



Given a set of observations y_i , what is the best model that fits the observations.

$$\text{Model: } \hat{y}_i = f(x_i) \rightarrow (1)$$

where \hat{y}_i is the prediction.

Then $y_i - \hat{y}_i$ is the residual or.

$y_i - (f(x_i))$ is the residual $e_i \rightarrow (2)$

In general f is a non linear function. but if f can be written as.

$f = \beta_1 x_{1i} + \beta_2 x_{2i} + \dots + \beta_n$ then f is obviously linear in the $(n-1)$ dimensional vector x_i

$$x_i = [x_{1i} \ x_{2i} \ \dots \ x_{(n-1)i}] \rightarrow (3)$$

$$\text{Then } \hat{y}_i = [x_{1i} \ x_{2i} \ \dots \ x_{(n-1)i}] \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{bmatrix} \rightarrow (4)$$

$$\text{or } \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_m \end{bmatrix} = \begin{bmatrix} x_{11} & x_{21} & \dots & x_{n-1,1} & 1 \\ x_{12} & x_{22} & \dots & x_{n-1,2} & 1 \\ \vdots & \vdots & & \vdots & \vdots \\ x_{1m} & x_{2m} & \dots & x_{n-1,m} & 1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_n \end{bmatrix} \rightarrow (5)$$

$$\hat{y}_{m \times 1} = X_{m \times n} \beta_{n \times 1} \rightarrow (6)$$

$$\text{Minimize } [y - \hat{y}]^T [y - \hat{y}]$$

$$\text{or } [y - X\beta]^T [y - X\beta] \rightarrow (7)$$

$$\text{or } [y^T - \beta^T X^T] [y - X\beta]$$

$$L = [y^T y - \beta^T X^T y - y^T X \beta + \beta^T X^T X \beta] \rightarrow (8)$$

The loss L is minimized when.

$\frac{dL}{d\beta}$ goes to zero

$$\frac{dL}{d\beta} = -x^T y - y^T x + 2x^T x \beta \rightarrow (9)$$

(from Matrix Calculus).

$$\frac{dL}{d\beta} = 0 \Rightarrow -2x^T y + 2x^T x \beta = 0.$$

$$\text{or } x^T x \beta = x^T y$$

$$\text{or } \boxed{\beta = [x^T x]^{-1} x^T y \rightarrow (10)}$$

is the pseudo inverse solution

→ When $m > n$ the system is overdetermined.

Due to noise the system is also inconsistent. Hence the least squares solution is the optimal estimate of the model parameters.

→ When $m = n$ the regular inverse solution exists if the equation

are consistent, i.e. $\beta = X^{-1}y$. However

if the model is not consistent with the data the least squares solution works.

→ When $m < n$ the system is underdetermined

Many solutions are possible. The minimum norm solution by the method of Lagrange multipliers is formulated as.

$$\min \beta^T \beta \rightarrow (11).$$

$$\text{s.t. } y = X\beta \rightarrow (12).$$

The Lagrange Multiplier gives

$$\min \beta^T \beta + \lambda (y - X\beta) \rightarrow (13).$$

which gives the pseudo inverse solution:

$$\boxed{\beta = X^T (X X^T)^{-1} y. \rightarrow (14)}$$

(14) is different from (10).

The Non Linear Least Squares:

$$Y_{n+1} = f(X_{n+1}, \beta). \text{ or } Y_i = f(X_i, \beta) \rightarrow (15)$$

$$\text{Minimize } [Y - f(X, \beta)]^T [Y - f(X, \beta)]. \rightarrow (16)$$

$$f(X, \beta) = f(X, \beta_0) + J \delta \beta \rightarrow (17)$$

The Taylor Series Approximation.

$$J = \left. \frac{\partial f}{\partial \beta} \right|_{\beta = \beta_0} \rightarrow (18)$$

$$(16) \text{ becomes Minimize } [Y - f(X, \beta_0) - J \delta \beta]^T [Y - f(X, \beta_0) - J \delta \beta]$$

Let $Y - f(X, \beta_0)$ be Y_n . or Y_{new}

$$\text{Then. Minimize } [Y_n - J \delta \beta]^T [Y_n - J \delta \beta] \rightarrow (19)$$

Then by the method of L.S

$$\boxed{\delta \beta = [J^T J]^{-1} J^T Y_n. \rightarrow (20)}$$

$$\text{Then } \beta_{n+1} = \beta_n + \delta \beta \rightarrow (21)$$

Linearize about the new β_{n+1} till such time $\|\beta_{n+1} - \beta_n\| < \epsilon$.

The LM Algorithm:

$$\delta \beta = [J^T J + \lambda I]^{-1} J^T y_n.$$

λ -updates: Look at Srinath Ranganathan's material on LM.