Least Squares Curve Fit

Example

°F	°C
32	0
212	100

Linear relationship

$y = mx + b$ where °F $\Rightarrow x$
°C $\rightarrow y$

x to be set
y to be measured
Solve for m + b

The measurement y is corrupted by many possible errors we would like to minimize.

$$Y_i' = mx_i + b + \varepsilon_i$$

Solve for the errors and minimize

$$\varepsilon_i = Y_i' - mx_i - b$$

Take N readings, sum the errors

$$\sum_{i=1}^{N} \varepsilon_i = \sum_{i=1}^{N} (Y_i - mx_i - b)$$

Properties of sums

$$\sum_{i=1}^{N} 1 = 1+1+1+ \cdots 1 \rightarrow \text{Add } 1 \text{ } N \text{ times}$$
$$= N$$

$$\sum_{i=1}^{N} c = c+c+ \cdots c \rightarrow \text{Add } c \text{ } N \text{ times}$$
$$= cN$$

$$\sum_{i=1}^{N} i = 1+2+3+ \cdots N = N(N+1)/2$$

We need a positive function to minimize like the sum of squares

$$\sum_{i=1}^{N} \varepsilon_i^2 = \sum_{i=1}^{N} (y_i - mx_i - b)^2$$

To minimize, we take the derivative and set to 0. Then solve for $m + b$.

$$\partial \sum_{i=1}^{N} \varepsilon_i^2 \Big/ \partial m = \sum_{i=1}^{N} 2(y_i - mx_i - b)(-x_i) = 0$$

$$\sum_{i=1}^{N} y_i x_i - m \sum_{i=1}^{N} x_i^2 - b \sum_{i=1}^{N} x_i = 0$$

$$S_{xy} - m S_{x^2} - b S_x = 0$$

$$\partial \sum_{i=1}^{N} \varepsilon_i^2 / \partial b = \sum_{i=1}^{N} 2(y_i - m x_i - b)(-1)$$

$$= \sum_{i=1}^{N} y_i - m \sum_{i=1}^{N} x_i - b \sum_{i=1}^{N} 1$$

$$S_y - m S_x - bN = 0$$

We have 2 equations, 2 unknowns
$m + b$ so solve

$$1) \quad S_{yx} - m S_{x^2} - b S_x$$
$$2) \quad S_y - m S_x - bN$$

solving for b from 2)

$$b = (S_y - m S_x)/N$$

plug b back into 1) and solve for m

$$S_{yx} - m S_{x^2} - S_x (S_y - m S_x)/N = 0$$

$$(S_{yx} - S_y S_x / N) + m (S_x^2 / N - S_{x^2}) = 0$$

$$m = \frac{(S_y S_x - N S_{yx})}{(S_x^2 - N S_{x^2})}$$

Check with the original $N=2$ exact values

x °F	y °C
32	0
212	100

$S_x = 32 + 212 = 244$

$S_y = 0 + 100 = 100$

$S_x^2 = 244^2 = 59{,}536$

$S_{xy} = 0 \cdot 32 + 100 \cdot 212 = 21{,}200$

$S_{x^2} = 32 \cdot 32 + 212 \cdot 212 = 1024 + 44944 = 45{,}968$

$$m = \frac{(S_y S_x - N S_{yx})}{(S_x^2 - N S_{x^2})} = \frac{(100 \cdot 244 - 2(21{,}200))}{(244^2 - 2(45968))}$$

$$= -18000/-32400 = 180/324$$

$$= 5 \cdot \cancel{36}/9 \cdot \cancel{36}$$

$$= 5/9$$

Then $b = (S_y - m S_x)/N$

$= (100 - 5/9\, 244)/2$

$= -5/9 \cdot 32$

So $y = 5/9\, x - 5/9 \cdot 32$

or $°C = 5/9(°F - 32)$

It Checks

Least Squares using any linear functional form

$\underline{f} = r\,\underline{c}$ Linear algebra

$f_i = \sum_{j=0}^{m} {}_i r_j \, c_j$ if polynomial of degree m $r_j = r^j$

but can be of any linea functional form
r_2 does not have to be r^2
Could be $\log r$ or $r \log r$

$$
\begin{aligned}
f_1 &= [\,{}_1r_0 \;\; {}_1r_1 \;\; {}_1r_2 \;\; {}_1r_3 \cdots {}_1r_m\,] \\
f_2 &= [\,{}_2r_0 \;\; {}_2r_1 \;\; {}_2r_2 \;\; {}_2r_3 \cdots {}_2r_m\,] \\
&\;\;\vdots \\
f_N &= [\,{}_Nr_0 \;\; {}_Nr_1 \;\; {}_Nr_2 \;\; {}_Nr_3 \cdots {}_Nr_m\,]
\end{aligned}
\begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix}
$$

$\underset{\text{Vector } N}{\underline{f}} = \underset{\substack{\text{MATRIX} \\ N \times m}}{r} \; \underset{\text{Vector } m}{\underline{c}} \longrightarrow \underline{f} = r\,\underline{c}$

$\underline{f}_{N \times 1} = r_{N \times m} \, \underline{c}_{m \times 1}$

Functional Form in Linear Algebra

$$\underline{f} = r\,\underline{c}$$

$$\underline{f}' = r\,\underline{c} + \underline{\varepsilon}$$

$r \rightarrow$ set
$f' \rightarrow$ measure
$\underline{\varepsilon} \rightarrow$ error in measure

Solving for $\underline{\varepsilon}$ + Sum of Squares

$$\underline{\varepsilon} = \underline{f}' - r\,\underline{c}$$

$$\underline{\varepsilon}^T\underline{\varepsilon} = \sum_{i=1}^{N} \varepsilon_i^2 = [\varepsilon_1\ \varepsilon_2 \cdots \varepsilon_N] \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_N \end{bmatrix}$$

$$\underline{\varepsilon}^T = \underline{\varepsilon}^T_{1\times N} \quad \text{row vector}$$

$$\underline{\varepsilon} = \underline{\varepsilon}_{N\times 1} \quad \text{column vector}$$

$$\underline{\varepsilon}^T_{1\times \cancel{N}}\ \underline{\varepsilon}_{\cancel{N}\times 1} = \text{Value}_{1\times 1}$$

Same type of solution as before
Take derivative and set to 0 to find the minimum.

$$\frac{\partial\, \underline{\varepsilon}^T \underline{\varepsilon}}{\partial\, \underline{c}} = \frac{\partial (\underline{f}' - r\underline{c})^T (\underline{f}' - r\underline{c})}{\partial\, \underline{c}}$$

$$0 = -2 r^T (\underline{f}' - r\underline{c})$$

$$0 = r^T \underline{f}' - r^T r \underline{c}$$

$$r^T r \underline{c} = r^T \underline{f}'$$

$$\underbrace{\cancel{(r^T r)^{-1} (r^T r)}}_{=1} \underline{c} = (r^T r)^{-1} r^T \underline{f}'$$

$$\underline{c} = (r^T r)^{-1} r^T \underline{f}'$$

$$= \left(r^T_{m \times N}\, r_{N \times m}\right)^{-1}_{m \times m} r^T_{m \times N}\, \underline{f}_{N \times 1}$$

$$= \text{Result}_{m \times 1}$$

Example solution for a linear function and how to invert a matrix

$y = mx + b \qquad m = 1 \qquad b = 2$

$\qquad\qquad\qquad c_1 = 1 \qquad c_0 = 2$

$y = x + 2$ or

$f = r + 2$

r	f
0	2
1	3

Data without measurement error

$\underline{f} = r\,\underline{c}$

$$\begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_0 \end{bmatrix} \rightarrow \begin{matrix} 2 = c_0 \\ 3 = c_1 + c_0 \end{matrix}$$

$$\underline{c} = (r^T r)^{-1} r^T f$$

$$r^T = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \qquad r = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$$

$$r^T r = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}$$

Invert the matrix

$$\left[\begin{array}{cc|cc} 1 & 1 & 1 & 0 \\ 1 & 2 & 0 & 1 \end{array}\right] \qquad [m : I] \qquad [I : m^{-1}]$$

$$2) - 1) \rightarrow 2) \quad \left[\begin{array}{cc|cc} 1 & 1 & 1 & 0 \\ 0 & 1 & -1 & 1 \end{array}\right]$$

$$1) - 2) \rightarrow 1 \quad \left[\begin{array}{cc|cc} 1 & 0 & 2 & -1 \\ 0 & 1 & -1 & 1 \end{array}\right]$$

$$(r^T r)^{-1} \qquad (r^T r) = I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$r^T \underline{f} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \end{bmatrix}$$

$$(r^T r)^{-1} r^T \underline{f} = \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} 3 \\ 5 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$$f = r + 2$$