

## 8.1 - Discrete Least Squares Approximation

# Motivation

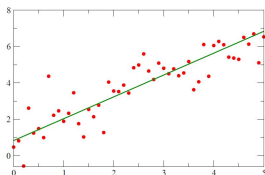


Figure: Dot: measured data; line: linear fit

Q:

Given  $m$  data point,  $\{(x_i, y_i)\}_{i=1}^m$ , how find the equation of straight line  $y = a_0 + a_1x$  which is the "best" fit for the data points.

Least squares error:

$$E \equiv E_2(a_0, a_1) = \sum_{i=1}^m [y_i - (a_0 + a_1x_i)]^2$$

# Linear least squares method

Ans. to Q: Solve a minimization problem

Find  $a_0, a_1$ , such that the least squares error  $E_2(a_0, a_1)$  is minimum, i.e.,  
 $\min_{a_0, a_1} E_2(a_0, a_1)$

At minimum of error, we have  $\frac{\partial E}{\partial a_0} = 0$ , and  $\frac{\partial E}{\partial a_1} = 0$ . This means:

$$0 = \frac{\partial E}{\partial a_0} = \frac{\partial}{\partial a_0} \sum_{i=1}^m [y_i - (a_0 + a_1 x_i)]^2 = 2 \sum_{i=1}^m [y_i - (a_0 + a_1 x_i)](-1); \quad (1)$$

$$0 = \frac{\partial E}{\partial a_1} = \frac{\partial}{\partial a_1} \sum_{i=1}^m [y_i - (a_0 + a_1 x_i)]^2 = 2 \sum_{i=1}^m [y_i - (a_0 + a_1 x_i)](-x_i). \quad (2)$$

Simplifying Eq. (1)  $\Rightarrow a_0 m + a_1 \sum_{i=1}^m x_i = \sum_{i=1}^m y_i$

Simplifying Eq. (2)  $\Rightarrow a_0 \sum_{i=1}^m x_i + a_1 \sum_{i=1}^m x_i^2 = \sum_{i=1}^m x_i y_i$

These lead to:

## Normal equations

$$a_0 m + a_1 \sum_{i=1}^m x_i = \sum_{i=1}^m y_i ;$$

$$a_0 \sum_{i=1}^m x_i + a_1 \sum_{i=1}^m x_i^2 = \sum_{i=1}^m x_i y_i .$$

$$a_0 = \frac{\sum_{i=1}^m x_i^2 \sum_{i=1}^m y_i - \sum_{i=1}^m x_i y_i \sum_{i=1}^m x_i}{m \sum_{i=1}^m x_i^2 - (\sum_{i=1}^m x_i)^2} \quad (3)$$

$$a_1 = \frac{m \sum_{i=1}^m x_i y_i - \sum_{i=1}^m x_i \sum_{i=1}^m y_i}{m \sum_{i=1}^m x_i^2 - (\sum_{i=1}^m x_i)^2} \quad (4)$$

# Polynomial Least squares

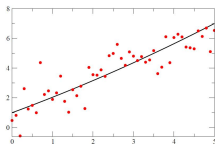


Figure: Dot: measured data; curve:  $1 + x + x^2/25$

Q:

Given  $m$  data point,  $\{(x_i, y_i)\}_{i=1}^m$ , find the equation of polynomial:  
 $P_n(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0$  which "best" fits for the data points. Here  $n < m - 1$ .

Ans to Q:

The coefficients  $\mathbf{a} = (a_0, \dots, a_n)^t$  are found by minimizing the least squares error  $E \equiv E_2(a_0, \dots, a_n) = \sum_{i=1}^m [y_i - P_n(x_i)]^2$

$$\begin{aligned}
 E &= \sum_{i=1}^m y_i^2 - 2 \sum_{i=1}^m P_n(x_i) y_i + \sum_{i=1}^m (P_n(x_i))^2 \\
 &= \sum_{i=1}^m y_i^2 - 2 \sum_{j=0}^n a_j \left( \sum_{i=1}^m y_i x_i^j \right) + \sum_{j=0}^n \sum_{k=0}^n a_j a_k \left( \sum_{i=1}^m x_i^{j+k} \right)
 \end{aligned} \tag{5}$$

At minimum of error, we have  $\frac{\partial E}{\partial a_0} = 0, \frac{\partial E}{\partial a_1} = 0, \dots, \frac{\partial E}{\partial a_n} = 0$ . These lead to:

Normal equations for polynomial fitting

$$\sum_{k=0}^n a_k \sum_{i=1}^m x_i^{j+k} = \sum_{i=1}^m y_i x_i^j, \quad \text{for each } j = 0, 1, \dots, n. \tag{6}$$

## Normal equations in matrix form

$$A^t A \mathbf{a} = A^t \mathbf{b} \quad (7)$$

where

$$A = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^n \\ 1 & x_2 & x_2^2 & \dots & x_2^n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_m & x_m^2 & \dots & x_m^n \end{bmatrix}; \quad \mathbf{b} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}; \quad (8)$$

and  $\mathbf{a} = (a_0, \dots, a_n)^t$ .

Remark: Eq. (7) has a unique solution if all  $x_i$  are unique.

Example. Fit the data in the table using quadratic polynomial least squares

	$i$	$x_i$	$y_i$
method.	1	0	1.0000
	2	0.25	1.2480
	3	0.50	1.6487
	4	0.75	2.1170
	5	1.00	2.7183

Soln: Let the quadratic polynomial be  $P_2(x) = a_2x^2 + a_1x + a_0$ . The matrix  $A$  and vector  $\mathbf{b}$  of the normal equation (7) are:

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0.25 & 0.25^2 \\ 1 & 0.5 & 0.5^2 \\ 1 & 0.75 & 0.75^2 \\ 1 & 1.00 & 1.0^2 \end{bmatrix}; \quad \mathbf{b} = \begin{bmatrix} 1.0 \\ 1.2840 \\ 1.6487 \\ 2.1170 \\ 2.7183 \end{bmatrix} \quad (9)$$



$$A^t = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 0.25 & 0.5 & 0.75 & 1.0 \\ 0 & 0.0625 & 0.25 & 0.5625 & 1 \end{bmatrix}$$

$$A^t A = \begin{bmatrix} 5.0 & 2.5 & 1.875 \\ 2.5 & 1.875 & 1.5625 \\ 1.875 & 1.5625 & 1.3828 \end{bmatrix}; \quad A^t \mathbf{b} = \begin{bmatrix} 8.768 \\ 5.4514 \\ 4.4015375 \end{bmatrix}$$

The normal equations are:

$$\begin{aligned} 5.0a_0 + 2.5a_1 + 1.875a_2 &= 8.768 \\ 2.5a_0 + 1.875a_1 + 1.5625a_2 &= 5.4514 \\ 1.875a_0 + 1.5625a_1 + 1.3828a_2 &= 4.4015375 \end{aligned} \tag{10}$$

Solving Eq. (10) for  $a_0, a_1, a_2$  yields  $P_2(x) = 1.0051 + 0.8642x + 0.8437x^2$ .  
Remark: See matlab code for solving this problem as well.