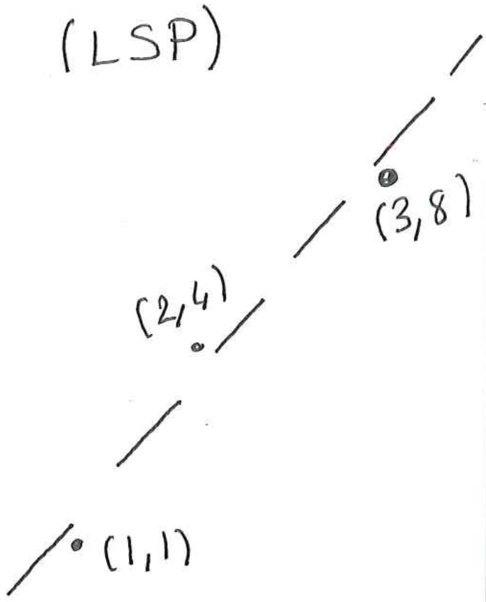
Least Squares Problem (LSP)



(1,1) (2,4) (3,8)

Find line

$$l(t) = x_2 t + x_1$$

through these points.

$$x_2 + x_1 = 1 \quad (\text{as } l(1) = 1)$$
$$2x_2 + x_1 = 4 \quad (\text{as } l(2) = 4)$$
$$3x_2 + x_1 = 8$$

No solution, no such line.

Instead find x_1, x_2 s.t.

$$\left\| \begin{bmatrix} 1 - (x_2 + x_1) \\ 4 - (2x_2 + x_1) \\ 8 - (3x_2 + x_1) \end{bmatrix} \right\|_2$$

is as small as possible. That is minimize

$$\left\| \begin{bmatrix} 1 \\ 4 \\ 8 \end{bmatrix} - \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right\|_2$$

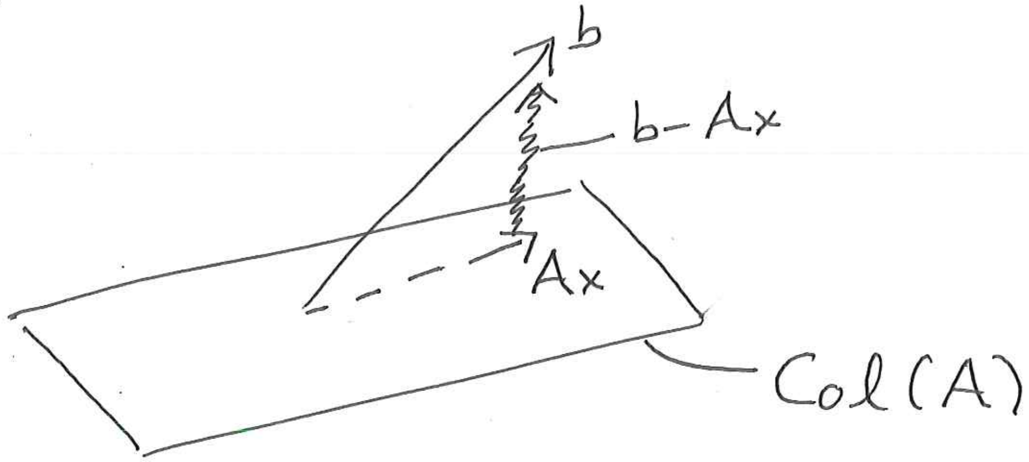
over x_1, x_2; a least squares problem.

Problem statement

Given $A \in \mathbb{C}^{n\times p}$, $b \in \mathbb{C}^n$. Solve

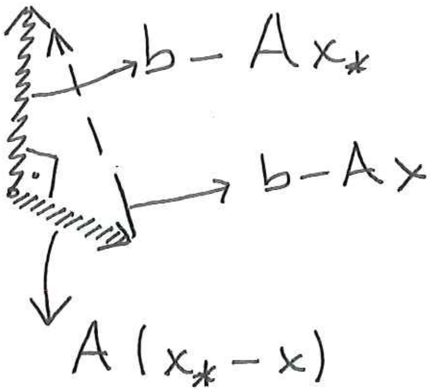
$$\min_{x\in\mathbb{C}^p} \|b - Ax\|_2 ,$$

find also minimizing $x \in \mathbb{C}^p$.



Let $x_* \in \mathbb{C}^p$ be such that

* $(b - Ax_*) \in \mathrm{Col}(A)^\perp$
* equivalently Ax_* is the orthogonal projection of b onto Col(A).



For every $x \in \mathbb{C}^p$ by the Pythagorean thm

$$\|b - Ax\|_2^2 = \|b - Ax_*\|_2^2 + \|A(x_* - x)\|_2^2$$

$$\Longrightarrow \|b - Ax_*\|_2 \leq \|b - Ax\|_2$$

(Indeed,

$$\|b - Ax_*\|_2 < \|b - Ax\|_2$$

unless Ax is not the orthogonal proj. of b onto $Col(A)$)

<u>THM</u>

The following are equivalent:

(1) $\|b - Ax_*\| \leq \|b - Ax\|_2 \; \forall x \in \mathbb{C}^p$.

(2) $(b - Ax_*) \in Col(A)^\perp$

(3) ~~to~~ Ax_* is the orthogonal projection of b onto $Col(A)$.

Ex

$$\min_{x_1, x_2} \left\| \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{2} \\ 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & -1/\sqrt{2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right\|_2$$

x_* such that

$$\begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{2} \\ 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & -1/\sqrt{2} \end{bmatrix} x_* = \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{2} \\ 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & -1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 5/6 \\ 1/3 \\ -1/6 \end{bmatrix}$$

solves the LSP, i.e., $x_* = \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{2} \end{bmatrix}$.

Numerical Solution

Most commonly using the (reduced) QR factor.

$$\underset{\substack{n\times p \\ n \geq p}}{A} = \underset{\substack{n\times p \\ \text{orthonormal} \\ \text{columns}}}{\hat{Q}} \; \underset{\substack{p\times p \\ \text{upper} \\ \text{triangular}}}{\hat{R}}$$

Assume rank $(A) = p$.

Orthogonal projector onto Col (A): $\hat{Q}\hat{Q}^*$

$$A x_* = \hat{Q}\hat{Q}^* b$$

$$\hat{Q}\hat{R} x_* = \hat{Q}\hat{Q}^* b$$

$$\Longrightarrow \quad \hat{R} x_* = \underbrace{\hat{Q}^* b}$$

Ex

$$\min_{x_1, x_2 \in \mathbb{R}} \left\| \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 1 & 3 \\ 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right\|_2$$

$$\begin{pmatrix} \text{Reduced} \\ \text{QR} \\ \text{factor.} \end{pmatrix} \quad \begin{bmatrix} 1 & 3 \\ 1 & 1 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{2} \\ 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & -1/\sqrt{2} \end{bmatrix} \begin{bmatrix} \sqrt{3} & \sqrt{3} \\ 0 & 2\sqrt{2} \end{bmatrix}$$

$$\begin{bmatrix} \sqrt{3} & \sqrt{3} \\ 0 & 2\sqrt{2} \end{bmatrix} x_* = \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{2} \end{bmatrix}$$

$x_* = \begin{bmatrix} 1/12 \\ 1/4 \end{bmatrix}$ solves the LSP.

Procedure

① Compute a reduced QR factor. by Householder reflectors

$$A = \hat{Q}\hat{R} \qquad \sim 2np^2 - \frac{2p^3}{3} \text{ flops}$$

② Form $\hat{b} = \hat{Q}^* b$ $\qquad \sim 4np - 2p^2$ flops

③ Solve

$$\hat{R} x_* = \hat{b} \qquad \sim p^2 \text{ flops}$$

by back substitution.

Stage ②

$$A = \underbrace{[\hat{Q} \;\; \tilde{Q}]}_{Q} \underbrace{\begin{bmatrix} \hat{R} \\ 0 \end{bmatrix}}_{R}$$

- full QR (led by the Householder reflectors)

$$\hat{b} = \underbrace{(Q^* b)(1:p)}_{\text{1st } p \text{ components of } Q^* b}$$

Recall

$$Q = Q_1 Q_2 \cdots Q_p$$

$$Q^* = Q_p^* \cdots Q_2^* Q_1^* = Q_p \cdots Q_2 Q_1$$

where $Q_j = \begin{bmatrix} I_{j-1} & 0 \\ 0 & I_{n-j+1} - 2q_j q_j^* \end{bmatrix}$ $j = 1, \dots, p$

$Q^* b$ can be formed as follows

$$b^{(1)} = Q_1 b$$

$$b^{(2)} = Q_2 b^{(1)}$$

$$\vdots$$

$$(Q^* b =) b^{(p)} = Q_p b^{(p-1)}$$

Pseudocode

for $j = 1, \dots, p$

$b(j:n) \longleftarrow b(j:n) - 2 q_j (q_j^* b(j:n))$

end

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① $\sim 2(n-j)$ flops

② $\sim (n-j)$ flops

③ $\sim (n-j)$ flops

Total # flops $\sim \sum_{j=1}^{p} 4(n-j)$

$\sim 4np - 2p^2$

Back-substitution to solve

$$\begin{bmatrix} \hat{r}_{11} & \cdots & \hat{r}_{1(n-1)} & \hat{r}_{1n} \\ & \ddots & & \vdots \\ 0 & & \hat{r}_{(n-1)(n-1)} & \hat{r}_{(n-1)n} \\ & & & \hat{r}_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_{n-1} \\ b_n \end{bmatrix}$$

$$x_n = b_n / \hat{r}_{nn}$$

$$x_{n-1} = \{ b_{n-1} - \hat{r}_{(n-1)n} x_n \} / \hat{r}_{(n-1)(n-1)}$$

$$\vdots$$

$$x_1 = \{ b_1 - \sum_{k=2}^{n} \hat{r}_{1k} x_k \} / \hat{r}_{11}$$

Pseudocode

for $j = n$ down to 1
  $x_j \leftarrow b_j$
  for $k = j+1, \ldots, n$
    $x_j \leftarrow x_j - \hat{r}_{jk} x_k$
  end
  $x_j \leftarrow x_j / \hat{r}_{jj}$
end

Total # flops $\sim \sum_{j=1}^{n} \sum_{k=j+1}^{n} 2$

$$= \sum_{j=1}^{n} 2(n-j) \sim n^2$$