Linear Least Squares

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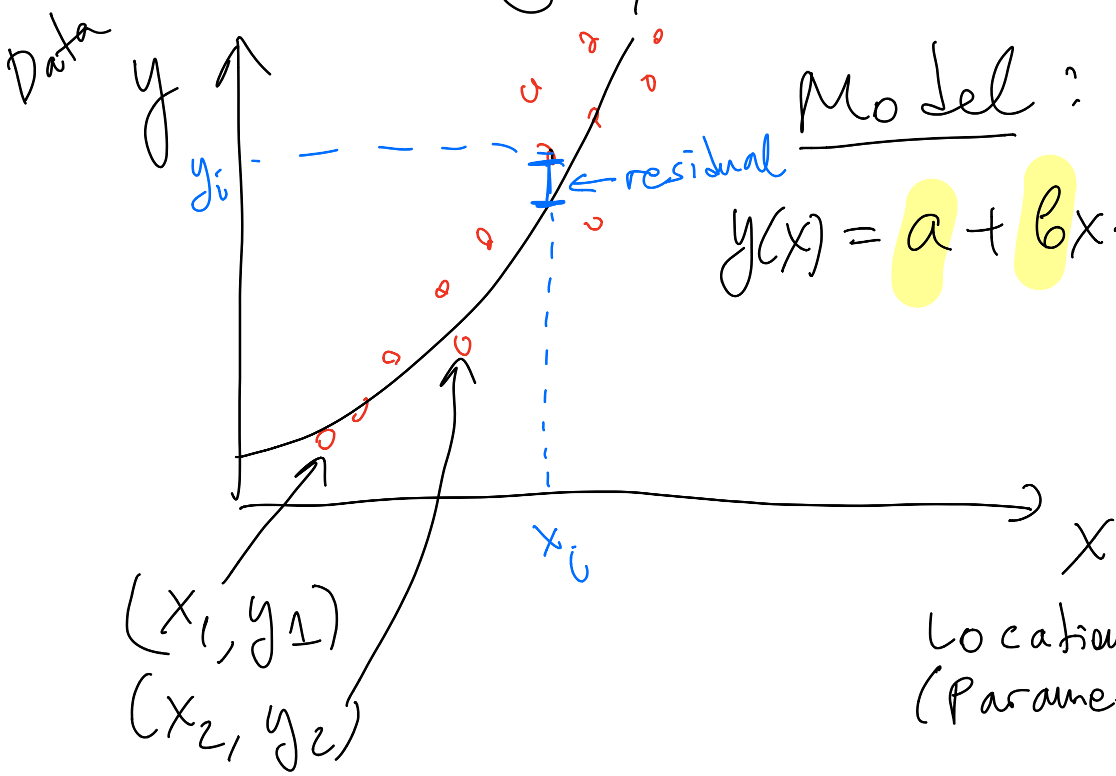
Fitting / regression



Model:

$$y(x) = a + bx + cx^2$$

Locations (Parameters)

$$y_i = a + b x_i + c x_i^2 + \varepsilon_i$$

$$|\varepsilon_i| \ll |y_i|$$

"noise" or "modeling error"

"Best fit"

$$r_i = y_i - (a + b x_i + c x_i^2) = \varepsilon_i$$

$\uparrow$ residual

$$(a,b,c)_{best} = \underset{a,b,c}{\arg\min} \|\vec{r}\|_2^2 = \sum_{i=1}^{n} |r_i|^2$$

Least squares fit

$$\overleftrightarrow{X} = \begin{array}{c} 1 \rightarrow \\ \\ \\ n \rightarrow \end{array} \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{bmatrix} \qquad \vec{p} = \begin{bmatrix} a \\ b \\ c \end{bmatrix}$$

$$\begin{array}{ccc} a & b & c \end{array}$$

$$\vec{r} = \overleftrightarrow{X}\,\vec{p} - \vec{y}$$

$$r_1 = (a + b x_1 + c x_1^2) - y_1$$

$$\vec{y}_{model}(\vec{p}) = \underbrace{\overleftrightarrow{X}\vec{p}}_{\text{linear mapping}}$$

linear least squares

Instead: $\cancel{y} = e^{-ax} \cdot \cos(bx)$

non linear least squares

$$y = a\cos(x) + b e^x \quad \checkmark$$

$$\boxed{\vec{p} = \arg\min_{\vec{p}} \left\| \overleftrightarrow{X}\vec{p} - \vec{y} \right\|_2^2}$$

How to find p?

$y = X p$ (notation)

Overdetermined

"p solves $y = Xp$ in the least squares sense"

$p = X \setminus y$ in Matlab works

$$Ax = b$$

Formula for the fit and x data

$A = [m \times n]$

$m \gg n$

$x = [n \times 1]$ unknown parameters

$b = [m \times 1]$ ydata

Linear Space of all solutions is $\mathrm{im}(A)$

If $b \in \mathrm{im}(A)$ there $\exists x$

$$\begin{cases} A x_1 = b \\ A x_2 = b \end{cases}$$

Imagine two distinct solutions

$$A x_1 - A x_2 = 0$$

If A is full-rank $x_1 = x_2$

$$A(x_1 - x_2) = 0$$

$$Ax = 0$$

- infinitely many
- no nonzero solutions

$$\begin{bmatrix} 1 & 2 \\ 1 & 2 \\ 1 & 2 \end{bmatrix}$$

$A = [m \times n] \quad m > n$

If cols are linearly independent, then $\text{rank}(A) = n$ (full-rank matrix)

$\Rightarrow x = 0$

$\Rightarrow$ If A is full-rank,
and $b \in \operatorname{im}(A)$,
then x is unique

$$y = a\,x + bx^2 + cx$$
$$= (a+c)x + bx^2$$

$\Rightarrow$ a/c not unique

$$A = \begin{bmatrix} x_1 & x_1^2 & x_1 \\ x_2 & x_2^2 & x_2 \\ - & - & - \\ x_n & x_n^2 & x_n \end{bmatrix}$$

$$y = x_1 f(x) + x_2 g(x) + x_3 h(x) \ldots$$

$f(x)$, $g(x)$ and $h(x)$ are linearly independent

$$f(x) = \cos(x)$$
$$g(x) = \sin(x)$$
$$h(x) = \cos(x + \pi/4)$$
$$= .. \cos(x) + .. \sin(x)$$

$Ax = b$, $A = [m \times n]$
$m > n$
full-rank

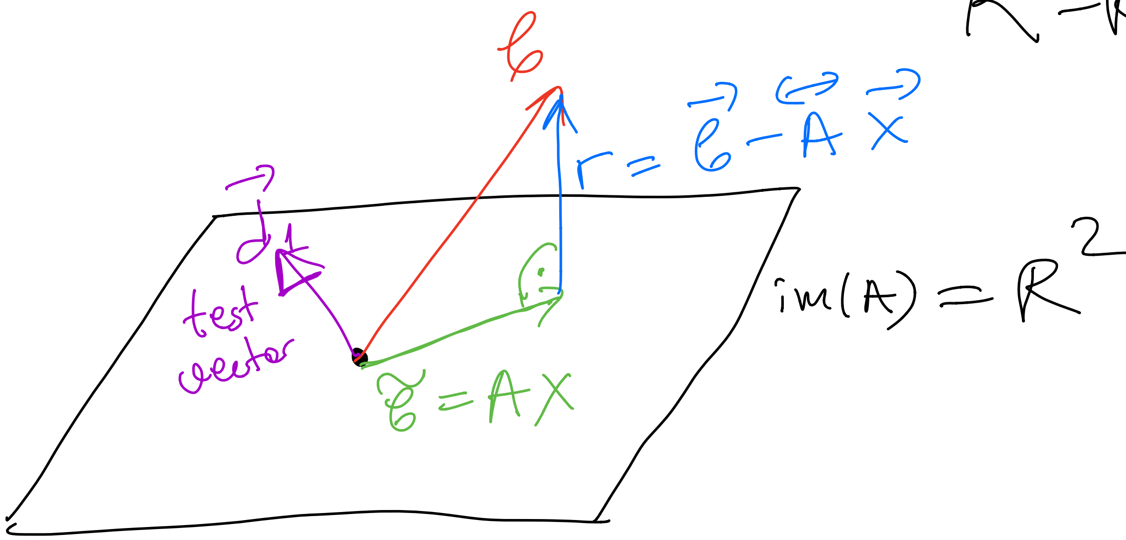
If $b \in \operatorname{Im}(A) \Rightarrow x$ is unique

$$Ax = \tilde{b} = \mathrm{Proj}_{\operatorname{Im}(A)} b$$

||| equivalent

least squares problem

$\mathbb{R}^m = \mathbb{R}^3$



$$r \perp \mathrm{im}(A)$$

$$(b - Ax) \perp \mathrm{im}(A)$$

$$r \cdot \mathrm{im}(A) = 0$$

$$\begin{cases} r \cdot d_1 = 0 \\ r \cdot d_2 = 0 \end{cases}$$

d_1 & d_2 lin. ind.

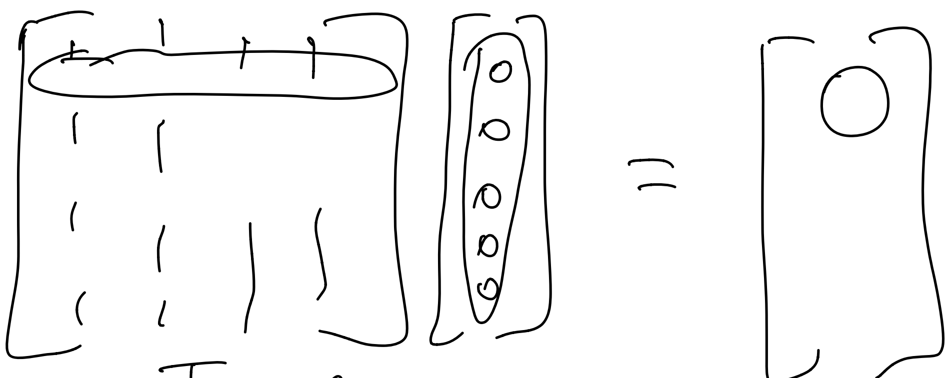
$\{d_1, d_2\}$ is a basis $\mathrm{im}(A)$

$\{a_1, a_2, \ldots, a_n\}$ are the basis of $m(A)$

$$a_i \cdot (b - Ax) = 0 \quad \forall i$$

$i = 1, \ldots, n$

columns of A
$=$
rows of A^T



$$A^T (b - Ax) = 0$$

$[n \times m][m \times 1] = [n \times 1]$

$$(A^T A)x = A^T b$$

normal equations

$$A^T A = [n \times m][m \times n] = [n \times n]$$

Square linear system of size n

If A is full-rank $\Rightarrow$
$A^T A$ is non-singular

$$B = A^T A$$

$$B^T = (A^T)(A^T)^T = A^T A = B$$

$B^T = B$, B is symmetric, positive definite

(all eigs are real & positive)

$$B = L L^T$$ Cholesky factorization

diagonal entries of L are positive

In Matlab

$$(A^T A)x = A^T b$$

$$x = (A' * A) \backslash (A' * b)$$ ✗

will use Cholesky

computes the same answer as

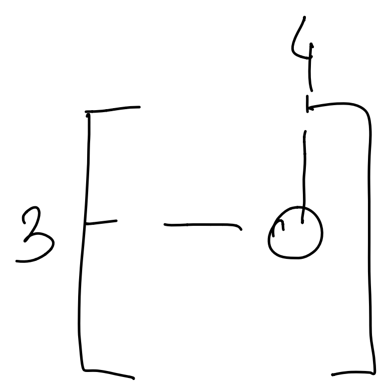
$$x = A \backslash b$$ ✓

<u>Cost</u> of normal equations method

$$B = A^T A$$

$$A = [m \times n]$$

$$A^T = [n \times m]$$



$$\text{FLOPS} = O(m n^2)$$

n^2 answers

$$\tilde{b} = A^T b = O(mn) \text{ FLOPS}$$

$$[n \times m] \times [m \times 1]$$

$$\underline{\underline{mn^2}} > mn$$

$$B x = \tilde{b} \xrightarrow{\text{solve}} O(n^3)$$

$$[n \times n] \times [n \times 1]$$

$$\begin{cases} mn^2 \gg n^3 \\ m \gg n \end{cases}$$

Total cost $\simeq O(mn^2)$