Convergence of QR Algorithm

Invariant Subspaces

Consider $A : \mathbb{F}^n \mapsto \mathbb{F}^n$. A subspace $V \subset \mathbb{F}^n$ is said to be invariant with respect to A, if $Av \in V$ for all $v \in V$.

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Examples:

1. For $A = \begin{bmatrix} 1 & 0 & -1 \\ 0 & -2 & 0 \\ 1 & 1 & -1 \end{bmatrix}$, $A\left(\mathrm{span}\{e_1, e_3\}\right) \subseteq \mathrm{span}\{e_1, e_3\}$.
2. For $A = \begin{bmatrix} 4 & 3 & -5 \\ 0 & -3 & 3 \\ 0 & -2 & 3 \end{bmatrix}$, $A(\mathrm{span}\{e_1\}) \subseteq \mathrm{span}\{e_1\}$ and $A\left(\mathrm{span}\{e_1 + e_2 + e_3, e_1 - e_2\}\right) \subseteq \mathrm{span}\{e_1 + e_2 + e_3, e_1 - e_2\}$.

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Facts:

1. The trivial subspaces $\mathbb{F}^n$ and $\{0\}$ are always invariant with respect to every $A \in \mathbb{F}^{n\times n}$.
2. $V \subseteq \mathbb{F}^n$ is a one dimensional subspace of $\mathbb{F}^n$ invariant with respect to $A \in \mathbb{F}^{n\times n}$ if and only if $V = \operatorname{span}\{v\}$ for some eigenvector v of A.
3. Eigenvectors of $A \in \mathbb{F}^{n\times n}$ span invariant subspaces.

Invariant Subspaces

Theorem: Let $A \in \mathbb{F}^{n \times n}$. The first k columns of an invertible $S \in \mathbb{F}^{n \times n}$ span a subspace of $\mathbb{F}^n$ invariant with respect to A if and only if

$$S^{-1}AS = \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline & A_{22} \end{array}\right]$$

where $A_{11} \in \mathbb{F}^{k \times k}$, $A_{12} \in \mathbb{F}^{k \times n-k}$ and $A_{22} \in \mathbb{F}^{n-k \times n-k}$.

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Corollary: Let $A \in \mathbb{F}^{n\times n}$ and $S = [s_1 \ \cdots \ s_n] \in \mathbb{F}^{n\times n}$ be a invertible matrix. Then the first k columns of S span subspaces of $\mathbb{F}^n$ that are invariant with respect to A $\underline{\text{for each } k = 1, \ldots, n-1,}$ if and only if $S^{-1}AS$ is an upper triangular matrix.

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Schur's Theorem: Given $A \in \mathbb{C}^{n\times n}$, there exists an orthonormal basis $\{q_1, \ldots, q_n\}$ of $\mathbb{C}^n$ such that

$$A(\mathrm{span}\{q_1, \ldots, q_k\}) \subseteq \mathrm{span}\{q_1, \ldots, q_k\}$$

for each $k = 1, \ldots, n-1$.

Subspace Iteration

Given $A \in \mathbb{F}^{n \times n}$, recall that the Power Method is essentially about producing a series of vectors

$$x, Ax, A^2x, \ldots$$

which under suitable scaling converges to a dominant eigenvector of A under suitable conditions.

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The scalings will replace x by other vectors in $\mathcal{S} := \mathrm{span}\{x\}$ and depending on their choices the iterations will converge to some vector in the one dimensional invariant eigenspace $\mathcal{T} := \mathrm{span}\{v\}$ where v is a dominant eigenvector of A.

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We could do this for higher dimensional subspaces $\mathcal{S}$!

Subspace iteration, Simultaneous iteration and the QR algorithm

Principal angles and distance between subspaces

Let $\mathcal{S}_1, \mathcal{S}_2$ be two subspaces of $\mathbb{F}^n$ with $\dim \mathcal{S}_1 = l$, $\dim \mathcal{S}_2 = m$ where $l \leq m$.

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Let the columns of $U_1 \in \mathbb{F}^{n \times l}$ and $U_2 \in \mathbb{F}^{n \times m}$ form orthonormal bases of $\mathcal{S}_1$ and $\mathcal{S}_2$ respectively. If

$$\sigma_1 \geq \cdots \geq \sigma_l \geq 0$$

are the singular values of $U_2^T U_1$ then the **principal angles between $\mathcal{S}_1$ and $\mathcal{S}_2$** are defined as

$$\theta_i = \arccos \sigma_i, \; i = 1, \ldots, l.$$

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Given a subspace $\mathcal{T}$ and sequence of subspaces $\{\mathcal{S}_m\}$ of $\mathbb{F}^n$,

$$\lim_{m\to\infty} \mathcal{S}_m = \mathcal{T} \Leftrightarrow d(\mathcal{S}_m, \mathcal{T}) \to 0 \text{ as } m \to \infty.$$

Convergence in Subspace iterations

Let $A \in \mathbb{F}^{n \times n}$ be diagonalizable with eigenvalues $\lambda_1, \ldots, \lambda_n$ such that

$$|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|.$$

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Suppose $|\lambda_k| > |\lambda_{k+1}|$ for some $1 \leq k \leq n-1$ and let

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Then for *any* subspace $\mathcal{S}$ of $\mathbb{F}^n$ such that $\dim \mathcal{S} = k$, and $\mathcal{S} \cap \mathcal{U}_k = \{0\}$,

$$\lim_{m \to \infty} A^m(\mathcal{S}) = \mathcal{T}_k$$

linearly at the rate $|\lambda_{k+1}|/|\lambda_k|$.

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Exercise: Since $|\lambda_k| > |\lambda_{k+1}|$, prove the following:

(a) $\mathrm{Null}(A^m) \subseteq \mathcal{U}_k$ for all $m = 1, 2, \ldots.$

(b) $\dim A^m(\mathcal{S}) = k$ for all $m = 1, 2, \ldots.$

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Not a good idea as there can be underflow and overflow. Also if $|\lambda_1| > |\lambda_2|$, then each of the sequences $\{A^m q_j\}, j = 1, 2, \ldots,$ could converge to some multiple of v_1 as $m \to \infty$ making $\{A^m q_1, \ldots, A^m q_k\}$ an ill conditioned basis for large m.

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(i) Compute $Aq_1^{(m)}, \ldots, Aq_k^{(m)}$;

(ii) Orthonormalize $Aq_1^{(m)}, \ldots, Aq_k^{(m)}$ to form an orthonormal basis $q_1^{(m+1)}, \ldots, q_k^{(m+1)}$ of $A^{m+1}(\mathcal{S})$.

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Let Q_m be a unitary matrix whose first k columns are $q_1^{(m)}, \ldots, q_k^{(m)}$. If the iterations have converged, then $A_m := Q_m^* A Q_m$ is of the form

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In particular if A is upper Hessenberg and the unitary Q_m are such that A_m are also always upper Hessenberg, then $a_{k+1,k}^{(m)}$ is the only nonzero entry of $A_{12}^{(m)}$ and

$$\lim_{m\to\infty} |a_{k+1,k}^{(m)}| = 0 \Leftrightarrow \lim_{m\to\infty} A^m(\mathcal{S}) = \mathcal{T}_k.$$

For either limits, the convergence is linear at the rate $|\lambda_{k+1}|/|\lambda_k|$.

Simultaneous iterations in subspace iterations

For each $j = 1, \ldots, m-1$, $q_1^{(m)}, \ldots, q_j^{(m)}$ is an orthonormal basis of $A^m(\mathrm{span}\{q_1^{(0)}, \ldots, q_j^{(0)}\})$

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So if for each $j = 1, \ldots, k$,

$$|\lambda_j| > |\lambda_{j+1}| \text{ and } \mathrm{span}\{q_1^{(0)}, \ldots, q_j^{(0)}\} \cap \mathrm{span}\{v_{j+1}, \ldots, v_n\} = \{0\},$$

then *for large enough* m,

$$\{q_1^{(m)}, \ldots, q_k^{(m)}\},$$

is *nearly* an orthonormal basis of the invariant subspace $\mathcal{T}_k$ with respect to A with the *additional* property that for each $j = 1, \ldots, k-1$,

$$\{q_1^{(m)}, \ldots, q_j^{(m)}\},$$

are *nearly* orthonormal bases of j-dimensional invariant subspaces $\mathrm{span}\{v_1, \ldots, v_j\}$ with respect to A.

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To check the progress of the simultaneous iterations set $Q_m = \left[\begin{array}{ccc} q_1^{(m)} & \cdots & q_n^{(m)} \end{array} \right]$ and check if $A_m := Q_m^* A Q_m$ is getting close to an upper triangular matrix.

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At this point we have the choice of performing the next iteration of simultaneous iteration either with respect to the standard basis $e_1, \ldots, e_n$ or the orthonormal basis formed by the columns say $q_1, \ldots, q_n$ of Q_0. If we go with $e_1, \ldots, e_n$, the operations are

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In iteration 1

(i) find $Ae_1, \ldots, Ae_n$, that is consider A;
(ii) orthonormalize by finding the Q, say Q_0, of a QR decomposition of A.

Feeling very optimistic about convergence, we find $A_1 := Q_0^* A Q_0$.

By now we have completed the first iteration of the QR algorithm!

At this point we have the choice of performing the next iteration of simultaneous iteration either with respect to the standard basis $e_1, \ldots, e_n$ or the orthonormal basis formed by the columns say $q_1, \ldots, q_n$ of Q_0. If we go with $e_1, \ldots, e_n$, the operations are

(i) find $Aq_1, \ldots, Aq_n$;
(ii) compute the Q of a QR decomposition of AQ_0.

QR algorithm and Simultaneous iterations

If we choose the basis of the columns of Q_0, A and $q_1, \ldots, q_n$ get replaced by their representations in the new basis.

QR algorithm and Simultaneous iterations

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So the iteration is

(i) find $Q_0^* A Q_0 (Q_0^* q_1)[= A_1 e_1], \ldots, Q_0^* A Q_0 (Q_0^* q_n)[= A_1 e_n]$, that is, consider A_1;

(ii) compute the Q, say Q_1, of a QR decomposition of A_1.

QR algorithm and Simultaneous iterations

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So the iteration is

(i) find $Q_0^* A Q_0 (Q_0^* q_1) [= A_1 e_1], \ldots, Q_0^* A Q_0 (Q_0^* q_n) [= A_1 e_n]$, that is, consider A_1;

(ii) compute the Q, say Q_1, of a QR decomposition of A_1.

Feeling very optimistic about the progress, we form $A_2 = Q_1^* A_1 Q_1$.

QR algorithm and Simultaneous iterations

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(ii) compute the Q, say Q_1, of a QR decomposition of A_1.

Feeling very optimistic about the progress, we form $A_2 = Q_1^* A_1 Q_1$.

This completes the second iteration of the QR algorithm!

QR algorithm and Simultaneous iterations

If we choose the basis of the columns of Q_0, A and $q_1, \ldots, q_n$ get replaced by their representations in the new basis.

So the iteration is

(i) find $Q_0^* A Q_0 (Q_0^* q_1) [= A_1 e_1], \ldots, Q_0^* A Q_0 (Q_0^* q_n) [= A_1 e_n]$, that is, consider A_1;

(ii) compute the Q, say Q_1, of a QR decomposition of A_1.

Feeling very optimistic about the progress, we form $A_2 = Q_1^* A_1 Q_1$.

This completes the second iteration of the QR algorithm!

Now we have the choice of performing the next iteration in three different bases, viz., $e_1, \ldots, e_n$, the columns of Q_0 or the columns of Q_1. If we choose the last option then the third iteration is

QR algorithm and Simultaneous iterations

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(i) find $Q_1^* A_1 Q_1 (Q_1^* Q_1 e_1), \ldots, Q_1^* A_1 Q_1 (Q_1^* Q_1 e_n)$, i.e., consider A_2;

(ii) compute the Q, say Q_2, of a QR decomposition of A_2.

QR algorithm and Simultaneous iterations

If we choose the basis of the columns of Q_0, A and $q_1, \ldots, q_n$ get replaced by their representations in the new basis.

So the iteration is

(i) find $Q_0^* A Q_0 (Q_0^* q_1) [= A_1 e_1], \ldots, Q_0^* A Q_0 (Q_0^* q_n) [= A_1 e_n]$, that is, consider A_1;

(ii) compute the Q, say Q_1, of a QR decomposition of A_1.

Feeling very optimistic about the progress, we form $A_2 = Q_1^* A_1 Q_1$.

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(i) find $Q_1^* A_1 Q_1 (Q_1^* Q_1 e_1), \ldots, Q_1^* A_1 Q_1 (Q_1^* Q_1 e_n)$, i.e., consider A_2;

(ii) compute the Q, say Q_2, of a QR decomposition of A_2.

To check for convergence form $A_3 := Q_2^* A_2 Q_2$.
This the third iteration of the QR algorithm!

QR algorithm and Simultaneous iterations

If we choose the basis of the columns of Q_0, A and $q_1, \ldots, q_n$ get replaced by their representations in the new basis.

So the iteration is

(i) find $Q_0^* A Q_0 (Q_0^* q_1) [= A_1 e_1], \ldots, Q_0^* A Q_0 (Q_0^* q_n) [= A_1 e_n]$, that is, consider A_1;

(ii) compute the Q, say Q_1, of a QR decomposition of A_1.

Feeling very optimistic about the progress, we form $A_2 = Q_1^* A_1 Q_1$.

This completes the second iteration of the QR algorithm!

Now we have the choice of performing the next iteration in three different bases, viz., $e_1, \ldots, e_n$, the columns of Q_0 or the columns of Q_1. If we choose the last option then the third iteration is

(i) find $Q_1^* A_1 Q_1 (Q_1^* Q_1 e_1), \ldots, Q_1^* A_1 Q_1 (Q_1^* Q_1 e_n)$, i.e., consider A_2;

(ii) compute the Q, say Q_2, of a QR decomposition of A_2.

To check for convergence form $A_3 := Q_2^* A_2 Q_2$.
This the third iteration of the QR algorithm!

Hence QR algorithm executes Simultaneous iteration with suitable change of basis at each iteration.