AMS526: Numerical Analysis I
(Numerical Linear Algebra)
Lecture 18: QR Algorithm and Simultaneous Iteration

Xiangmin Jiao

SUNY Stony Brook
QR Algorithm

- Most basic version of QR algorithm is remarkably simple:

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

- 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?
To understand QR algorithm, first consider simple algorithm

Simultaneous iteration is power iteration applied to several vectors

Start with linearly independent $v_1^{(0)}, \ldots, v_n^{(0)}$

We know from power iteration that $A^k v_1^{(0)}$ converge to $q_1$

With some assumptions, the space $\langle A^k v_1^{(0)}, \ldots, A^k v_n^{(0)} \rangle$ should converge to $\langle q_1, \ldots, q_n \rangle$

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 $\hat{Q}^{(k)}$. 
Simultaneous Iteration

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

Algorithm: Simultaneous Iteration

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

for $k = 1, 2, \ldots$

$$\mathbf{Z} = \mathbf{A} \hat{\mathbf{Q}}^{(k-1)}$$

$$\hat{\mathbf{Q}}^{(k)} \hat{\mathbf{R}}^{(k)} = \mathbf{Z}$$

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

Algorithm: Simultaneous Iteration

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

for $k = 1, 2, \ldots$

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

Algorithm: "Pure" QR Algorithm

\[
\begin{align*}
A^{(0)} &= A \\
\text{for } k = 1, 2, \ldots \\
Q^{(k)} R^{(k)} &= A^{(k-1)} \\
A^{(k)} &= R^{(k)} Q^{(k)}
\end{align*}
\]

- 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

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

Simultaneous iteration

\[
\begin{align*}
Q^{(0)} &= I \\
Z &= A Q^{(k-1)} \\
Q^{(k)} R^{(k)} &= Z \\
A^{(k)} &= \left( Q^{(k)} \right)^T A Q^{(k)}
\end{align*}
\]

QR algorithm

\[
\begin{align*}
A^{(0)} &= A \\
Q^{(k)} R^{(k)} &= A^{(k-1)} \\
A^{(k)} &= R^{(k)} Q^{(k)} \\
Q^{(k)} &= Q^{(1)} Q^{(2)} \ldots Q^{(k)}
\end{align*}
\]
Simultaneous Iteration $\iff$ QR Algorithm

- $Q^{(k)} = Q^{(1)} Q^{(2)} \cdots Q^{(k)}$. Let $R^{(k)} = R^{(k)} R^{(k-1)} \cdots R^{(1)}$
- 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

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

For $k \geq 1$ with QR algorithm,

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

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 eigenvalues if $A$ has distinct eigenvalues.
- From $A^{(k)} = \left( Q^{(k)} \right)^T A Q^{(k)}$, 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, $A = Q^{(k)} A^{(k)} \left( Q^{(k)} \right)^T$. For a symmetric matrix, it converges to eigenvalue decomposition of $A$. 