QR-method lecture 2

SF2524 - Matrix Computations for Large-scale Systems

Agenda QR-method

1. Decompositions (previous lecture)
   - Jordan form
   - Schur decomposition
   - QR-factorization
2. Basic QR-method
3. Improvement 1: Two-phase approach
   - Hessenberg reduction (previous lecture)
   - **Hessenberg QR-method**
4. Improvement 2: Acceleration with shifts
5. Convergence theory

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Reading instructions

Point 1: TB Lecture 24

Points 2-4: Lecture notes "QR-method" on course web page

Point 5: TB Chapter 28

(Extra reading: TB Chapter 25-26, 28-29)

Basic QR-method (previous lecture)

Basic QR-method = basic QR-algorithm

Simple basic idea: Let $A_0 = A$ and iterate:

- Compute QR-factorization of $A_k = QR$
- Set $A_{k+1} = RQ$.

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- The method often requires many iterations.

Improvement 1: Two-phase approach

We will separate the computation into two phases:

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Phases

- Phase 1: Reduce the matrix to a Hessenberg with similarity transformations (Section 2.2.1 in lecture notes)
- Phase 2: Specialize the QR-method to Hessenberg matrices (Section 2.2.2 in lecture notes)

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Idea

- Householder reflector:

$$P = I - 2uu^* \quad \text{where } u \in \mathbb{C}^m \text{ and } \|u\| = 1,$$

- Apply one Householder reflector at a time to eliminate the column by column.

Phase 2: Hessenberg QR-method

A QR-step on a Hessenberg matrix is a Hessenberg matrix:

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If the basic QR-method is applied to a Hessenberg matrix, then all iterates A_k are Hessenberg matrices.

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Recall: basic QR-step is $\mathcal{O}(m^3)$.

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Hessenberg structure can be exploited such that we can carry out a QR-step with less operations.

Definition (Givens rotation)

The matrix $G(i,j,c,s) \in \mathbb{R}^{n\times n}$ corresponding to a Givens rotation is defined by

$$G(i,j,c,s) := \begin{bmatrix} I & & & & \\ & c & & -s & \\ & & I & & \\ & s & & c & \\ & & & & I \end{bmatrix},$$

which deviates from identity at row and column i and j.

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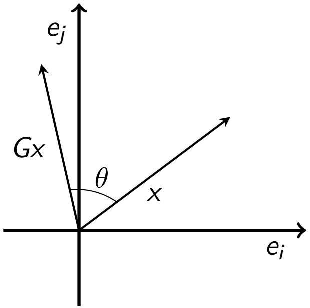

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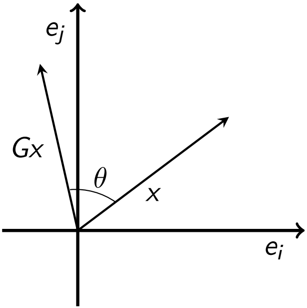

Properties

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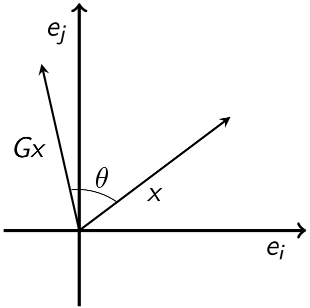

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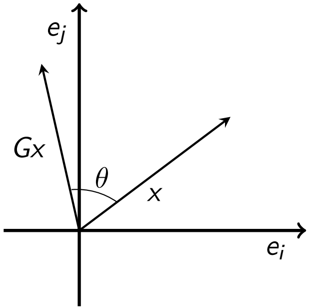

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Theorem (Theorem 2.2.6)

Suppose $A \in \mathbb{C}^{m\times m}$ is a Hessenberg matrix. Let H_i be generated as follows $H_1 = A$

$$H_{i+1} = G_i^T H_i, \quad i = 1, \dots, m-1$$

where $G_i = G(i, i+1, (H_i)_{i,i}/r_i, (H_i)_{i+1,i}/r_i)$ and $r_i = \sqrt{(H_i)_{i,i}^2 + (H_i)_{i+1,i}^2}$ and we assume $r_i \neq 0$. Then, H_n is upper triangular and

$$A = (G_1 G_2 \cdots G_{m-1}) H_n = QR$$

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Proof idea: Only one rotator required to bring one column of a Hessenberg matrix to a triangular.

* Matlab: Explicit QR-factorization of Hessenberg $\mathtt{qr}_g ivens.m$ *

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$\Rightarrow$

$$\text{the complexity of one Hessenberg QR step} = \mathcal{O}(m^2)$$

Givens rotators only modify very few elements.
Several optimizations possible. $\Rightarrow$

Algorithm 3 Hessenberg QR algorithm

Input: A Hessenberg matrix $A \in \mathbb{C}^{n\times n}$

Output: Upper triangular T such that $A = UTU^*$ for an orthogonal matrix U.

Set $A_0 := A$
for $k = 1,\ldots$ **do**
  // One Hessenberg QR step
  $H = A_{k-1}$
  for $i = 1,\ldots,n-1$ **do**
    $[c_i, s_i] = \text{givens}(h_{i,i}, h_{i+1,i})$
    $H_{i:i+1,i:n} = \begin{bmatrix} c_i & s_i \\ -s_i & c_i \end{bmatrix} H_{i:i+1,i:n}$
  end for
  for $i = 1,\ldots,n-1$ **do**
    $H_{1:i+1,i:i+1} = H_{1:i+1,i:i+1} \begin{bmatrix} c_i & -s_i \\ s_i & c_i \end{bmatrix}$
  end for
  $A_k = H$
end for
Return $T = A_\infty$

Show animation again:

http://www.youtube.com/watch?v=qmgxzsWWsNc

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Acceleration still remains

Outline:

- Basic QR-method
- Improvement 1: Two-phase approach
  - Hessenberg reduction
  - Hessenberg QR-method
- **Improvement 2: Acceleration with shifts**
- Convergence theory

Improvement 2: Acceleration with shifts (Section 2.3)

Shifted QR-method

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$\Rightarrow$ One step of shifted QR-method is a similarity transformation, with a different Q matrix.

Idealized situation: Let $\mu = \lambda(H)$

Suppose μ is an eigenvalue:
$\Rightarrow$ $H - \mu I$ is a singular Hessenberg matrix.

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QR-factorization of singular Hessenberg matrices (Lemma 2.3.1)

The R-matrix in the QR-decomposition of a singular unreduced Hessenberg matrix has the structure

$$R = \begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & & \times & \times & \times \\ & & & \times & \times \\ & & & & 0 \end{bmatrix}.$$

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* Matlab demo: Show QR-factorization of singular Hessenberg matrix in matlab *

Shifted QR for exact shift: $\mu = \lambda$

If $\mu = \lambda$ is an eigenvalue of H, then $H - \mu I$ is singular. Suppose Q, R a QR-factorization of a Hessenberg matrix and

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* Prove on blackboard *

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$\Rightarrow \lambda$ is an eigenvalue of $\bar{H}$.

More precisely:

Lemma (Lemma 2.3.2)

Suppose λ is an eigenvalue of the Hessenberg matrix H. Let $\bar{H}$ be the result of one shifted QR-step. Then,

$$\begin{aligned} \bar{h}_{n,n-1} &= 0 \\ \bar{h}_{n,n} &= \lambda. \end{aligned}$$

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Explanation

- The QR-method can be interpreted as equivalent to variant of Power Method applied to A. (Will be shown later)
- The QR-method can be interpreted as equivalent to variant of Power Method applied to A^{-1}. (Proof sketched in TB Chapter 29) $\Rightarrow$ Rayleigh shifts can be interpreted as Rayleigh quotient iteration.

Deflation

QR-step on reduced Hessenberg matrix

Suppose

$$H = \begin{pmatrix} H_0 & H_1 \\ 0 & H_3 \end{pmatrix},$$

where H_3 is upper triangular and let

$$\bar{H} = \begin{pmatrix} \bar{H}_0 & \bar{H}_1 \\ \bar{H}_2 & \bar{H}_3 \end{pmatrix},$$

be the result of one (shifted) QR-step.

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be the result of one (shifted) QR-step. Then, $\bar{H}_2 = 0$, $\bar{H}_3 = H_3$ and $\bar{H}_0$ is the result of one (shifted) QR-step applied to H_0.

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QR-step on reduced Hessenberg matrix

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This is called deflation.

Rayleigh shifts can be combined with deflation $\Rightarrow$

Algorithm 4 Hessenberg QR algorithm with Rayleigh quotient shift and deflation

Input: A Hessenberg matrix $A \in \mathbb{C}^{n\times n}$

Set $H^{(0)} := A$
for $m = n, \ldots, 2$ **do**
  $k = 0$
  repeat
    $k = k + 1$
    $\sigma_k = h_{m,m}^{(k-1)}$
    $H_{k-1} - \sigma_k I =: Q_k R_k$
    $H_k := R_k Q_k + \sigma_k I$
  until $|h_{m,m-1}^{(k)}|$ is sufficiently small
  Save $h_{m,m}^{(k)}$ as a converged eigenvalue
  Set $H^{(0)} = H_{1:(m-1),1:(m-1)}^{(k)} \in \mathbb{C}^{(m-1)\times(m-1)}$
end for

* show Hessenberg qr with shifts in matlab *
* `http://www.youtube.com/watch?v=qmgxzsWWsNc` *

Outline:

- Basic QR-method
- Improvement 1: Two-phase approach
  - Hessenberg reduction
  - Hessenberg QR-method
- Improvement 2: Acceleration with shifts
- **Convergence theory**

Convergence theory - TB Chapter 28

Didactic simplification for convergence of QR-method: Assume $A = A^T$.

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(4) Show: USI $\Leftrightarrow$ NSI $\Leftrightarrow$ QR-method

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Theorem (TB Theorem 28.1)

Suppose simultaneous iteration is started with $V^{(0)}$ and assumptions above are satisfied. Let q_j, $j = 1, \ldots, n$ be the first n eigenvectors of A. Then, as $k \to \infty$, the columns of the matrices $\hat{Q}^{(k)}$ convergence linearly to q_j

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* Show matlab demo on USI (video) *