Linear Least-Squares Problem (LSP)
QR Method

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Outline

- QR method for LSP

Special matrices

Complex matrix	Real matrix
Hermitian: $A^* = A$	Symmetric: $A^\top = A$
Unitary: $AA^* = A^*A = I$	Orthogonal: $AA^\top = A^\top A = I$
Isometry: $A^*A = I$	Isometry: $A^\top A = I$

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Example: The matrix $U := \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$ is unitary and $P := \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$ is orthogonal.

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Exercise: An $n \times n$ matrix U is unitary (resp., orthogonal) if and only if $\langle Ux, Uy \rangle = \langle x, y \rangle$ for all x and y. An $m \times n$ matrix Q is an isometry if and only if $\langle Qx, Qy \rangle = \langle x, y \rangle$ for all x and y.

QR factorization

Theorem: Let $A \in \mathbb{C}^{m\times n}$. Then there is a unitary matrix $Q \in \mathbb{C}^{m\times m}$ and an upper triangular matrix $\mathcal{R} \in \mathbb{C}^{m\times n}$ such that $A = Q\mathcal{R}$.

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$$A = Q\mathcal{R} = \begin{bmatrix} Q_n & Q_{m-n} \end{bmatrix} \begin{bmatrix} R \\ 0 \end{bmatrix} = Q_n R. \quad \blacksquare$$

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Example:

$$\underbrace{\begin{bmatrix} 1 & 3 & 1 \\ 1 & 3 & 7 \\ 1 & -1 & -4 \\ 1 & -1 & 2 \end{bmatrix}}_{A} = \underbrace{\frac{1}{2}\begin{bmatrix} 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \end{bmatrix}}_{Q} \underbrace{\begin{bmatrix} 2 & 2 & 3 \\ 0 & 4 & 5 \\ 0 & 0 & 6 \\ 0 & 0 & 0 \end{bmatrix}}_{\mathcal{R}}.$$

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$$\|Ax - b\|_2 = \|Q^*(Ax - b)\|_2 = \left\| \begin{bmatrix} R \\ 0 \end{bmatrix} x - \begin{bmatrix} c \\ d \end{bmatrix} \right\|_2 = \sqrt{\|Rx - c\|_2^2 + \|d\|_2^2}.$$

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2. Set $\begin{bmatrix} c \\ d \end{bmatrix} := Q^* b$, where $c \in \mathbb{C}^n$ and $d \in \mathbb{C}^{m-n}$.
3. Solve upper triangular system $Rx = c$.
4. Compute the residual $\|d\|_2$.

Example

Given $A = \begin{bmatrix} 3 & -6 \\ 4 & -8 \\ 0 & 1 \end{bmatrix}$ and $b = \begin{bmatrix} -1 \\ 7 \\ 2 \end{bmatrix}$, solve the LSP $Ax \approx b$.

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3. Solve $\begin{bmatrix} -5 & 10 \\ 0 & -1 \end{bmatrix} x = \begin{bmatrix} -5 \\ -2 \end{bmatrix} \Longrightarrow x = \begin{bmatrix} 5 \\ 2 \end{bmatrix}$.
4. The residual $\|d\|_2 = 5$.

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- Compute QR factorization `[A, b] = QR`.
- Solve the upper triangular sytem `R(1:n, 1:n)x = R(1:n, n+1)`.
- Compute residual norm `|d| = abs( R(n+1, n+1) )`.

QR method for rank deficient LSP

Theorem: Let $A \in \mathbb{C}^{m \times n}$. Suppose that $\mathrm{rank}(A) = r$. Then there is a unitary matrix $Q \in \mathbb{C}^{m \times m}$ and a nonsingular upper triangular matrix $R_{11} \in \mathbb{C}^{r \times r}$ such that

$$AP = Q \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix} = Q\mathcal{R},$$

where $P \in \mathbb{R}^{n \times n}$ is a permutation matrix and $R_{12} \in \mathbb{C}^{r \times (n-r)}$. ■

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Remark: If x is a solution of LSP $Ax \approx b$ then $x + z$ is also a solution for any $z \in N(A)$. Hence the LSP has $n - r$ linearly independent solutions.

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Remark: If x is a solution of LSP $Ax \approx b$ then $x + z$ is also a solution for any $z \in N(A)$. Hence the LSP has $n - r$ linearly independent solutions.

A rank deficient LSP is an ill-posed problem and solutions are strongly dependent on the rank of A. Numerical rank determination is a tricky problem.

QR method for rank deficient LSP

Algorithm: Solution of LSP $Ax \approx b$ when $\mathrm{rank}(A) = r$.

1. Compute QR factorization $AP = Q \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix}$, where $Q \in \mathbb{C}^{m\times m}$ is unitary, $R_{11} \in \mathbb{C}^{r\times r}$ is nonsingular and upper triangular.
2. Set $\begin{bmatrix} c \\ d \end{bmatrix} := Q^* b$, where $c \in \mathbb{C}^r$ and $d \in \mathbb{C}^{m-r}$.
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The MATLAB command `[Q,R,P] = qr(A)` computes a QR factorization $AP = QR$.

Uniqueness of QR factorization

Theorem: Let $A \in \mathbb{R}^{m\times n}$ and $\mathrm{rank}(A) = n$. Then there exist unique isometry $Q \in \mathbb{R}^{m\times n}$ and an upper triangular matrix $R \in \mathbb{R}^{n\times n}$ with positive diagonal entries such that $A = QR$.

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Proof: Let $A = \hat{Q}\hat{R}$ be a QR factroziation of A, where $\hat{Q} \in R^{m\times n}$ is an isometry and $\hat{R} \in \mathbb{R}^{n\times n}$ is upper triangular.

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Then D is unitary, $Q := \hat{Q}D$ is an isometry, $R := D\hat{R}$ is upper triangular with positive diagonal entries, and $A = QR$.

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Then $A^\top A = R_1^\top R_1 = R_2^\top R_2$ are Cholesky factorizations of $A^\top A$. By uniqueness of Cholesky factorization, $R_1 = R_2$ which gives $Q_1 = Q_2$. ■

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