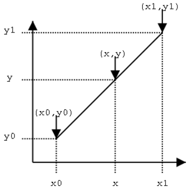
Interpolation and data fitting

Commonly, typically in experiments, we know $f(x_i)$ at various x_i, not necessarily equally spaced. Additionally, we may not quite know the analytical expression of $f(x)$ that describes the data and allow to calculate its value at arbitrary $x \neq x_i$.

If the desired x is/are between largest and smallest x_i's, the problem is of *interpolation*. If outside, then it is *extrapolation*.

Extrapolation is terribly risky endeavor unless backed up by solid theoretical idea(s). Here we study only *interpolation*.

Interpolating (x, y) between (x_0, y_0) and (x_1, y_1) with a straight line,



$$\frac{y - y_0}{x - x_0} = \frac{y_1 - y_0}{x_1 - x_0} \Rightarrow y = y_0 + \frac{x - x_0}{x_1 - x_0}(y_1 - y_0)$$

Generalize this idea by considering a polynomial of degree N to approximate a function from a set of $N+1$ points

$$P_N(x_i) \equiv f(x_i) = y_i \quad \text{where } i = 0, 1, \ldots, N$$

The general form of $P_N(x)$ is

$$\begin{aligned}
P_N(x) &= a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \cdots + \\
&\quad a_N(x - x_0)(x - x_2)\ldots(x - x_{N-1}) \\
P_0(x_0) &= a_0 = y_0 = f(x_0) \\
P_1(x_1) &= a_0 + a_1(x_1 - x_0) = y_1 = f(x_1) \\
P_2(x_2) &= a_0 + a_1(x_2 - x_0) + a_2(x_2 - x_0)(x_2 - x_1) = y_2 = f(x_2) \quad \text{etc.}
\end{aligned}$$

For linear interpolation $N = 1$,

$$a_0 = y_0, \quad a_1 = \frac{y_1 - y_0}{x_1 - x_0} \;\Rightarrow\; P_1(x) = y(x) = y_0 + \frac{x - x_0}{x_1 - x_0}(y_1 - y_0)$$

A particularly useful form, although looks complicated, is

$$P_1(x) = y_0 - \frac{x - x_0}{x_1 - x_0}y_0 + \frac{x - x_0}{x_1 - x_0}y_1 = \frac{x - x_1}{x_0 - x_1}y_0 + \frac{x - x_0}{x_1 - x_0}y_1$$

This is most suitable for iterative processes.

Generalized interpolation formula by Lagrange

$$P_N(x) = \sum_{i=0}^{N} \prod_{k \neq i} \frac{x - x_k}{x_i - x_k} \, y_i$$

As an example, show that (DIY)

$$P_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} y_0 + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} y_1 + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} y_2$$

Ex 1. Consider the following data table and show the $f(x = 4) = 20$

x	2	3	5	8	12
$f(x)$	10	15	25	40	60

Ex 2. To understand what is going on, take a smaller data set

x	0	10	20	30
$f(x)$	-250	0	50	-100

Each term in Lagrange formula *i.e.* coefficient of y_i

$$i=1 \qquad \frac{(x-10)(x-20)(x-30)}{0-10)(0-20)(0-30)} = -\frac{x^3}{6000} + \frac{x^2}{100} - \frac{11x}{60} + 1$$

$$i=2 \qquad \frac{(x-0)(x-20)(x-30)}{(10-0)(10-20)(10-30)} = \frac{x^3}{2000} - \frac{x^2}{40} + \frac{3x}{10}$$

$$i=3 \qquad \frac{(x-0)(x-10)(x-30)}{20-0)(20-10)(20-30)} = -\frac{x^3}{2000} + \frac{x^2}{50} - \frac{3x}{20}$$

$$i=4 \qquad \frac{(x-0)(x-10)(x-20)}{(30-0)(30-10)(30-20)} = \frac{x^3}{6000} - \frac{x^2}{200} + \frac{x}{30}$$

Multiply each line with the corresponding $f(x_i)$ and add together the terms of like power to obtain

$$y(x) \equiv P_4(x) = -x^2 + 35x - 250$$

Lagrange's formula gives a simple quadratic description of the data.

If required, we can calculate, say, $f(x=15)$ either using the quadratic formula or directly from Lagrange's formula.

DIY : Find both way $f(x=1969)$ from the data

x	1951	1961	1971
$f(x)$	2.8	3.2	4.5

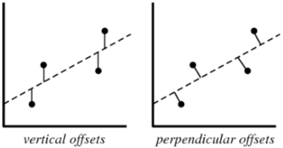
Least square fitting

Set of data points generated (x_i, y_i) are expected to be described by a **known** function $f(x)$ but with undetermined coefficients.

Examples – stress-strain data points within elastic limit, voltage-current data points. Task is to determine modulus of elasticity and Resistance of the material under consideration.

$$V = \mathbf{R}\, i \quad \text{and} \quad \text{stress} = \mathbf{k} \times \text{strain}$$

Least square fitting is a way to do this and for that we need *sum of squares of the offset (residual)* of the data points from the curve $f(x)$. Offsets can be either *vertical* or *perpendicular*



Vertical offsets allow uncertainties of data points along x, y-axes to be independent of each other.

Why squares and not absolute values?

Squares permit offsets to be treated as continuous differentiable quantities.

Absolute values result in discontinuous derivatives.

Fit N data points (x_i, y_i, σ_i) to a model $f(x_i; a_1, a_2, \ldots, a_M)$ with M parameters ($M < N$). Least square suggests to minimize squares of weighted offsets with respect to the parameters a_k's

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - f(x_i; a_1, a_2, \ldots, a_M)}{\sigma_i} \right)^2 \rightarrow \frac{\partial \chi^2}{\partial a_j} = 0$$

Linear regression : model the data points with a straight line

$$f(x) = a_1 + a_2 x \;\Rightarrow\; \chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - a_1 - a_2 x_i}{\sigma_i} \right)^2$$

Minimizing χ^2 w.r.t. a_1, a_2 yields

$$\begin{aligned}
\frac{\partial \chi^2}{\partial a_1} &= -2 \sum_{i=1}^{N} \frac{y_i - a_1 - a_2 x_i}{\sigma_i^2} = 0 \\
\frac{\partial \chi^2}{\partial a_2} &= -2 \sum_{i=1}^{N} \frac{x_i (y_i - a_1 - a_2 x_i)}{\sigma_i^2} = 0
\end{aligned}$$

Introducing a shorthand symbol $\sum_{i=1}^{N} \equiv \sum_i$, we ended up with

$$\left.\begin{array}{l} \displaystyle\sum_i \frac{y_i}{\sigma_i^2} = a_1 \sum_i \frac{1}{\sigma_i^2} + a_2 \sum_i \frac{x_i}{\sigma_i^2} \\[2ex] \displaystyle\sum_i \frac{x_i y_i}{\sigma_i^2} = a_1 \sum_i \frac{x_i}{\sigma_i^2} + a_2 \sum_i \frac{x_i^2}{\sigma_i^2} \end{array}\right. \equiv \begin{array}{l} \mathcal{S}_y = a_1 \mathcal{S} + a_2 \mathcal{S}_x \\[2ex] \mathcal{S}_{xy} = a_1 \mathcal{S}_x + a_2 \mathcal{S}_{xx} \end{array}$$

The solution of these equations are absolutely straight forward,

$$a_1 = \frac{\mathcal{S}_{xx}\mathcal{S}_y - \mathcal{S}_x\mathcal{S}_{xy}}{\Delta}, \quad a_2 = \frac{\mathcal{S}_{xy}\mathcal{S} - \mathcal{S}_x\mathcal{S}_y}{\Delta} \text{ where } \Delta = \mathcal{S}\mathcal{S}_{xx} - \mathcal{S}_x^2$$

Estimating the errors σ_{a_i} on the parameters a_i determined above

$$\sigma_{a_i}^2 = \sum_i \sigma_i^2 \left(\frac{\partial a_i}{\partial y_i}\right)^2$$

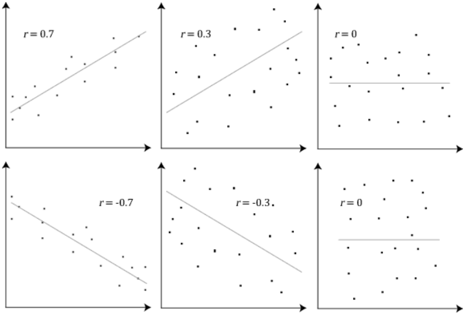
$$\Rightarrow \qquad \frac{\partial a_1}{\partial y_i} = \frac{\mathcal{S}_{xx} - \mathcal{S}_x\, x_i}{\Delta\ \sigma_i^2}, \quad \frac{\partial a_2}{\partial y_i} = \frac{\mathcal{S}\, x_i - \mathcal{S}_x}{\Delta\ \sigma_i^2}$$

$$\Rightarrow \qquad \sigma_{a_1}^2 = \frac{\mathcal{S}_{xx}}{\Delta} \quad \text{and} \quad \sigma_{a_2}^2 = \frac{\mathcal{S}}{\Delta}$$

To this end, in order to get some idea about how *good* is the **linear** fit we define an estimate called *Pearson's correlation coefficient* r

$$r^2 = \frac{\mathcal{S}_{xy}}{\mathcal{S}_{xx}\mathcal{S}_{yy}} \quad \text{where} \quad 0 \le r^2 \le 1$$

As $r^2 \to 1$ fit gets better.



NB : But is the straight line model itself good to fit the data? To address this requires ideas of *goodness of fit*, *confidence level*, testing some *null hypothesis* against χ^2 probability distribution and so on.

The straight line model is generic enough for use in a few other models which can be reduced to straight line form usually by taking logarithms,

$$\begin{aligned}
\text{exponential :} &\quad f(x) = a\, e^{b\,x} \quad \rightarrow \quad \log f(x) = \log a + bx \\
\text{logarithm :} &\quad f(x) = a + b\, \log x \\
\text{power law :} &\quad f(x) = a\, x^{b} \quad \rightarrow \quad \log f(x) = \log a + b\, \log x
\end{aligned}$$

Least square polynomial fitting

Polynomial model $f(x) = \sum_{k=0}^{n} a_k x^k$ can also be subjected to linear fitting. For simplified expressions, we put all the errors $\sigma_i^2 = 1$ without any loss of generality. In such case, $\chi^2 \rightarrow R^2$

$$\begin{aligned}
R^2 &= \sum_{i=1}^{n} \left[y_i - \left(a_0 + a_1 x_i + \cdots + a_k x_i^k \right) \right]^2 \\
\frac{\partial R^2}{\partial a_0} &= -2 \sum \left[y_i - \left(a_0 + a_1 x_i + \cdots + a_k x_i^k \right) \right] = 0 \\
\frac{\partial R^2}{\partial a_1} &= -2 \sum \left[y_i - \left(a_0 + a_1 x_i + \cdots + a_k x_i^k \right) \right] x_i = 0 \\
&\cdots \\
\frac{\partial R^2}{\partial a_k} &= -2 \sum \left[y_i - \left(a_0 + a_1 x_i + \cdots + a_k x_i^k \right) \right] x_i^k = 0
\end{aligned}$$

Set of equations for a_i's are,

$$\begin{aligned}
a_0 n + a_1 \sum x_i + \cdots + a_k \sum x_i^k &= \sum y_i \\
a_0 \sum x_i + a_1 \sum x_i^2 + \cdots + a_k \sum x_i^{k+1} &= \sum x_i y_i \\
&\cdots \\
a_0 \sum x_i^k + a_1 \sum x_i^{k+1} + \cdots + a_k \sum x_i^{2k} &= \sum x_i^k y_i
\end{aligned}$$

which when written in matrix form becomes a problem of matrix inversion, and you are free to use your favorite inverter.

$$\begin{pmatrix} n & \sum x_i & \cdots & \sum x_i^k \\ \sum x_i & \sum x_i^2 & \cdots & \sum x_i^{k+1} \\ \vdots & \vdots & \ddots & \vdots \\ \sum x_i^k & \sum x_i^{k+1} & \cdots & \sum x_i^{2k} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_k \end{pmatrix} = \begin{pmatrix} \sum y_i \\ \sum x_i y_i \\ \vdots \\ \sum x_i^k y_i \end{pmatrix}$$

$$\Rightarrow \quad \mathbf{X} \cdot \mathbf{a} = \mathbf{Y} \quad \rightarrow \quad \mathbf{a} = \mathbf{X}^{-1}\mathbf{Y}$$

DIY fitting

1. A time versus angular velocity data set on deceleration of a rotating disc is in the file `fit1.dat`. Fit it with the following functions (*i*) $\omega(t) = \omega_0 + \omega_c t$ and (*ii*) $\omega(t) = \omega_0 \, e^{-\omega_c t}$. Determine $\omega_0, \, \omega_c$ and the quality of fit for both the functions by *Pearson's* r.

2. Distance (r) versus height (h) of the trajectory of a test missile is given in the datafile `fit2.dat`. Try quadratic fit $h = a_0 + a_1 r + a_2 r^2$ and determine the highest point reached by the missile.