Least Squares Problem
(Reminders from Lecture 13)

Problem Statement

Given $A \in \mathbb{C}^{n \times p}$ with $n > p$, and $b \in \mathbb{C}^{n}$,

- solve
$$\min_{x \in \mathbb{C}^p} \|b - Ax\|_2,$$
- find also minimizing x.

Optimal Solution

Theorem

The following are equivalent:

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

(2) Ax_* *is the orthogonal projection of b onto* $Col(A)$.

Numerical Solution

Let $A = \widehat{Q}\widehat{R}$ be a reduced QR factorization. The solution x_* of LSP satisfies

$$\widehat{R}x_* = \widehat{Q}^* b.$$

Numerical Procedure

1. Compute a QR factorization

$$A = QR = \begin{bmatrix} \underbrace{\widehat{Q}}_{n\times p} & \underbrace{\widetilde{Q}}_{n\times n-p} \end{bmatrix} \begin{bmatrix} \underbrace{\widehat{R}}_{p\times p} \\ \underbrace{0}_{n-p\times p} \end{bmatrix}$$

   by Householder reflectors. $\sim 2np^2 - 2p^3/3$ flops

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

3. Solve

$$\widehat{R}x_* = \widehat{b}$$

   by back substitution. $\sim p^2$ flops

Forming $\widehat{b} = \widehat{Q}^* b$

$\widehat{b} = (Q^* b)(1:p)$,
QR factorization algorithm returns vectors $q_1, \ldots q_p$ s.t.

$$Q = Q_1 Q_2 \ldots Q_p, \quad Q_j = \begin{bmatrix} I_{j-1} & 0 \\ 0 & I_{n-j+1} - 2 q_j q_j^* \end{bmatrix}$$

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Pseudocode to form $Q^* b$

for $j = 1, 2, \dots, p$ **do**
$\quad b(j:n) \leftarrow b(j:n) - 2q_j(q_j^* b(j:n))$
end for

Back Substitution

$$\begin{bmatrix} \widehat{r}_{11} & \cdots & \widehat{r}_{1(p-1)} & \widehat{r}_{1p} \\ 0 & \ddots & & \vdots \\ & & \widehat{r}_{(p-1)(p-1)} & \widehat{r}_{(p-1)p} \\ 0 & & 0 & \widehat{r}_{pp} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_{p-1} \\ x_p \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_{p-1} \\ b_p \end{bmatrix}$$

$$\begin{aligned} x_p &= b_p / \widehat{r}_{pp} \\ x_{p-1} &= \left\{ b_{p-1} - \widehat{r}_{(p-1)p} x_p \right\} / \widehat{r}_{(p-1)(p-1)} \\ x_j &= \left\{ b_j - \widehat{r}_{j(j+1)} x_{j+1} - \cdots - \widehat{r}_{jp} x_p \right\} / \widehat{r}_{jj} \end{aligned}$$

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