Discrete Least Square Problems:

Example Given $(x_i, y_i)_{i=1}^{m}$

Can we find $a_0, \dots, a_n \in \mathbb{R}$

such that $P(x) = \sum_{j=0}^{n} a_j x^j$

Satisfies $P(x_i) = y_i \quad i=1, \dots, m$?

(Fit (x_i, y_i) with a polynomial $y = P(x)$)

Ans: Case 1: $m = n+1$

Yes (Lagrange polynomial interp.)

Case 2 $\quad n+1 > m$ (do not consider)

Case 3 $\quad n+1 < m$

Use a low order polynomial

to reconstruct the model as $y = P(x)$.

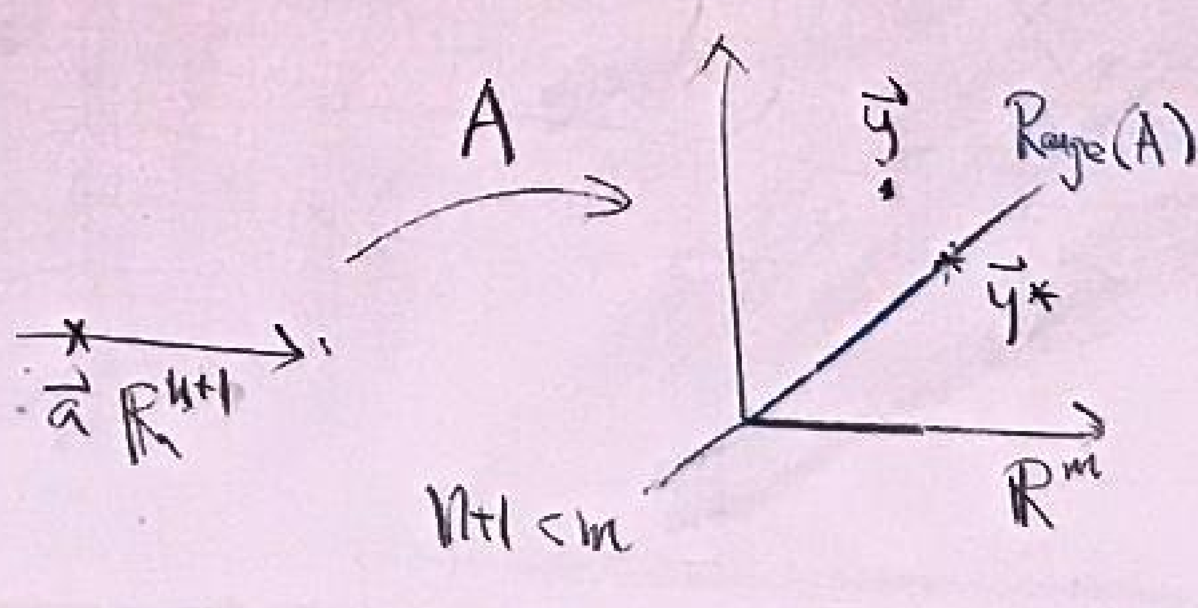
$n+1 < m$

$$a_0 + a_1 x_1^1 + \cdots + a_n x_1^n = y_1$$
$$\vdots \qquad\qquad\qquad\qquad \vdots$$
$$a_0 + a_1 x_m^1 + \cdots + a_n x_m^n = y_m$$

A linear system for the unknowns $(a_0, \cdots, a_n)$

$$A\vec{a} = \vec{y}$$

$\vec{a} \in \mathbb{R}^{n+1}$ $\quad \vec{y} \in \mathbb{R}^m$



$A\vec{a} = \vec{y}$ has no solution

if $\vec{y} \notin \text{Range}(A)$.

Instead, we can do

(1) Find $\vec{y}^* = \begin{pmatrix} \text{Projection of } \vec{y} \\ \text{onto Range}(A) \end{pmatrix}$

$\Updownarrow$ and solve $A\vec{a} = \vec{y}^*$

(2) $\underset{\vec{a} \in \mathbb{R}^{n+1}}{\text{Minimize}} \; \|A\vec{a} - \vec{y}\|^2$

where $\vec{x} \in \mathbb{R}^m$, $\|\vec{x}\|^2 = \sum_{i=1}^{m} x_i^2$

Reformulate Find $a_0 \dots a_n$

to minimize $E = \sum_{i=1}^{m} (y_i - P(x_i))^2$

where $P(x) = a_0 + a_1 x + \dots + a_n x^n$.

Solve. $E = \sum_{i=1}^{m} \left(y_i - \sum_{j=0}^{n} a_j x_i^j\right)^2$

Formally $E = \|A\vec{a} - \vec{y}\|^2 = (A\vec{a} - \vec{y})^T (A\vec{a} - \vec{y})$

$$= \vec{a}^T A^T A \vec{a} - \vec{y}^T A \vec{a} - \vec{a}^T A^T \vec{y} + \vec{y}^T \vec{y}$$

$$= \vec{a}^T \underline{A^T A} \vec{a} - 2(\vec{a}^T A^T \vec{y}) + \underline{\vec{y}^T \vec{y}}$$

$$\partial_{\vec{a}} = 0 \Rightarrow 2A^T A \vec{a} - 2A^T \vec{y} = 0$$

$A^T A \vec{a} = A^T \vec{y}$ (normal equation)

<u>Example</u> Find $a, b \in \mathbb{R}$ that minimizes $\sum_{k=1}^{3} ((ax_k+b)-y_k)^2$

<u>Ans</u>: $E = \sum_{k=1}^{3} ((ax_k+b)-y_k)^2$

$$\frac{\partial E}{\partial a} = 2\sum_{k=1}^{3} ((ax_k+b)-y_k)(x_k) = 0$$

$$\frac{\partial E}{\partial b} = 2\sum_{k=1}^{3} ((ax_k+b)-y_k)(1) = 0$$

$$\cancel{2} \begin{pmatrix} \sum_{k=1}^{3} x_k^2 & \sum_{k=1}^{3} x_k^1 \\ \sum_{k=1}^{3} x_k^1 & \sum_{k=1}^{3} \underbrace{x_k^0}_{1} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \cancel{2} \begin{pmatrix} \sum x_k y_k \\ \sum 1 \cdot y_k \end{pmatrix}$$

<u>Note</u>: $A\vec{a} = \begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$ $\quad \vec{y} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$

$A^T A \vec{a} = ?$ $\quad A^T \vec{y} = ?$

Rm

$$\begin{pmatrix} \sum_{k=1}^{3} x_k^0 & \sum_{k=1}^{3} x_k^1 \\ \sum_{k=1}^{3} x_k^1 & \sum_{k=1}^{3} x_k^2 \end{pmatrix} \begin{pmatrix} b \\ a \end{pmatrix} = RHS$$

In general

$$\begin{pmatrix} \sum_{k=1}^{m} x_k^0 & \sum_{k=1}^{m} x_k^1 & \cdots & \sum_{k=1}^{m} x_k^n \\ \vdots & & & \\ \sum_{k=1}^{m} x_k^n & \sum_{k=1}^{m} x_k^{n+1} & \cdots & \sum_{k=1}^{m} x_k^{2n} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} = RHS$$

(similar to Hilbert matrix

$$\parallel$$

H ~~(Hilbert matrix)~~

(Hilbert matix: see page 486 and 519)

$$H_{\tilde{i}\tilde{j}} = \sum_{k=1}^{m} x_k^{\tilde{i}+\tilde{j}} \quad 0 \le \tilde{i}, \tilde{j} \le n$$

or

$$H_{ij} = \sum_{k=1}^{m} x_k^{i+j-2} \quad 1 \le i, j \le n+1$$

Note For this problem,

rank $(A) = n+1$, if $m \ge n+1$

A has full rank, $A^T A$ is nonsingular

Example How to fit the data

$(x_k, y_k)_{k=1}^{m}$ with $y = be^{ax}$

or $y = bx^a$?

Ans. $\min_{a,b\in\mathbb{R}} \begin{cases} (y_k - be^{ax_k})^2 \\ (y_k - bx_k^a)^2 \end{cases}$

For example

take $E = \sum (y_k - be^{ax_k})^2$

$$\frac{\partial E}{\partial a} = 2\sum_k (y_k - be^{ax_k})(-bx_k e^{ax_k}) = 0$$

$$\frac{\partial E}{\partial b} = 2\sum_k (y_k - be^{ax_k})(-e^{ax_k}) = 0$$

Solve for (a, b)

Nonlinear system of equations

Not a good model

Alternative

$$y = b e^{ax}$$
$$(\text{or } b x^a)$$

$$\Rightarrow \ln y = \ln b + ax$$
$$\text{or } (\ln b + a \ln x)$$

$$\tilde{E} = \sum_k \left((\ln b + a x_k) - \ln y_k \right)^2$$
$$\text{or } \sum_k \left((\ln b + a \ln x_k) - \ln y_k \right)^2$$

= Quadratic in $(a, \ln b)$

$\Rightarrow$ Get linear system in $(a, \ln b)$