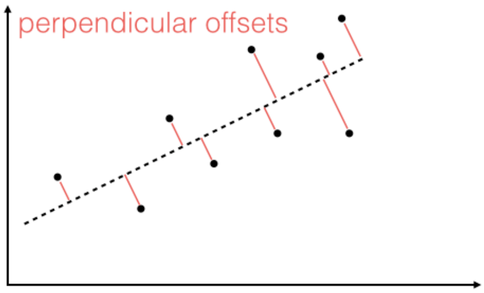
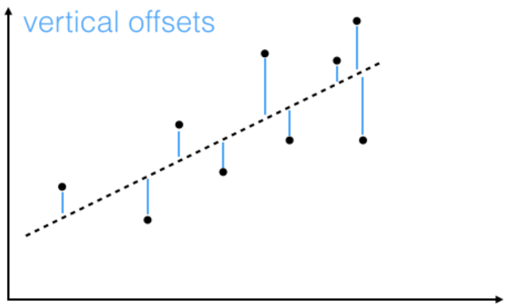
Least-squares fitting

Least-squares fitting (Gauss 1795, Legendre earlier)

- a mathematical procedure for finding the best fitting curve
- minimizing the sum of squares of the offsets (**the residuals**) of the points of the curve
- use **squares** of the offsets instead of absolute values
- but because of squares outlying points have disproportionate effect on the fit





- in practice: best to work with vertical offset (easier to work with experimental data, x and y values with uncertainty)
- for a reasonalbe number of noisy data points difference between vertical and perpendicular offset is **small**
- the **linear** least squares fitting method is the simplest and most commonly applied form of **linear regression**

→ fitting a **straight line** through a set of points

- best practice tip: When plotting and also fitting data, transform data i such a way that the resulting line is a straight line.
- e.g. Period of a pendulum as a function of its length $\left(T \approx 2\pi\sqrt{\frac{l}{g}}\right)$; plot T vs. $\sqrt{l}$ instead of T vs. l
- for this reason: standard forms for exponential, logarithmic and power laws are often explicitly computed.
- vertical least-squares fitting works by finding the sum of the squares of the vertical deviations R^2 of a set of n data points

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

for a function f. (Note: This procedure dos `not` minimize the actual deviations from the line. you need to use perpendicular offsets for that.) Again, it might be more intuitive to use the unsquared sum, but this can lead to discontinuous derivatives that cannot be treated analytically. The condition for R^2 to be minimal is given by:

$$\frac{\partial(R^2)}{\partial a_i} = 0 \qquad \text{for } i = 1 \ldots n \tag{2}$$

For a linear fit that means

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

and

$$R^2(a,b,x) = \sum_{i=1}^{N} \left[y_i - (a + bx_i)\right]^2 \tag{4}$$

$$\frac{\partial(R^2)}{\partial a} = -2\sum_{i=1}^{N} \left[y_i - (a + bx_i)\right] = 0 \tag{5}$$

$$\frac{\partial(R^2)}{\partial b} = -2\sum_{i=1}^{N} \left[y_i - (a + bx_i)\right] x_i = 0 \tag{6}$$

This leads to the following equations:

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

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

Now let us write the same equations in matrix form. (All sums are $\sum_{i=1}^{n}$)

$$\begin{pmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \sum y_i \\ \sum x_i y_i \end{pmatrix} \tag{9}$$

We want to solve this for $\begin{pmatrix} a \\ b \end{pmatrix}$:

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{pmatrix}^{-1} \begin{pmatrix} \sum y_i \\ \sum x_i y_i \end{pmatrix} \tag{10}$$

As a reminder: the inverse of a 2x2 matrix A is given by:

$$A^{-1} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{\det(A)} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \tag{11}$$

For our matrix above that means:

$$\frac{1}{n \sum x_i^2 - (\sum x_i)^2} \begin{pmatrix} \sum x_i^2 & -\sum x_i \\ -\sum x_i & n \end{pmatrix} \tag{12}$$

with this Eq. (10) becomes

$$\begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{n \sum x_i^2 - (\sum x_i)^2} \begin{pmatrix} \sum x_i^2 \sum y_i - \sum x_i \sum x_i y_i \\ -\sum x_i \sum y_i + n \sum x_i y_i \end{pmatrix} \tag{13}$$

The solutions for a and b are then given by

$$a = \frac{\sum y_i \sum x_i^2 - \sum x_i \sum x_i y_i}{n \sum x_i^2 - (\sum x_i)^2}, \tag{14}$$

and

$$b = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - (\sum x_i)^2}. \tag{15}$$

Which we can write as

$$\boxed{a = \frac{\bar{y} \left(\sum x_i^2\right) - \bar{x} \sum x_i y_i}{n \sum x_i^2 - n \bar{x}^2}} \tag{16}$$

and

$$\boxed{b = \frac{\left(\sum x_i y_i\right) - n \bar{x} \bar{y}}{\sum x_i^2 - n \bar{x}^2}} \tag{17}$$

A simplified version by Kenny and Kipping [1962] is using the following definitions (sums of squares ss):

$$ss_{xx} := \sum_{i=1}^{n} (x_i - \bar{x})^2 = \left(\sum_{i=1}^{n} x_i^2 \right) - n\bar{x}^2, \tag{18}$$

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

and finally

$$ss_{xy} := \sum_{i=1}^{n} (x_i - \bar{x}) (y_i - \bar{y}) = \left(\sum_{i=1}^{n} x_i y_i \right) - n\bar{x}\bar{y}. \tag{20}$$

They can be rewritten as

$$\sigma_x^2 = \frac{ss_{xx}}{n}, \tag{21}$$

$$\sigma_y^2 = \frac{ss_{yy}}{n}, \tag{22}$$

and

$$\mathrm{cov}(x, y) = \frac{ss_{xy}}{n}. \tag{23}$$

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

$$\sum_{i=1}^{n} x_i y_i = \vec{x} \cdot \vec{y} \tag{24}$$

and

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

Now in terms of the sums of squares the regression coefficient b is given by

$$\boxed{b = \frac{\mathrm{cov}(x, y)}{\sigma_x^2} = \frac{ss_{xy}}{ss_{xx}}.} \tag{26}$$

With the knowledge of b we can calculate a as follows

$$\boxed{a = \bar{y} - b\bar{x}.} \tag{27}$$

The overall quality of the fit is then parameterized by a quantity known as the **correlation** coefficient

$$r^2 := \frac{ss_{xy}^2}{ss_{xx}ss_{yy}}. \tag{28}$$

Now we need an estimator for the error of our fitting parameters. Let $\hat{y}_i$ be the vertical coordinate of the best fit line with x-coordinate x_i, so that

$$\hat{y}_i \equiv a + bx_i. \tag{29}$$

Then the error between the actual point with coordinates $(x_{,i}, y_i)$ and the fitted point $(x_i, \hat{y}_i)$ is given by

$$e_i \equiv y_i - \hat{y}_i \tag{30}$$

We define s^2 as an estimator for the variance of e_i

$$s^2 := \sum_{i=1}^{n} \frac{e_i^2}{n-2} \tag{31}$$

Then s is given by

$$s = \sqrt{\frac{ss_{yy} - bss_{xy}}{n-2}} = \sqrt{\frac{ss_{yy} - \frac{ss_{xy}^2}{ss_{xx}}}{n-2}} \tag{32}$$

The **standard errors** for our fitting parameters a and b are then given by

$$\boxed{\mathrm{SE}(a) = s\sqrt{\frac{1}{n} + \frac{\bar{x}^2}{ss_{xx}}}} \tag{33}$$

and

$$\boxed{\mathrm{SE}(b) = \frac{s}{\sqrt{ss_{xx}}}} \tag{34}$$

Taken from: Weisstein, Eric W. "Least Squares Fitting." From MathWorld–A Wolfram Web Resource. `http://mathworld.wolfram.com/LeastSquaresFitting.html`