

AMS526: Numerical Analysis I (Numerical Linear Algebra)

Lecture 19: QR Algorithm and Simultaneous Iteration

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QR Algorithm

- Most basic version of QR algorithm is remarkably simple:

Algorithm: "Pure" QR Algorithm

$$\mathbf{A}^{(0)} = \mathbf{A}$$

for $k = 1, 2, \dots$

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

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

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

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

- 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 $\mathbf{v}_1^{(0)}, \dots, \mathbf{v}_n^{(0)}$
- We know from power iteration that $\mathbf{A}^k \mathbf{v}_1^{(0)}$ converge to \mathbf{q}_1
- With some assumptions, the space $\langle \mathbf{A}^k \mathbf{v}_1^{(0)}, \dots, \mathbf{A}^k \mathbf{v}_n^{(0)} \rangle$ should converge to $\langle \mathbf{q}_1, \dots, \mathbf{q}_n \rangle$
- Notation: Define initial matrix $\mathbf{V}^{(0)}$ and matrix $\mathbf{V}^{(k)}$ at step k :

$$\mathbf{V}^{(0)} = \left[\mathbf{v}_1^{(0)} \mid \dots \mid \mathbf{v}_n^{(0)} \right], \quad \mathbf{V}^{(k)} = \mathbf{A}^k \mathbf{V}^{(0)} = \left[\mathbf{v}_1^{(k)} \mid \dots \mid \mathbf{v}_n^{(k)} \right]$$

Unnormalized Simultaneous Iteration

- Define orthogonal basis for column space of $\mathbf{V}^{(k)}$ by reduced QR factorization $\hat{\mathbf{Q}}^{(k)} \hat{\mathbf{R}}^{(k)} = \mathbf{V}^{(k)}$
- We assume that
 - 1 leading $n + 1$ eigenvalues are distinct, and
 - 2 all leading principal submatrices of $\hat{\mathbf{Q}}^T \mathbf{V}^{(0)}$ are nonsingular where $\hat{\mathbf{Q}} = [\mathbf{q}_1 | \cdots | \mathbf{q}_n]$

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

$$\|\mathbf{q}_j^{(k)} - (\pm \mathbf{q}_j)\| = O(c^k),$$

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

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

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 $k = 1, 2, \dots$

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

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

- 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

- QR algorithm is equivalent to simultaneous iteration with $\hat{Q}^{(0)} = I$
- Notation: Replace $\hat{R}^{(k)}$ by $R^{(k)}$ and $\hat{Q}^{(k)}$ by $\underline{Q}^{(k)}$

Algorithm: Simultaneous Iteration

$$\underline{Q}^{(0)} = I$$

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

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

$$\underline{A}^{(k)} = \left(\underline{Q}^{(k)}\right)^T \underline{A}\underline{Q}^{(k)}$$

QR Algorithm

$$\underline{A}^{(0)} = \underline{A}$$

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

$$\underline{A}^{(k)} = \underline{R}^{(k)}\underline{Q}^{(k)}$$

$$\underline{Q}^{(k)} = \underline{Q}^{(1)}\underline{Q}^{(2)}\dots\underline{Q}^{(k)}$$

Simultaneous Iteration \iff QR Algorithm

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

Proof by induction. For $k = 0$ it is trivial for both algorithms.

For $k \geq 1$ with simultaneous iteration, $\mathbf{A}^{(k)}$ is given by definition, and

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

For $k \geq 1$ with QR algorithm,

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

and

$$\mathbf{A}^{(k)} = \left(\underline{Q}^{(k)}\right)^T \mathbf{A}^{(k-1)} \underline{Q}^{(k)} = \left(\underline{Q}^{(k)}\right)^T \mathbf{A} \underline{Q}^{(k)}$$