Least Squares

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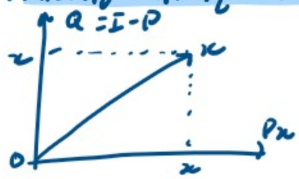
Pythagoras Theorem

Let $x \in \mathbb{R}^n$, $P \rightarrow$ orthogonal projection matrix, $Q = I - P$.

$\therefore \|x\|_2^2 = \|P\|_2^2 + \|Qx\|_2^2$



$$\|x\|_2^2 = \langle x, x\rangle = \langle Ix, Ix\rangle$$
$$= \langle (P+Q)x, (P+Q)x\rangle$$
$$= \langle Px, Px\rangle + \langle Px, Qx\rangle + \langle Qx, Px\rangle + \langle Qx, Qx\rangle$$
$$= \|Px\|_2^2 + 2\langle Px, Qx\rangle + \|Qx\|_2^2$$

If $\langle Px, Qx\rangle = 0$, $\langle Px, Qx\rangle = Px^T Qx = x^T P^T Qx$

$P^T = P$ $\quad : x^T \underbrace{PQ}_{0} x = 0 \longrightarrow \|x\|_2^2 = \|Px\|_2^2 + \|Qx\|_2^2$

1.3 Least Squares & Projection onto R(A)

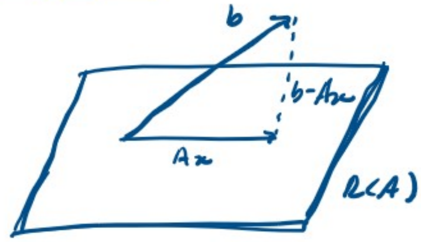
$Ax = b$ has soln. if $b \in R(A)$. What if $b \notin R(A)$? ($Ax = \vec{b} \longrightarrow$ no solution)

Find vector x s.t. $Ax \in R(A)$ & Ax is as close as possible to $\vec{b}$ in $R(A)$

$\rightarrow$ Find vector x_0 s.t. $Ax_0 \in R(A)$ & $\|Ax_0 - b\|$ is minimized

$\rightarrow Ax_0 = \text{proj}_{R(A)} b$, $P_{R(A)}$ is proj matrix onto $R(A)$

$Q\vec{b} = \underbrace{(I-P)\vec{b}}_{= b - Ax_0} \perp R(A) \rightarrow b - Ax_0 \perp R(A)$



$R(A)^T = N(A)^T \rightarrow Ax_0 - b \in R(A)^T = N(A^T)$

$\rightarrow A^T(Ax_0 - b) = 0$

$\rightarrow A^T A x_0 = A^T b \longrightarrow$ Least Squares equation

$\therefore$ every x_0 satisfying eqn. = least square solution.
Ax_0 = proj of b onto $R(A)$

Properties

- L.S.E. always has a solution
  - $\hookrightarrow A^T A x = A^T b$ has soln. if $A^T b \in R(A^T A)$. $R(A^T) = R(A^T A)$ $\therefore N(A) = N(A^T A)$
- If $A^T A$ is invertible, least square soln. is unique
  - $\hookrightarrow A^T A x_0 = A^T b \quad x_0 = (A^T A)^{-1} A^T b$ $\therefore$ unique soln.
- let A be an orthogonal projection matrix ($A^2 = A$, $A^T = A$)

LSE: $A^T A x = A^T b \longrightarrow AAx = A^T b$
$A^T = A \longrightarrow A^2 x = Ab$
$A^2 = A \longrightarrow Ax = Ab$

$\therefore x = Ab \rightarrow$ soln. of least square eqn.

ex. $A = \begin{bmatrix} 0 & 1 \\ 0 & -1 \\ 0 & 0 \end{bmatrix}$ $b = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$ is $b \in R(A)$?

→ no soln. for $b = Ax$ ∴ Find L.S. soln.

$Ax = b \longrightarrow A^T A x = A^T b$

$$A^T A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & -1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix} \quad A^T b = \begin{bmatrix} 1 & 0 & 0 \\ 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\therefore A^T A x = A^T b \longrightarrow \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix} x = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$\because \det \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix} = 2-1 \neq 0$, $\begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}$ → invertible.

$\therefore x_{LS} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{2-1} \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \begin{bmatrix} 3 \\ -2 \end{bmatrix}$ → unique soln. for $A^T A x = A^T b$

l_2 dist. b/w Ax_{LS} & b: $Ax_{LS} = \begin{bmatrix} 1 & 1 \\ 0 & -1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 3 \\ -2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix}$

$\left\| \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} - \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix} \right\|_2^2 = \sqrt{9} = 3$ ∴ min. dist. b/w b & $R(A) = 3$

orthog. proj onto $R(A)$: $P = A(A^T A)^{-1} A^T$

$$Pb = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

- If $A^T A$ not invertible:
  - Cols of A = lin. dependent

Find proj. onto $R(A)$:

i) Find basis for $R(A)$ → G.E.

ii) Write basis vectors as column vectors in matrix $\tilde{A}$

iii) ∵ columns of $\tilde{A}$ = lin. independent, $\tilde{A}^T A$ = invertible & proj. onto $R(\tilde{A})$:

→ $P_{R(\tilde{A})} = \tilde{A}(\tilde{A}^T \tilde{A})^{-1} \tilde{A}^T$

− ∵ columns of $\tilde{A}$ form basis for $R(A)$, $R(\tilde{A}) = R(A)$

& $P_{R(A)} = \tilde{A}(\tilde{A}^T \tilde{A})^{-1} \tilde{A}^T$

Least Square equation always has a soln.

→ Prove that $N(A) = N(A^T A)$

$N(A) \subseteq N(A^T A)$: $x \in N(A)$, then $Ax = 0 \rightarrow A A^T x = 0 \rightarrow x \in N(A^T A)$

$N(A^T A) \subseteq N(A)$: $x \in N(A^T A)$, then $A^T A = 0 \rightarrow Ax \in N(A^T) = [R(A)]^\perp$

$\rightarrow Ax \in [R(A)]^\perp$ $Ax \perp R(A)$ $Ax \perp \{Ay : y \in \mathbb{R}^m\}$ $Ax \perp Ay$ for $y \in \mathbb{R}^m$

$Ax \perp Ax \longrightarrow Ax = 0$ $x \in N(A)$