AMS526: Numerical Analysis I
(Numerical Linear Algebra)
Lecture 16: QR Algorithm and Simultaneous Iteration

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QR Algorithm

- Most basic version of QR algorithm is remarkably simple:

\[
\text{Algorithm: “Pure” QR Algorithm} \\
A^{(0)} = A \\
\text{for } k = 1, 2, \ldots \\
Q^{(k)} R^{(k)} = A^{(k-1)} \\
A^{(k)} = R^{(k)} Q^{(k)}
\]

- With some suitable assumptions, \(A^{(k)}\) converge to Schur form of \(A\) (diagonal if \(A\) is symmetric)
- Similarity transformation of \(A\):

\[
A^{(k)} = R^{(k)} Q^{(k)} = \left(Q^{(k)}\right)^T A^{(k-1)} Q^{(k)}
\]

- But why it works?
Unnormalized Simultaneous Iteration

- To understand QR algorithm, first consider simple algorithm
- Simultaneous iteration is power iteration applied to several vectors
- Start with linearly independent $v_1^{(0)}, \cdots, v_n^{(0)}$
- We know from power iteration that $A^k v_1^{(0)}$ converge to $q_1$
- With some assumptions, the space $\langle A^k v_1^{(0)}, \cdots, A^k v_n^{(0)} \rangle$ should converge to $\langle q_1, \cdots, q_n \rangle$
- Notation: Define initial matrix $V^{(0)}$ and matrix $V^{(k)}$ at step $k$:

$$V^{(0)} = \begin{bmatrix} v_1^{(0)} & \cdots & v_n^{(0)} \end{bmatrix}, \quad V^{(k)} = A^k V^{(0)} = \begin{bmatrix} v_1^{(k)} & \cdots & v_n^{(k)} \end{bmatrix}$$
Unnormalized Simultaneous Iteration

- Define orthogonal basis for column space of $V^{(k)}$ by reduced QR factorization $\hat{Q}^{(k)}\hat{R}^{(k)} = V^{(k)}$

- We assume that
  1. leading $n + 1$ eigenvalues are distinct, and
  2. all leading principal submatrices of $\hat{Q}^T V^{(0)}$ are nonsingular where $\hat{Q} = [q_1| \cdots |q_n]$

- We then have columns of $\hat{Q}^{(k)}$ converge to eigenvectors of $A$:

  $$\|q_j^{(k)} - (\pm q_j)\| = O(c^k),$$

  where $c = \max_{1 \leq k \leq n} |\lambda_{k+1}|/|\lambda_k|$

- Proof idea: Show that subspace of any leading $j$ columns of $V^{(k)} = A^k V^{(0)}$ converges to subspace of first $j$ eigenvectors of $A$, so does the subspace of any leading $j$ columns of $\hat{Q}^{(k)}$. 

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Numerical Analysis I
Simultaneous Iteration

- Matrices $V^{(k)} = A^k V^{(0)}$ are highly ill-conditioned
- Orthonormalize at each step rather than at the end

Algorithm: Simultaneous Iteration

Pick $\hat{Q}^{(0)} \in \mathbb{R}^{m \times n}$

\[
\begin{align*}
\text{for } k = 1, 2, \ldots \\
Z &= A\hat{Q}^{(k-1)} \\
\hat{Q}^{(k)}\hat{R}^{(k)} &= Z
\end{align*}
\]

- Column spaces of $\hat{Q}^{(k)}$ and $Z^{(k)}$ are both equal to column space of $A^k \hat{Q}^{(0)}$, therefore same convergence as before
Simultaneous Iteration $\iff$ QR Algorithm

Algorithm: Simultaneous Iteration

Pick $\hat{Q}^{(0)} \in \mathbb{R}^{m \times n}$

for $k = 1, 2, \ldots$

\[
Z = A\hat{Q}^{(k-1)}
\]

\[
\hat{Q}^{(k)} \hat{R}^{(k)} = Z
\]

Algorithm: “Pure” QR Algorithm

\[
A^{(0)} = A
\]

for $k = 1, 2, \ldots$

\[
Q^{(k)} R^{(k)} = A^{(k-1)}
\]

\[
A^{(k)} = R^{(k)} Q^{(k)}
\]

- QR algorithm is equivalent to simultaneous iteration with $\hat{Q}^{(0)} = I$
- Replace $\hat{R}^{(k)}$ by $R^{(k)}$ and $\hat{Q}^{(k)}$ by $Q^{(k)}$, and introduce new statement

\[
A^{(k)} = \left( Q^{(k)} \right)^T \hat{A} Q^{(k)}
\] in simultaneous iteration

Simultaneous iteration

\[
\underline{Q}^{(0)} = I
\]

\[
Z = A\underline{Q}^{(k-1)}
\]

\[
\underline{Q}^{(k)} \underline{R}^{(k)} = Z
\]

\[
A^{(k)} = \left( Q^{(k)} \right)^T \hat{A} Q^{(k)}
\]
Simultaneous Iteration $\iff$ QR Algorithm

- $Q^{(k)} = Q^{(1)} Q^{(2)} \ldots Q^{(k)}$. Let $R^{(k)} = R^{(k)} R^{(k-1)} \ldots R^{(1)}$
- Both schemes generate QR factorization $A^k = Q^{(k)} R^{(k)}$ and projection $A^{(k)} = \left( Q^{(k)} \right)^T A Q^{(k)}$

Proof by induction. For $k = 0$ it is trivial for both algorithms. For $k \geq 1$ with simultaneous iteration, $A^{(k)}$ is given by definition, and

$$A^k = A Q^{(k-1)} R^{(k-1)} = Q^{(k)} R^{(k)} R^{(k-1)} = Q^{(k)} R^{(k)}$$

For $k \geq 1$ with QR algorithm,

$$A^k = A Q^{(k-1)} R^{(k-1)} = Q^{(k-1)} A^{(k-1)} R^{(k-1)} = Q^{(k)} R^{(k)}$$

and

$$A^{(k)} = \left( Q^{(k)} \right)^T A^{(k-1)} Q^{(k)} = \left( Q^{(k)} \right)^T A Q^{(k)}$$
Convergence of QR Algorithm

- Since \( Q^{(k)} = \hat{Q}^{(k)} \) in simultaneous iteration, column vectors of \( Q^{(k)} \) converge linearly to eigenvectors if \( A \) has distinct eigenvalues.

- From \( A^{(k)} = (Q^{(k)})^T A Q^{(k)} \), diagonal entries of \( A^{(k)} \) are Rayleigh quotients of column vectors of \( Q^{(k)} \), so they converge linearly to eigenvalues of \( A \).

- Off-diagonal entries of \( A^{(k)} \) converge to zeros, as they are generalized Rayleigh quotients involving approximations of distinct eigenvectors.

- Overall, \( A = Q^{(k)} A^{(k)} (Q^{(k)})^T \). For a symmetric matrix, it converges to eigenvalue decomposition of \( A \).

- Convergence rate is only linear: columns of \( \hat{Q}^{(k)} \) converge to eigenvectors of \( A \) \( \| q_j^{(k)} - (\pm q_j) \| = O(c^k) \), where \( c = \max_{1 \leq k \leq n} |\lambda_{k+1}|/|\lambda_k| \). 

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