. The errors in fitted parameters should also be small.
- Ensure that there is a large number of data points for fitting. Linear least squares depends strongly on the problem being overdetermined
- Rule of thumb: the number of points should be at least thrice the number of parameters to be fitted.