

Least Squares Curve Fit

Example

$^{\circ}\text{F}$	$^{\circ}\text{C}$
32	0
212	100

Linear relationship

$$y = mx + b \quad \text{where } ^{\circ}\text{F} \Rightarrow x \\ ^{\circ}\text{C} \Rightarrow y$$

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

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

$$\sum_{i=1}^N C = C + C + \dots + C \rightarrow \text{Add } C \text{ } n \text{ times} \\ = CN$$

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

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

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

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

$$2 \frac{\sum_{i=1}^N \epsilon_i^2}{2m} = \sum_{i=1}^N 2(y_i - mx_i - b)(-x_i) = 0$$

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

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

$$\begin{aligned} 2 \sum_{i=1}^N \varepsilon_i^2 / 2b &= \sum_{i=1}^N 2(y_i - mx_i - b)(-1) \\ &= \sum_{i=1}^N y_i - m \sum_{i=1}^N x_i - b \sum_{i=1}^N 1 \end{aligned}$$

$$S_y - m S_x - b N = 0$$

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

$$\begin{array}{l} 1) \quad S_{yx} - m S_{x^2} - b S_x \\ 2) \quad S_y - m S_x - b N \end{array}$$

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	Y
$^{\circ}\text{F}$	$^{\circ}\text{C}$
32	0
212	100

$$S_x = 32 + 212 = 244$$

$$S_y = 0 + 100 = 100$$

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

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

$$S_x^2 = 32 \cdot 32 + 212 \cdot 212 = 1024 + 44944 = 45,968$$

$$m = \frac{(S_y S_x - n S_{xy})}{(S_x^2 - n S_x^2)} = \frac{(100 \cdot 244 - 2(21,200))}{(244^2 - 2(45,968))}$$

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

$$= 5.76 / 9.76$$

$$= \boxed{5/9}$$

$$\begin{aligned} \text{Then } b &= (S_y - m S_x) / n \\ &= (100 - 5/9 \cdot 244) / 2 \\ &= -5/9 \cdot 32 \end{aligned}$$

$$\text{So } y = 5/9 x - 5/9 \cdot 32$$

$$\text{or } \underline{\underline{^{\circ}\text{C} = 5/9(^{\circ}\text{F} - 32)}}$$

I + Checks

Least Squares using any linear functional form

$$\underline{f} = \underline{r} \underline{c} \quad \text{Linear algebra}$$

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

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

$$\begin{aligned} f_1 &= [r_0 \ r_1 \ r_2 \ r_3 \ \dots \ r_m] \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} \\ f_2 &= [2r_0 \ 2r_1 \ 2r_2 \ 2r_3 \ \dots \ 2r_m] \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} \\ &\vdots \\ f_N &= [r_N \ r_1 \ r_2 \ r_3 \ \dots \ r_m] \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} \end{aligned}$$

$$\underset{\text{vector } N}{\underline{f}} = \underset{\substack{\text{MATRIX} \\ N \times m}}{\underline{r}} \underset{\text{vector } m}{\underline{c}} \rightarrow \underline{f} = \underline{r} \underline{c}$$

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

Functional Form in Linear Algebra

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

$$\underline{f}' = r \underline{c} + \underline{e}$$

$r \rightarrow$ set

$f' \rightarrow$ measure

$\underline{e} \rightarrow$ error in measure

Solving for \underline{e} + Sum of Squares

$$\underline{e} = \underline{f}' - r \underline{c}$$

$$\underline{e}^T \underline{e} = \sum_{i=1}^N e_i^2 = \begin{bmatrix} e_1 & e_2 & \dots & e_N \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_N \end{bmatrix}$$

$$\underline{e}^T = \underline{e}_{1 \times N} \quad \text{row vector}$$

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

$$\underline{e}_{1 \times N} / \underline{e}_{N \times 1} = \text{Value}_{1 \times 1}$$

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

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

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

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

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

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

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

$$= \begin{pmatrix} \underline{r}_{m \times n}^T & \underline{r}_{n \times m} \end{pmatrix}_{m \times m}^{-1} \underline{r}_{m \times n}^T \underline{f}_{n \times 1}$$

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

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

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

$$C_1 = 1 \quad C_0 = 2$$

$$y = x + 2 \quad \text{or}$$

$$f = r + 2$$

r	f
0	2
1	3

↙ Data without
measurement error

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

$$\begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} C_1 \\ C_0 \end{bmatrix} \rightarrow \begin{aligned} 2 &= C_0 \\ 3 &= C_1 + C_0 \end{aligned}$$

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

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

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

Invert the matrix

$$\begin{bmatrix} 1 & 1 & | & 1 & 0 \\ 1 & 2 & | & 0 & 1 \end{bmatrix} \quad \begin{matrix} [m; I] \\ [I; m^{-1}] \end{matrix}$$

$$2) - 1) \rightarrow 2) \quad \begin{bmatrix} 1 & 1 & | & 1 & 0 \\ 0 & 1 & | & -1 & 1 \end{bmatrix}$$

$$1) - 2) \rightarrow 1) \quad \begin{bmatrix} 1 & 0 & | & 2 & -1 \\ 0 & 1 & | & -1 & 1 \end{bmatrix}$$

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

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

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

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

$$\underline{f} = r + 2$$