Math 381 - Fall 2022

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Week 9

Last Time

1. Projection matrices
2. A little linear algebra review
3. Overview of least squares problem
4. Least squares solution theorem
5. Full-rank least squares problem: normal equations

Today

1. Strategies for solving the full-rank least squares problem ($m > n$)
    1. LU decomposition (Cholesky decomposition)
    2. QR decomposition
    3. SVD decomposition

Daily linear algebra

2-norm invariance to orthogonal (unitary) multiplication

Let $Q \in \mathbb{R}^{n\times n}$ be an orthogonal matrix. Then, we have that $\|Qx\|_2 = \|x\|_2$ and $\|QA\|_2 = \|A\|_2$, for any $x \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n\times n}$.

Review from last time

Least squares solution theorem

The length of residual $r = b - Ax$ is minimized if x is a solution to $Ax = Pb$, where P is an *orthogonal* projection onto $R(A)$ so that $r = (I - P)b \in R(A)^{\perp}$.

Full rank least squares problems with Cholesky decomposition

Normal equations

For a full rank matrix $A \in \mathbb{R}^{m \times n}$ (with $m > n$) and $b \in \mathbb{R}^n$, the least squares solution to $Ax = b$ is the solution to

$$A^T A x = A^T b.$$

$$Mx = A^T b$$

$$M = A^T A$$

Full rank least squares problems with Cholesky decomposition

$M = LU \quad LU = (LU)^T = U^T L^T$

Cholesky decomposition

Let $M \in \mathbb{R}^{n \times n}$ be symmetric and nonsingular. There is an upper triangular matrix R such that

$$M = R^T R.$$

Backward stable

Full rank least squares problems with Cholesky decomposition

1. Compute matrix-matrix product

$$M = A^T A \qquad O(mn^2)$$

2. Compute Cholesky factorization

$$M = R^T R \qquad O(n^3)$$

3. Forward substitution

$$R^T y = A^T b \qquad O(n^2)$$

4. Backward substitution

$$Rx = y \qquad O(n^2)$$

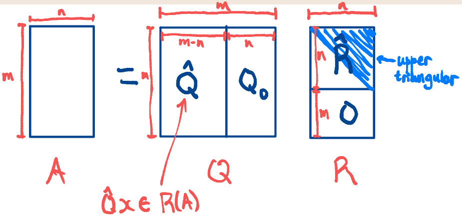
Backward stable, but can be less accurate than other methods for certain problems (next week)

Full rank least squares problems with QR decomposition

QR decomposition

Let $A \in \mathbb{R}^{m\times n}$ be a full rank matrix (with $m > n$). There exists an orthogonal matrix $Q \in \mathbb{R}^{m\times m}$ and an upper triangular matrix $R \in \mathbb{R}^{m\times n}$ such that

$$A = QR.$$



Reduced QR

$A = \hat{Q}\hat{R}$

Backward Stable

Full rank least squares problems with QR decomposition

Least squares solution using QR

Let $A = QR = \hat{Q}\hat{R}$ be the QR and reduced QR factorization of A, respectively. Since Q is orthogonal and the columns of $\hat{Q}$ span $R(A)$, an orthogonal projection matrix for $R(A)$ is given by $P = \hat{Q}\hat{Q}^T$. Hence, the unique solution to

$$Ax = \hat{Q}\hat{Q}^T b,$$

is the unique solution to the least squares problem.

Full rank least squares problems with QR decomposition

$$\underset{A}{\boxed{}}\;\underset{x}{\boxed{}} = \underset{Q}{\begin{bmatrix}\hat{Q} & Q_0\end{bmatrix}}\;\underset{R}{\begin{bmatrix}\hat{R}\\ 0\end{bmatrix}}\;\underset{x}{\boxed{}} = \underset{b}{\boxed{}}$$

① compute $A = \hat{Q}\hat{R}$ $\mathcal{O}(n^3)$

② compute $z = \hat{Q}^T b$ $\mathcal{O}(mn)$

③ Backward substitution $\hat{R}x = z$

$$\underset{R}{\begin{bmatrix}\hat{R}\\ 0\end{bmatrix}}\;\underset{x}{\boxed{}} = \underset{Q^T}{\begin{bmatrix}\hat{Q}^T\\ Q_0^T\end{bmatrix}}\;\underset{b}{\boxed{}}$$

$$\hat{R}x = \hat{Q}^T b \Rightarrow x = \hat{R}^{-1}\hat{Q}^T b$$

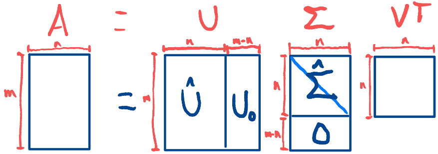
Fredholm Alternative

$$0 \cdot x = \underbrace{Q_0^T b}_{\text{residual}} \neq 0 \text{ in general for LS problems}$$

General least squares problems with SVD decomposition

Singular value decomposition (SVD)

Let $A \in \mathbb{R}^{m\times n}$ be a full rank matrix (with $m > n$). There exists orthogonal matrices $U \in \mathbb{R}^{m\times m}$, $V \in \mathbb{R}^{n\times n}$ and a diagonal matrix $\Sigma \in \mathbb{R}^{m\times n}$ such that $A = U\Sigma V^T$.



Reduced SVD

$A = \hat{U}\hat{\Sigma}V^T$

Backward Stable

General least squares problems with SVD decomposition

Least squares solution using SVD

Let $A = U\Sigma V^T = \hat{U}\hat{\Sigma}V^T$ be the SVD and reduced SVD of the matrix A, respectively. Since U is orthogonal and the columns of $\hat{U}$ span $R(A)$, an orthogonal projection matrix for $R(A)$ is given by $P = \hat{U}\hat{U}^T$. Hence, the unique solution to

$$Ax = \hat{U}\hat{U}^T b,$$

is the unique solution to the least squares problem.

Pseudoinverse matrices for the full rank least squares problem

$$\begin{aligned} \text{Normal Equations:} \qquad & A^+ = (A^T A)^{-1} A^T \\ \text{QR:} \qquad & A^+ = \hat{R}^{-1} \hat{Q}^T \\ \text{SVD:} \qquad & A^+ = V \hat{\Sigma}^{-1} \hat{U}^T \end{aligned}$$