Lecture 11
Scientific and Data Computing I

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Lecture

- Monday – Singular Value Decomposition (SVD)
- Wednesday – Principle Component Analysis (PCA)
- No Office Hours This Week Due to Admin Meeting
Orthogonal Matrices

Definition 4.2. An orthogonal matrix is a square matrix whose columns are orthogonal vectors.

Theorem 4.4. Suppose $Q$ is an $n \times n$ matrix.
1. $Q$ is an orthogonal matrix if and only if $Q^{-1} = Q^T$.
2. $Q$ is an orthogonal matrix if and only if its rows are orthogonal vectors.
3. If $Q$ is an orthogonal matrix, then $|\det(Q)| = 1$.

Example:

$$R = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$
QR Method Properties

**Definition 4.3.** If $A$ is an $n \times n$ matrix with entries $a_{ij}$, then the trace $tr(A)$ is defined as:

$$tr(A) = \sum_{i=1}^{n} a_{ii}$$

**Theorem 4.5.** Let $A$ be an $n \times n$ matrix, with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ (listed according to their algebraic multiplicities), then

$$tr(A) = \sum_{i=1}^{n} \lambda_i,$$

$$tr(A^k) = \sum_{i=1}^{n} \lambda_i^k,$$

where $k$ is a positive integer.
What Really Is QR?

- Recall Gram-Schmidt

\[ q_1 = \frac{a_1}{r_{11}} \]

\[ q_2 = \frac{a_2 - r_{12}q_1}{r_{22}} \]

\[ q_3 = \frac{a_3 - r_{13}q_1 - r_{23}q_2}{r_{33}} \]
What Really Is QR (continued)?

• Classic Gram-Schmidt (unstable)

for \( j = 1 \) to \( n \)
\[
    v_j = a_j
\]
for \( i = 1 \) to \( j-1 \)
\[
    r_{ij} = q_i^* a_j
\]
\[
    v_j = v_j - r_{ij} q_i
\]
\[
    r_{jj} = \|v_j\|_2
\]
\[
    q_j = v_j / r_{jj}
\]

Trefethen and Bau, Numerical Linear Algebra
What Really Is QR (continued)?

- Modified Gram-Schmidt

\[
\begin{align*}
\text{for } i &= 1 \text{ to } n \\
v_i &= a_i \\
\text{for } i &= 1 \text{ to } n \\
r_{ii} &= \| v_i \| \\
q_i &= v_i / r_{ii} \\
\text{for } j &= i+1 \text{ to } n \\
r_{ij} &= q_i^* v_j \\
v_j &= v_j - r_{ij} q_i
\end{align*}
\]
QR Operation Count

• Assume an $m \times n$ matrix
• Previous algorithms: complexity $\sim 2mn^2$ flops to compute a QR factorization
Three Ways to Compute QR

- Gram-Schmidt Orthogonalization
- Householder Triangularization
- Givens Rotations
Theorem 4.6. If $A$ is a symmetric matrix, then it is possible to factor $A$ as:

$$A = QDQ^T$$

General matrix:

$$A = U\Sigma V^T$$

$$\Sigma = \begin{pmatrix} S \\ O \end{pmatrix}$$
Lemma 1 Assuming $A$ is an $m \times n$ matrix, with $n \leq m$, then:

1. $A^T A$ and $AA^T$ are symmetric with non-negative eigenvalues.

2. If $\lambda$ is an eigenvalue of $AA^T$, with eigenvector $u$, then either $\lambda$ is an eigenvalue of $A^T A$ with eigenvector $A^T u$ or else $\lambda = 0$ and $A^T u = 0$. 
Observations

• The left-singular vectors of $A$ are a set of orthonormal eigenvectors of $AA^T$.
• The right-singular vectors of $A$ are a set of orthonormal eigenvectors of $A^TA$.
• The non-zero singular values of $A$ (found on the diagonal entries of $\Sigma$) are the square roots of the non-zero eigenvalues of both $A^TA$ and $AA^T$. 
Algorithm (continued)

- Golub-Kahan Bidiagonalization
- Pattern resembles two Householder QR factorizations interleaved with each other, one operating on an $m \times n$ matrix, the other on the $n \times m$ matrix $A^T$.
- Complexity:

$$4mn^2 - \frac{4}{3}n^3$$
Theorem 4.7. If $A$ is symmetric, then its singular values are the absolute value of its eigenvalues. For its SVD, if $u_i$ is the $i$th column of $U$, then the $i$th column of $V$ is $\pm u_i$, where the $-$ is used if the corresponding eigenvalue is negative, otherwise the $+$ is used.

\[
(A^T A) = (U \Sigma V^T)^T (U \Sigma V^T) = V \Sigma U^T U \Sigma V^T = V (\Sigma \Sigma) V^T
\]

\[
(A^T A) V = V (\Sigma^T \Sigma)
\]

Note: $V (\Sigma^T \Sigma) = (\Sigma^T \Sigma) V$ because of diagonal matrix $\Sigma$
Theorem 4.8. The matrix $A$ has rank $r$, and only if, $A$ has exactly $r$ nonzero singular values.
For Next Time

• Read Chapter 4 and 9 (for volatility)
• Look ahead at Chapters 5 and 6
• Start working on Practicums
• Start working on Homework 3