QR-method lecture 1 SF2524 - Matrix Computations for Large-scale Systems

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Methods suitable for large sparse matrices

• Power method:

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Methods suitable for large sparse matrices

• Power method: largest eigenvalue

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- Inverse iteration:

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 - Outer isolated eigenvalues
 - Only requires matrix vector products Ay
 - Underlying the matlab command: eigs

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- Computes all eigenvalues

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Now: QR-method

- Underlying the matlab command: eig
- Computes all eigenvalues
- Suitable for dense problems
- Small matrices in comparison to previous algorithms

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Agenda QR-method

- Occompositions
 - Jordan form
 - Schur decomposition
 - QR-factorization
- Basic QR-method
- Improvement 1: Two-phase approach
 - Hessenberg reduction
 - Hessenberg QR-method
- Improvement 2: Acceleration with shifts
- Onvergence theory

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Reading instructions

Point 1: TB Lecture 24 (background.pdf) Points 2-4: Lecture notes (qrmethod.pdf) Point 5: Lecture notes (qrmethod.pdf) (TB Chapter 28) (Extra reading: TB Chapter 25-26, 28-29)

Occompositions

- Jordan form
- Schur decomposition
- QR-factorization
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- Improvement 1: Two-phase approach
 - Hessenberg reduction
 - Hessenberg QR-method
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- **5** Convergence theory

Similarity transformation

Suppose $A \in \mathbb{C}^{n \times n}$ and $V \in \mathbb{C}^{n \times n}$ is an invertible matrix. Then

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and

$$B = VAV^{-1}$$

have the same eigenvalues.

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Numerical methods based on similarity transformations

- If *B* is triangular we can read-off the eigenvalues from the diagonal.
- Idea of numerical method: Compute V such that B is triangular.

First idea: compute the Jordan canonical form

Jordan canonical form (JCF)

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Jordan canonical form (JCF)

Suppose $A \in \mathbb{C}^{n \times n}$. There exists an invertible matrix $V \in \mathbb{C}^{n \times n}$ and a block diagonal matrix such that

 $A = V \Lambda V^{-1}$

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$$A = V \Lambda V^{-1}$$

where

$$\Lambda = \begin{pmatrix} J_1 & & \\ & \ddots & \\ & & J_k \end{pmatrix},$$

where

$$J_{i} = \begin{pmatrix} \lambda_{i} & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_{i} \end{pmatrix}, i = 1, \dots, k$$

Common case: distinct eigenvalues Suppose $\lambda_i \neq \lambda_j$, i = 1, ..., n. Then, $\Lambda = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_m \end{pmatrix}.$

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Common case: symmetric matrix

Suppose $A = A^T \in \mathbb{R}^{n \times n}$. Then,

$$\Lambda = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}.$$

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Consider

$$A = \begin{pmatrix} 2 & 1 \\ & 2 & 1 \\ \varepsilon & & 2 \end{pmatrix}$$

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If $\varepsilon = 0$. Then, the Jordan canonical form (JCF) is

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If $\varepsilon > 0$. Then, the eigenvalues are distinct and

$$\Lambda = \begin{pmatrix} 2 + O(\varepsilon^{1/3}) & & \\ & 2 + O(\varepsilon^{1/3}) & \\ & & 2 + O(\varepsilon^{1/3}) \end{pmatrix}$$

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 \Rightarrow JCF not continuous with respect to ε \Rightarrow JCF is often not numerically stable

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Schur decomposition (essentially TB Theorem 24.9) Suppose $A \in \mathbb{C}^{n \times n}$. There exists an unitary matrix P

$$P^{-1} = P^*$$

and a triangular matrix T such that

 $A = PTP^*$.

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The Schur decomposition is numerically stable. Goal with QR-method: Numercally compute a Schur factorization

Outline:

Decompositions

- Jordan form
- Schur decomposition
- QR-factorization

Basic QR-method

- Improvement 1: Two-phase approach
 - Hessenberg reduction
 - Hessenberg QR-method
- Improvement 2: Acceleration with shifts
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QR-factorization

Suppose $A \in \mathbb{C}^{n \times n}$. There exists a unitary matrix $Q \in \mathbb{C}^{n \times n}$ and an upper triangular matrix $R \in \mathbb{C}^{n \times n}$ such that

A = QR

QR-factorization

Suppose $A \in \mathbb{C}^{n \times n}$. There exists a unitary matrix $Q \in \mathbb{C}^{n \times n}$ and an upper triangular matrix $R \in \mathbb{C}^{n \times n}$ such that

$$A = QR$$

Note: Very different from Schur factorization

 $A = PTP^*$

- QR-factorization can be computed with a finite number of operations
- Schur decomposition directly gives us the eigenvalues

Didactic simplifying assumption: All eigenvalues are real

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Didactic simplifying assumption: All eigenvalues are real

 ${\sf Basic} \ {\sf QR}{\sf -method} = {\sf basic} \ {\sf QR}{\sf -algorithm}$

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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Basic QR-method = basic QR-algorithm

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Note:

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$$A_1 = RQ = Q^*A_0Q \Rightarrow A_0, A_1, \dots$$
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Simple basic idea: Let $A_0 = A$ and iterate:

- Compute QR-factorization of $A_k = QR$
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Note:

- $A_1 = RQ = Q^*A_0Q \Rightarrow A_0, A_1, \dots$ have the same eigenvalues
- More remarkable: $A_k \rightarrow$ triangular matrix (except special cases)

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$A_k \rightarrow \text{triangular matrix:}$



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 $A_k \rightarrow \text{triangular matrix:}$



* Time for matlab demo *

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Elegant and robust but not very efficient:

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Elegant and robust but not very efficient:

Disadvantages

• Computing a QR-factorization is quite expensive. One iteration of the basic QR-method

 $\mathcal{O}(n^3).$

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• Computing a QR-factorization is quite expensive. One iteration of the basic QR-method

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• The method often requires many iterations.

Improvement demo:

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

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