QR-method - Lecture 2

SF2524 - Matrix Computations for Large-scale Systems

Outline QR-method:

1. Decompositions (last lecture)
2. Basic QR-method (last lecture)
3. Improvement 1: Two-phase approach
   - Hessenberg reduction
   - Hessenberg QR-method
4. Improvement 2: Acceleration with shifts
5. Convergence theory

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 (repetition last lecture)

- Method for dense eigenvalue problems
- Computes a Schur factorization

$$A = Q^* TQ$$

by using QR-factorizations

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Basic QR-method

$$\begin{aligned} A_{k-1} &= Q_k R_k \\ A_k &:= R_k Q_k \end{aligned}$$

Generates a sequence of matrices A_k with same eigenvalues, and in general converge to a triangular matrix.

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Disadvantages

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- The method often requires many iterations. (HW3, problem 1)

Improvement 1: Two-phase approach

We will separate the computation into two phases:

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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)

Phase 1: Hessenberg reduction

We will need matrices called Householder reflectors.

Definition

A matrix $P \in \mathbb{C}^{m\times m}$ of the form

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

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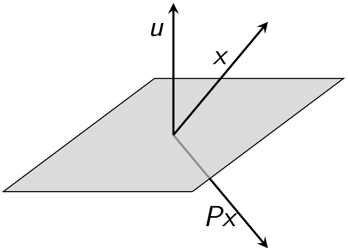

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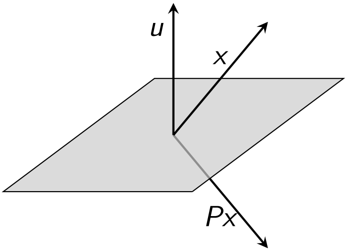

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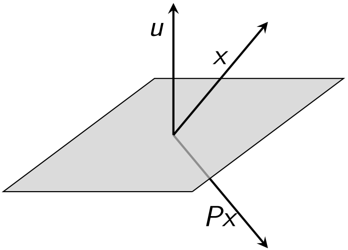

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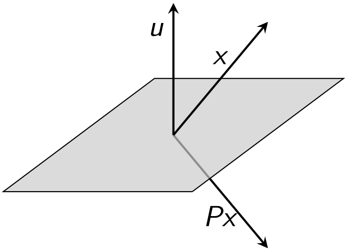

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Let $\rho = \text{sign}(x_1)$,

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* Matlab demo showing Householder reflectors *

We will be able to construct $m-2$ householder reflectors that bring the matrix to Hessenberg form.

Elimination for first column

$$P_1 := \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \end{bmatrix} = \begin{bmatrix} 1 & 0^T \\ 0 & I - 2u_1u_1^T \end{bmatrix}.$$

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$$P_1 A = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \end{bmatrix}$$

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In order to have a similarity transformation mult from right:

$$P_1AP_1^{-1} = P_1AP_1 = \text{same structure as } P_1A.$$

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Elimination for second column

Repeat the process with:

$$P_2 = \begin{bmatrix} 1 & 0 & 0^T \\ 0 & 1 & 0^T \\ 0 & 0 & I - 2u_2 u_2^T \end{bmatrix}$$

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where u_2 is constructed from the $n-2$ last elements of the second column of $P_1 A P_1^*$.

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* Matlab demo of the first two steps of the Hessenberg reduction *

The iteration can be implemented without explicit use of the P matrices.

Algorithm 2 Reduction to Hessenberg form

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

Output: A Hessenberg matrix H such that $H = U^*AU$.

for $k = 1, \ldots, n-2$ **do**

  Compute u_k using (2.4) where $x^T = [a_{k+1,k}, \cdots, a_{n,k}]$

  Compute P_kA: $A_{k+1:n,k:n} := A_{k+1:n,k:n} - 2u_k(u_k^* A_{k+1:n,k:n})$

  Compute $P_kAP_k^*$: $A_{1:n,k+1:n} := A_{1:n,k+1:n} - 2(A_{1:n,k+1:n}u_k)u_k^*$

end for

Let H be the Hessenberg part of A.

Phase 2: Hessenberg QR-method

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

* Matlab demo showing QR-step of Hessenberg is Hessenberg *

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

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

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

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

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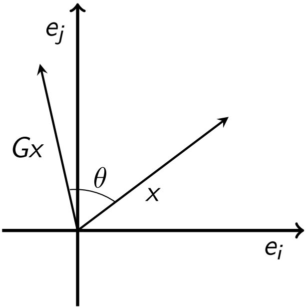

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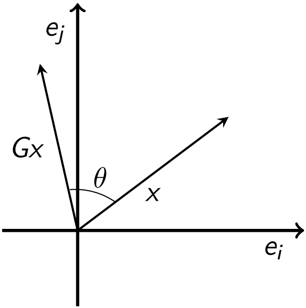

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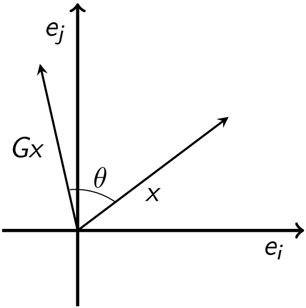

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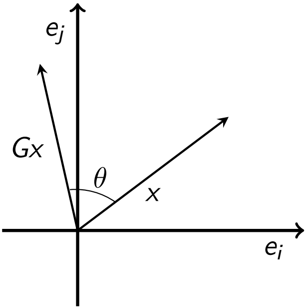

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Theorem

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

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

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.

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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, ... do
    // One Hessenberg QR step
    H = A_{k-1}
    for i = 1, ..., n-1 do
        [c_i, s_i] = givens(h_{i,i}, h_{i+1,i})
        H_{i:i+1,i:n} = [c_i  s_i; -s_i  c_i] H_{i:i+1,i:n}
    end for
    for i = 1, ..., n-1 do
        H_{1:i+1,i:i+1} = H_{1:i+1,i:i+1} [c_i  -s_i; s_i  c_i]
    end for
    A_k = H
end for
Return T = A_∞
```

$$H_{i:i+1,i:n} = \begin{bmatrix} c_i & s_i \\ -s_i & c_i \end{bmatrix} H_{i:i+1,i:n}, \qquad H_{1:i+1,i:i+1} = H_{1:i+1,i:i+1} \begin{bmatrix} c_i & -s_i \\ s_i & c_i \end{bmatrix}$$

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

One step of shifted QR-method:

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$$\begin{aligned} H - \mu I &= QR \\ \bar{H} &= RQ + \mu I \end{aligned}$$

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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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* Show QR-factorization of singular Hessenberg matrix in matlab *

Suppose Q, R a QR-factorization of a Hessenberg matrix and

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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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How to select the shifts?

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Explanation

- The QR-method can be interpreted as equivalent to variant of Power Method applied to A. (Will be shown next)
- 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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$\Rightarrow$ We can reduce the active matrix when an eigenvalue is converged.

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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

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

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    until $|h_{m,m-1}^{(k)}|$ is sufficiently small
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Convergence theory - TB Chapter 28

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

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- Show USI $\Leftrightarrow$ NSI $\Leftrightarrow$ QR-method

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- Let eigenvalues ordered and assume:

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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, $1, \ldots, n$ 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

$$\|q_j^{(k)} - \pm q_j\| = \mathcal{O}(C^k), \;\; j = 1, \ldots, n,$$

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Normalized Simultaneous Iteration (NSI)

Variants of the power method. Equivalent:

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Algorithm: (Normalized) Simultaneous Iteration

- Input $\hat{Q}^{(0)} \in \mathbb{R}^{m \times n}$
- For $k = 1, \ldots,$
    - Set $Z = A\hat{Q}^{k-1}$
    - Compute QR-factorization $\hat{Q}^{(k)}\hat{R}^{(k)} = Z$

USI and NSI are equivalent.

USI and NSI are equivalent. More precisely:

Equivalence USI and NSI (TB Thm 28.2)

Suppose assumptions above are satisfied. If USI and NSI are started with the same vector they will generate the same sequence of matrices $\hat{Q}^k$ and $\hat{R}^k$.

Simultaneous iteration and QR-method

We will establish:

$$\text{basic QR-method} \Leftrightarrow \text{Simultaneous iteration with } \hat{Q}^{(0)} = I \in \mathbb{R}^{m\times m}.$$

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More precisely ...

TB Theorem 38.3:

Theorem (Equivalence simultaneous iteration and QR-method)

The above processes generate identical sequences of vectors. In particular,

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

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Beware: QR-factorization is not unique and equivalence only holds with one QR-factorization.

Important property:

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

Consequences

- Recall from USI-NSI equivalence and USI convergence. The columns in $\hat{Q}^{(k)}$ satisfy
$$q_i^{(k)} = \pm q_i + O(C^k).$$
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  - Off-diagonal $i \neq j$: $(A^{(k)})_{i,j}$

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

Consequences

- Recall from USI-NSI equivalence and USI convergence. The columns in $\hat{Q}^{(k)}$ satisfy
$$q_i^{(k)} = \pm q_i + O(C^k).$$
where $C = \max_{1<i<n} |\lambda_{i+1}|/|\lambda_i|$.
- $(A^k)_{i,j} = (q_i^{(k)})^T A q_j^{(k)}$
  - Diagonal $i = j$: $(A^{(k)})_{i,i} = (q_i^{(k)})^T A q_i^{(k)} = r(q_i^{(k)})$ =Rayleigh quotient $\Rightarrow (A^{(k)})_{i,i} = \lambda_i + O(C^{2k})$
  - Off-diagonal $i \neq j$: $(A^{(k)})_{i,j} = (q_i^{(k)})^T A q_j^{(k)} = O(C^k)$

Important property:

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

Consequences

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Hence, $A^{(k)}$ will approach a triangular matrix

* Matlab demo *