Chapter 6

Least Squares Approximation

How do we find approximate solutions to over determined system?

Overdetermined System?

$$\left.\begin{aligned} 5x_1 + 2x_2 + 3x_3 &= 7 \\ 2x_1 + 7x_2 + 8x_3 &= 5 \\ 3x_1 + 9x_2 + 2x_3 &= 6 \end{aligned}\right\}$$

This is a linear system where, number of equations = number of unknown variables

We can solve this using inverse matrix, gaussian elimination or LU Decomposition.

But if this system had another equation,

$$\left.\begin{aligned} 5x_1 + 2x_2 + 3x_3 &= 7 \\ 2x_1 + 7x_2 + 8x_3 &= 5 \\ 3x_1 + 9x_2 + 2x_3 &= 6 \\ 4x_1 + 2x_2 + 5x_3 &= 10 \end{aligned}\right\}$$

In this linear system,

coefficient matrix, $A = \begin{bmatrix} 5 & 2 & 3 \\ 2 & 7 & 8 \\ 3 & 9 & 2 \\ 4 & 2 & 5 \end{bmatrix}$ $[m \times n]$ $m > n$

This is a $[4 \times 3]$ matrix and not a square matrix.

If the coefficient matrix A is an $m \times n$ rectengular matrix with $m > n$, then the linear system $Ax = b$ is a $\boxed{\text{overdetermined system.}}$

This type of system usually don't have an exact solution as all equation may not be consistent with each other.

So, we can not directly solve this using Gaussin, LU or inverse matrix. But we can still look for approximation.

Summary: $\boxed{\text{number of equation} > \text{number of unknowns/variables}}$

Before moving on how to work with this, we need to revisit some terms.

Orthonormality → A set of vector that are **both** orthogonal & Normal.

Orthogonal ↓

Every pair of vector are perpendicular (Dot product $= 0$)

$$\boxed{\begin{aligned} x^T y &= 0 \\ y^T z &= 0 \\ &\vdots \end{aligned}}$$

Normal (Norm) ↓

Each vector has a unit length. (magnitude $= 1$)

$$\boxed{\begin{aligned} x^T \cdot x &= 1 \\ y^T \cdot y &= 1 \\ &\vdots \end{aligned}}$$

Row matrix,

$$[x_1, x_2, x_3, \dots x_n]$$

$[1 \times n]$ matrix

Column matrix,

$$[n \times 1] \qquad \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Example: Check if the following vector set is $\boxed{\text{orthonormal}}$.

$$S = \left\{ \frac{1}{\sqrt{5}} (2, 1)^T , \frac{1}{\sqrt{5}} (1, -2)^T \right\}$$

To find orthonormality, we need to verify both orthogonality & normality.

Orthogonality, $x^T y = 0$

$$x^T y = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 & 1 \end{bmatrix} \times \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ -2 \end{bmatrix}$$

$$= \frac{1}{5} \begin{bmatrix} 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -2 \end{bmatrix}$$

$$= \frac{1}{5} (2-2)$$

$$= 0$$

$$\therefore x^T y = 0 \longrightarrow \text{True}$$

Normal,

$$x^T x = 1 \quad \text{and} \quad y^T y = 1$$

$$x^T x = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 & 1 \end{bmatrix} \times \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

$$= \frac{1}{5} \begin{bmatrix} 2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

$$= \frac{1}{5} (4+1)$$

$$= \frac{5}{5}$$

$$x^T x = 1 \longleftarrow \text{True}$$

$$y^T y = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 & -2 \end{bmatrix} \times \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ -2 \end{bmatrix}$$

$$= \frac{1}{5} \begin{bmatrix} 1 & -2 \end{bmatrix} \begin{bmatrix} 1 \\ -2 \end{bmatrix}$$

$$= \frac{1}{5} (1+4)$$

$$= \frac{5}{5}$$

$$y^T y = 1 \longleftarrow \text{True}$$

Since both orthogonality & normality has been proven, so the matrix has orthonormal properties.

Kronecker Delta

Summerizes orthogonality & normality

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \qquad \begin{matrix} u^T u \ \{\text{normal/norm/normality}\} \\ u^T v \ \{\text{orthogonality}\} \end{matrix}$$

Discrete Least Square

We use Least square method to solve overdetermined system.

Since the coefficient matrix is not a square matrix in the overdetermined system, we will try to obtain a square matrix.

$$\underbrace{A}_{[m \times n]} x = b$$

By multiplying transposed matrix, A^T in both side,

$$\underbrace{\underbrace{A^T}_{[n \times m]} \underbrace{A}_{[m \times n]}}_{[n \times n]} x = A^T b$$

Square Matrix

Now, we can solve this using any known methods like gaussian, LU or inverse matrix. In exams, follow the approach that is mentioned.

Example: Fit a least square straight line (degree = 1) to the given data

$$\left.\begin{aligned} f(-3) &= 0 \\ f(0) &= 0 \\ f(6) &= 2 \end{aligned}\right\}$$

Here

node 3, degree = 2

$$P_2(x) = a_0 + a_1 x + a_2 x^2$$

But we are asked to fit a straight line. (degree = 1)

$$\therefore \quad P_1(x) = a_0 + a_1 x$$

Then,

$$P_1(-3) = a_0 + (-3)a_1 = 0$$

$$P_1(0) = a_0 + (0)\,a_1 = 0$$

$$P_1(6) = a_0 + (6)\,a_1 = 2$$

$$\therefore \text{ coefficient matrix, } A = \begin{bmatrix} 1 & -3 \\ 1 & 0 \\ 1 & 6 \end{bmatrix}$$

$$A^T A x = A^T b$$

$$\underbrace{\begin{bmatrix} 1 & 1 & 1 \\ -3 & 0 & 6 \end{bmatrix}}_{A^T} \underbrace{\begin{bmatrix} 1 & -3 \\ 1 & 0 \\ 1 & 6 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} a_0 \\ a_1 \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} 1 & 1 & 1 \\ -3 & 0 & 6 \end{bmatrix}}_{A^T} \underbrace{\begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}}_{b}$$

$$\begin{bmatrix} 3 & 3 \\ 3 & 45 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 2 \\ 12 \end{bmatrix}$$

Using gaussian,

$$\left[\begin{array}{cc|c} 3 & 3 & 2 \\ 3 & 45 & 12 \end{array}\right] \qquad R_2 = R_2 - \tfrac{3}{3} R_1$$

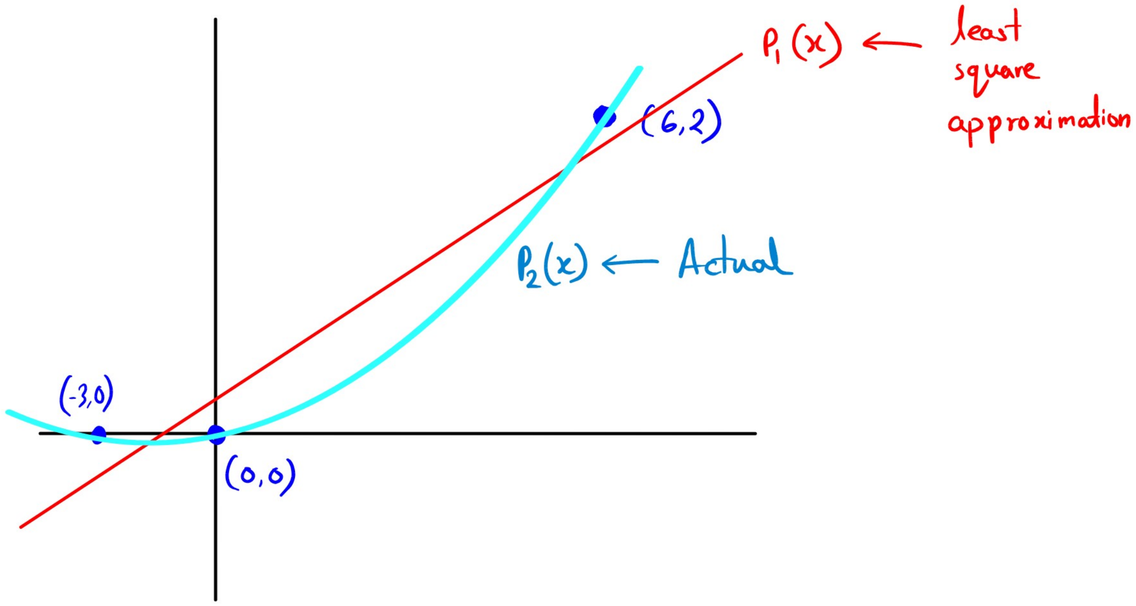
$$\left[\begin{array}{cc:c} 3 & 3 & 2 \\ 0 & 42 & 10 \end{array}\right]$$

$$\therefore \; 42\,a_1 = 10 \;, \quad a_1 = \frac{10}{42} = \frac{5}{21}$$

$$\therefore \; 3a_0 + 3a_1 = 2 \;, \quad a_0 = \frac{2 - 3\left(\frac{5}{21}\right)}{3} = \frac{3}{7}$$

$\therefore$ Least square approximation straight line is, $P_1(x) = \frac{3}{7} + \frac{5}{21}x$

Graphical Representation



Example 2: Find a two degree polynomial from the given points using least square approximation.

$$f(2) = 3 \qquad f(3) = 5 \qquad f(5) = 12 \qquad f(6) = 15$$

We know,

$$P_2(x) = a_0 + a_1 x + a_2 x^2$$

Therefore,

$$P_2(2) = a_0 + 2a_1 + 4a_2 = 3$$

$$P_2(3) = a_0 + 3a_1 + 9a_2 = 5$$

$$P_2(5) = a_0 + 5a_1 + 25a_2 = 12$$

$$P_2(6) = a_0 + 6a_1 + 36a_2 = 15$$

$$\therefore A = \begin{bmatrix} 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 5 & 25 \\ 1 & 6 & 36 \end{bmatrix}$$

$$A^T A x = A^T b$$

$$\Rightarrow \underset{3\times 4}{\begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 3 & 5 & 6 \\ 4 & 9 & 25 & 36 \end{bmatrix}} \underset{4\times 3}{\begin{bmatrix} 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 5 & 25 \\ 1 & 6 & 36 \end{bmatrix}} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 3 & 5 & 6 \\ 4 & 9 & 25 & 36 \end{bmatrix} \begin{bmatrix} 3 \\ 5 \\ 12 \\ 15 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} 4 & 16 & 74 \\ 16 & 74 & 376 \\ 74 & 376 & 2018 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 35 \\ 171 \\ 879 \end{bmatrix}$$

Solving using Gaussian

$$\left[\begin{array}{ccc|c} 4 & 16 & 74 & 35 \\ 16 & 74 & 376 & 171 \\ 74 & 376 & 2018 & 879 \end{array}\right]$$

$$R_2 = R_2 - \left(\frac{16}{4}\right) R_1$$

$$R_3 = R_3 - \left(\frac{74}{4}\right) R_1$$

$$\left[\begin{array}{ccc|c} 4 & 16 & 74 & 35 \\ 0 & 10 & 80 & 31 \\ 0 & 86 & 649 & 231.5 \end{array}\right]$$

$$R_3 = R_3 - \left(\frac{86}{10}\right) R_2$$

$$\left[\begin{array}{ccc|c} 4 & 16 & 74 & 35 \\ 0 & 10 & 80 & 31 \\ 0 & 0 & 9 & -16.5 \end{array}\right]$$

$$\therefore \quad 9a_2 = -16.5 \quad , \quad a_2 = -1.83$$

$$\therefore \quad 10a_1 + 80a_2 = 31 \quad , \quad a_1 = \frac{31 - 10(-1.83)}{10}$$

$$= 17.74$$

$$\therefore \quad 4a_0 + 16a_1 + 74a_2 = 35 \quad , \quad a_0 = \frac{35 - 16(17.74) - 74(-1.83)}{4}$$

$$= -28.355$$

$$\therefore \quad P_2(x) = -28.355 + 17.74x - 1.83x^2$$