MA580H Matrix Computations

Least-Squares Problem(LSP)

Lecture 12: QR method for LSP

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Outline

- QR method for LSP
- Augmented QR method for LSP
- Rank revealing QR method for rank deficient LSP

Unitary matrices

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

Fact: An $n \times n$ matrix A is unitary (resp., orthogonal) if and only if columns of A are orthonormal. An $m \times n$ matrix is isometry if and only if columns of A are orthonormal.

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. The matrix $Q := \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{3}} \\ 0 & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \end{bmatrix}$ is an isometry.

Let $Q \in \mathbb{R}^{n\times n}$ be orthogonal. Then $\|Qx\|_2 = \sqrt{\langle Qx, Qx\rangle} = \sqrt{\langle x, Q^\top Qx\rangle} = \sqrt{\langle x, x\rangle} = \|x\|_2$.

Let $Q \in \mathbb{C}^{n\times n}$ be unitary. Then $\|Qx\|_2 = \sqrt{\langle Qx, Qx\rangle} = \sqrt{\langle x, Q^* Qx\rangle} = \sqrt{\langle x, x\rangle} = \|x\|_2$.

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 $A = Q\mathcal{R}$. If $\mathrm{rank}(A) = n$ then $\mathcal{R}$ is of the form $\mathcal{R} = \begin{bmatrix} R \\ 0 \end{bmatrix}$ for some nonsingular upper triangular matrix $R \in \mathbb{C}^{n\times n}$. Let $Q = \begin{bmatrix} Q_n & Q_{m-n} \end{bmatrix}$ with $Q_n \in \mathbb{C}^{m\times n}$. Then Q_n is an isometry and

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

Remark: The factorization $A = Q\mathcal{R}$ is called a full QR factorization and $A = Q_n R$ is called a compact (or economy size) QR factorization of A. MATLAB commands: `[Q,R] = qr(A)` and `[Q,R] = qr(A,0)`, respectively, compute full and compact QR factorization of A

Example:

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

QR method for LSP

A QR factorization of A provides an efficient method for solution of the LSP $Ax \approx b$.

Suppose that $\mathrm{rank}(A) = n$. Set $\begin{bmatrix} c \\ d \end{bmatrix} := Q^* b$, where $c \in \mathbb{C}^n$ and $d \in \mathbb{C}^{m-n}$. Then

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

This shows that $\min \|Ax - b\|_2 = \|d\|_2 \iff Rx = c$. Hence $x = R^{-1}c$ is a unique solution of the LSP and $\|d\|_2$ is the residual. [If $Q \in \mathbb{C}^{n \times n}$ is unitary then $\|Qx\|_2 = \|x\|_2$ for all x.]

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

1. Compute QR factorization $A = Q \begin{bmatrix} R \\ 0 \end{bmatrix}$.
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 $Ax \approx b$.

1. Compute QR factorization: $A = \begin{bmatrix} -\frac{3}{5} & 0 & \frac{4}{5} \\ -\frac{4}{5} & 0 & -\frac{3}{5} \\ 0 & -1 & 0 \end{bmatrix} \left[\begin{array}{cc} -5 & 10 \\ 0 & -1 \\ \hline 0 & 0 \end{array}\right] = Q \begin{bmatrix} R \\ 0 \end{bmatrix}$.
2. Compute $Q^\top b = \left[\begin{array}{c} -5 \\ -2 \\ \hline -5 \end{array}\right]$.
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 $\|r\|_2 = 5$.

QR factorization of augmented matrix

If the matrix Q in the QR factorization $A = QR$ is not required, then the LSP $Ax \approx b$ can be solved more efficiently by computing QR factorization of the augmented matrix $\begin{bmatrix} A & b \end{bmatrix}$.

Suppose that $\mathrm{rank}(A) = n$. Then

$$Ax - b = \begin{bmatrix} A & b \end{bmatrix} \begin{bmatrix} x \\ -1 \end{bmatrix} \text{ and } \begin{bmatrix} A & b \end{bmatrix} = Q \left[\begin{array}{c|c} R & c \\ 0 & d \\ \hline \multicolumn{2}{c}{\mathbf{0}} \end{array}\right] = Q\mathcal{R}, \text{ where } d \in \mathbb{C}.$$

Hence $\|Ax - b\|_2 = \sqrt{\|Rx - c\|_2 + |d|^2} \Longrightarrow \min \|Ax - b\|_2 = |d| \iff Rx = c$.

Hence the LSP $Ax \approx b$ can be solved in three steps:

- 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 $R_{12} \in \mathbb{C}^{r\times(n-r)}$. ■

Set $\begin{bmatrix} c \\ d \end{bmatrix} := Q^* b$, where $c \in \mathbb{C}^r$ and $d \in \mathbb{C}^{m-r}$. Then

$$\begin{aligned} \|Ax - b\|_2 &= \|Q^*(APP^\top x - b)\|_2 = \left\| \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix} - \begin{bmatrix} c \\ d \end{bmatrix} \right\|_2 \\ &= \sqrt{\|R_{11}y + R_{12}z - c\|_2^2 + \|d\|_2^2}. \end{aligned}$$

This shows that $\min \|Ax - b\|_2 = \|d\|_2 \iff R_{11}y = c - R_{12}z$. Hence $x = P\begin{bmatrix} y \\ z \end{bmatrix}$ is a solution of the LSP for any $z \in \mathbb{C}^{n-r}$ and $\|d\|_2$ is the residual. Setting $z = 0$ we obtain a unique solution with smallest norm.

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 $d \in \mathbb{C}^{m-r}$.
3. Solve upper triangular system $R_{11} y = c$.
4. Set $x = P \begin{bmatrix} y \\ 0 \end{bmatrix}$. Then x is a unique solution of $Ax \approx b$.
5. Compute the residual $\|d\|_2$.

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.