LECTURE 12

SOLUTION OF THE LEAST SQUARES PROBLEM BY QR FACTORIZATION

$$\text{(LSP)} \quad \underset{x \in \mathbb{C}^n}{\text{minimize}} \; \|Ax - b\|_2$$

$$A = \begin{bmatrix} \; \end{bmatrix} \in \mathbb{C}^{m \times n} \qquad x = \begin{bmatrix} \; \end{bmatrix} \in \mathbb{C}^n \qquad b = \begin{bmatrix} \; \end{bmatrix} \in \mathbb{C}^m$$

where $m > n$

Recall that the 2-norm is invariant under unitary transformations (that is $\|Qb\|_2 = \|b\|_2$ for all unitary $Q \in \mathbb{C}^{m \times m}$).

Therefore

$$\begin{aligned} \|Ax - b\|_2 &= \|QRx - b\|_2 \\ &= \|Q^*QRx - Q^*b\|_2 \\ &= \|Rx - Q^*b\|_2 \end{aligned}$$

implying

$$\underset{x \in \mathbb{C}^n}{\text{minimize}} \; \|Ax - b\| = \underset{x \in \mathbb{C}^n}{\text{minimize}} \; \|Rx - Q^*b\|.$$

Partition $R \in \mathbb{C}^{m \times n}$ and $Q^* b$ as follows.

$$R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = \begin{bmatrix} \\ 0 \end{bmatrix} \quad \text{where } R_1 \in \mathbb{C}^{n \times n} \text{ is upper triangular}$$

$$Q^* b = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad \text{where} \quad \begin{matrix} b_1 \in \mathbb{C}^{n} \\ b_2 \in \mathbb{C}^{m-n} \end{matrix}$$

Notice that

$$\| Ax - b \|_2 = \Bigg\| \underbrace{\begin{bmatrix} R_1 \\ 0 \end{bmatrix}}_{R} x - \underbrace{\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}}_{b} \Bigg\|_2$$

$$= \left\| \begin{bmatrix} R_1 x - b_1 \\ -b_2 \end{bmatrix} \right\|_2$$

$$= \sqrt{\begin{bmatrix} (R_1 x - b_1)^* & (-b_2)^* \end{bmatrix} \begin{bmatrix} R_1 x - b_1 \\ -b_2 \end{bmatrix}}$$

$$= \sqrt{(R_1 x - b_1)^* (R_1 x - b_1) + b_2^* b_2}$$

$$= \sqrt{\| R_1 x - b_1 \|_2^2 + \underbrace{\| b_2 \|^2}_{\substack{\text{positive constant} \\ \text{(independent of } x)}}}$$

Consequently

$$\boxed{\begin{aligned} &\underset{x\in\mathbb{C}^n}{\text{minimize}}\ \|Ax-b\|_2 = \|A\hat{x}-b\|_2 \\ &\qquad\qquad\qquad\qquad = \|b_2\|_2 \\ &\text{where} \\ &\hat{x} \text{ is a solution of } \underbrace{R_1}_{\substack{n\times n \\ \text{upper} \\ \text{triangular}}} x = \underbrace{b_1}_{\text{in } \mathbb{C}^n} \end{aligned}}$$

EXAMPLE

- Consider the LSP

$$\underset{x\in\mathbb{R}^2}{\text{minimize}} \left\| \underbrace{\begin{bmatrix} 1 & 2 \\ 1 & 2 \\ 0 & 1 \end{bmatrix}}_{A} x - \underbrace{\begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}}_{b} \right\|_2 .$$

- Given the QR factorization

$$\underbrace{\begin{bmatrix} 1 & 2 \\ 1 & 2 \\ 0 & 1 \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 \end{bmatrix}}_{Q} \underbrace{\begin{bmatrix} \overbrace{\begin{matrix} \sqrt{2} & 2\sqrt{2} \\ 0 & 1 \end{matrix}}^{R_1} \\ \begin{matrix} 0 & 0 \end{matrix} \end{bmatrix}}_{R}$$

Exploiting the QR factorization

$$\|Ax-b\|_2 = \|Rx - Q^*b\|_2 = \left\| \begin{bmatrix} \overbrace{\begin{matrix} \sqrt{2} & 2\sqrt{2} \\ 0 & 1 \end{matrix}}^{R_1} \\ \begin{matrix} 0 & 0 \end{matrix} \end{bmatrix} x - \begin{bmatrix} \overbrace{\begin{matrix} -1/\sqrt{2} \\ 1 \end{matrix}}^{b_1} \\ \underbrace{-3/\sqrt{2}}_{b_2} \end{bmatrix} \right\|_2$$

Therefore

$$\underset{}{\text{minimize}} \; \|Ax-b\|_2 = \|A\hat{x}-b\|_2 = \|b_2\|_2 = 3/\sqrt{2}$$

where $\hat{x}$ is the solution of

$$\underbrace{\begin{bmatrix} \sqrt{2} & 2\sqrt{2} \\ 0 & 1 \end{bmatrix}}_{R_1} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \underbrace{\begin{bmatrix} -1/\sqrt{2} \\ 1 \end{bmatrix}}_{b_1}$$

$$\Longrightarrow \hat{x} = \begin{bmatrix} -5/2 \\ 1 \end{bmatrix},$$

PROCEDURE (TO SOLVE LSP)

1. Compute a full QR factorization

$$A = \underbrace{Q}_{m\times m}\underbrace{R}_{m\times n}$$

2. Partition R and Q^*b

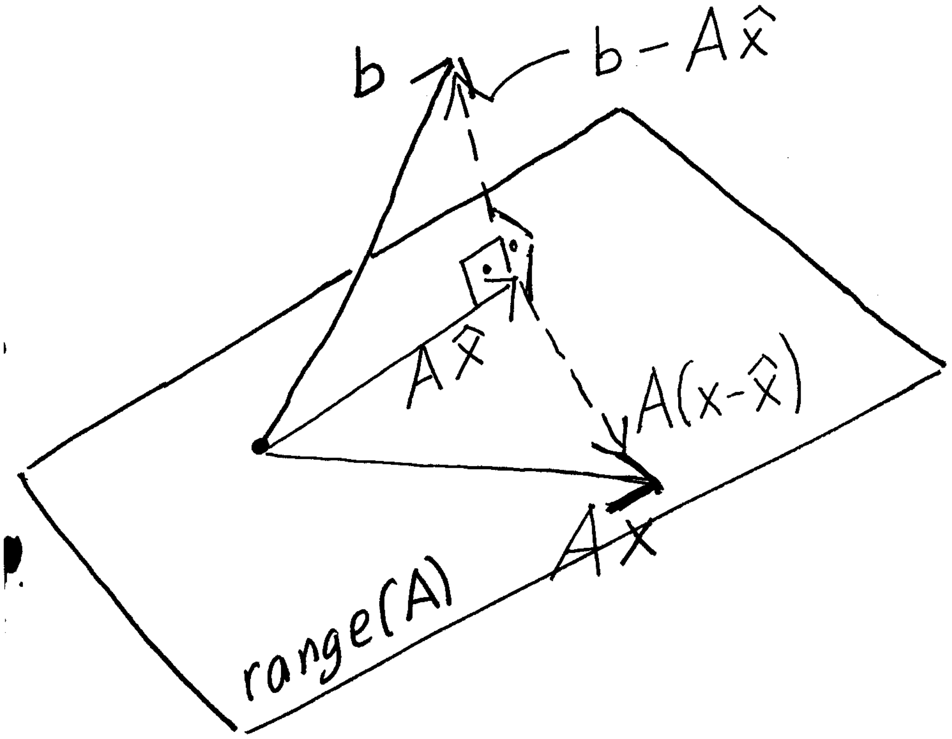
$$R = \begin{bmatrix} R_1 \\ R_2 \end{bmatrix} \begin{matrix} \leftarrow n\times n \\ \leftarrow (m-n)\times n \end{matrix} \qquad Q^*b = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \begin{matrix} \text{in } \mathbb{C}^n \\ \text{in } \mathbb{C}^{m-n} \end{matrix}$$

3. Solve the upper triangular system

$$R_1\hat{x} = b_1$$

4. $$\underset{x\in\mathbb{C}^n}{\text{minimize}} \; \|Ax-b\|_2 = \underbrace{\|b_2\|_2}_{\text{minimal distance}} = \|A\underbrace{\hat{x}}_{\text{minimizing } x}-b\|_2$$

NORMAL EQUATIONS FOR THE LEAST SQUARES PROBLEM



THM

A solution $\hat{x} \in \mathbb{C}^n$ of LSP must satisfy

$$(*) \quad b - A\hat{x} \perp \operatorname{range}(A)$$

PROOF

Suppose $\hat{x}$ is such that

$$b - A\hat{x} \perp \operatorname{range}(A)$$

and $x \neq \hat{x}$ is any vector such that

$$b - Ax \not\perp \operatorname{range}(A).$$

But then by the Pythagorean thm

$$\|b - Ax\|_2^2 = \|b - A\hat{x}\|_2^2 + \underbrace{\|A(x-\hat{x})\|_2}_{>0}$$

Therefore

$$\|b - Ax\|_2 > \|b - A\hat{x}\|_2$$

implying x is not a solution to LSP. $\square$

Eqn (*) implies

$$a_1^* (b - A\hat{x}) = 0$$
$$a_2^* (b - A\hat{x}) = 0$$
$$\vdots$$
$$a_n^* (b - A\hat{x}) = 0$$

$$\Longrightarrow$$

$$\underbrace{\begin{bmatrix} a_1^* \\ \vdots \\ a_n^* \end{bmatrix}}_{A^*} (b - A\hat{x}) = 0$$

The solution $\hat{x} \in \mathbb{C}^n$ of LSP satisfies

$$\boxed{\text{NORMAL EQUATION}} \quad \underbrace{A^* A}_{n \times n} \hat{x} = \underbrace{A^* b}_{\text{in } \mathbb{C}^n}$$