SF2524 - Matrix computations for large-scale systems

SF3580 - Numerical linear algebra (PhD level course)

Intro lecture, November 4, 2014

Elias Jarlebring
KTH Royal Institute of Technology
Mathematics Dept. - NA division

Lecture 1

- About the lecturer
- About the topic
- About the course

- Fundamental eigenvalue techniques:
  - Rayleigh quotient
  - Power method
  - Inverse iteration
  - Rayleigh qoutient iteration

About the Lecturer

Associate Professor - teacher - researcher

CV - Elias Jarlebring

- MSc: KTH, Stockholm
- PhD: TU Braunschweig, Germany
- Topic: Mathematics (applied & computational mathematics)
  Specialization: Numerical linear algebra

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Awards / grants

Gustafsson-pris för unga forskare, Elgersburg best presentation award, Vetenskaprsådets bidrag till yngre forskare, ...

Countries

Sweden, Germany, Belgium, USA, Ireland

Other

Language-nerd: Swedish, English, German, Flemish
Former indie game-developer: freecol, nenem, ...
Former programming consultant

Social media

- Facebook (not for students)
- Scientific microblog, twitter: @ejarlebring
  Tweeting about science, mathematical elegance, nerdy stuff and numerical linear algebra.

Teaching portfolio

Teaching - Elias Jarlebring

- Experience: All university levels
  bachelor, master, PhD-level (+high-shool level)
- Semi-classical lecturing style:
  slides, blackboard, computer demos, additional online material

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- Germany 2006: Clear explanations
- Sweden ∼2012: Authorative style. Strict. Structured and competent.

About the topic

Definition: Numerical linear algebra

Numerical linear algebra is the study of numerical methods for linear algebra operations

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Large-scale matrix computations

- Algorithms and methods that involve matrices of large size
- Large-scale matrix computations $\subset$ Numerical linear algebra

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Applications arise in essentially all scientific fields

- Molecular properties in chemistry
- Black holes in astronomy
- Microvascular networks in cell biology
- Most importantly: Discretizations of PDEs
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The predictive power of the model is often limited by the performance of the algorithms. We study the details of the algorithms.

The course is about the methods and details, not the applications.

About the course - SF2524

Course contents - SF2524

A selection of topics in numerical linear algebra:

- Numerical methods for eigenvalue problems
- Numerical methods for linear systems of equations
- Numerical methods for matrix functions
- (Numerical methods for matrix equations - PhD level)

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Not-so-serious answers:

- Answer 1: Elias thinks they are cool and full of mathematical elegance
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Why these topics?

Not-so-serious answers:

- Answer 1: Elias thinks they are cool and full of mathematical elegance
- Answer 2: Elias thinks they are useful in applications.

More serious answers:

- They are mature well-represented active topics in the research field of numerical linear algebra.
- Many applications lead to one of these problems, and future approaches (for instance used in industry/companies) are likely to be based on these methods.

Practicalities

Course webpage

KTH Social = Course web. Please read news-feed.

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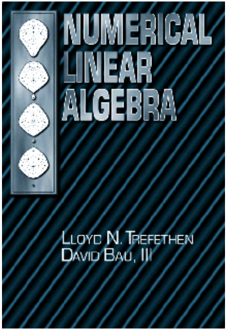
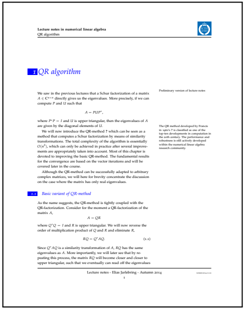
Homework

- Three sets of homework on theory and hands-on practice of the methods (four for PhD students)
- Work in groups of at most two
- Compulsary, can give bonus points for exam
- Hand in correct solutions (in the form of a report) before deadline ⇒ bonus points for exam. One report per group.

Literature

- *Numerical Linear Algebra* by Lloyd N. Trefethen and David Bau, available in kårbokhandeln
- Additional handouts downloadable on web:
  - Lecture notes on the convergence of the Arnoldi method
  - Lecture notes on the QR-method
- Additional material on matrix functions





Lecture notes in numerical linear algebra
QR algorithm

1 QR algorithm

Preliminary version of lecture notes

We saw in the previous lectures that a Schur factorization of a matrix $A \in \mathbb{C}^{n\times n}$ directly gives us the eigenvalues. More precisely, if we can compute P and U such that

$$A = PUP^*,$$

where $P^*P = I$ and U is upper triangular, then the eigenvalues of A are given by the diagonal elements of U.

We will now introduce the QR-method ? which can be seen as a method that computes a Schur factorization by means of similarity transformations. The total complexity of the algorithm is essentially $O(n^3)$, which can only be achieved in practice after several improvements are appropriately taken into account. Most of this chapter is devoted to improving the basic QR-method. The fundamental results for the convergence are based on the vector iterations and will be covered later in the course.

The QR method developed by Francis in 1960's ? is classified as one of the top-ten developments in computation in the 20th century. The performance and robustness is still actively developed within the numerical linear algebra research community.

Although the QR-method can be successfully adapted to arbitrary complex matrices, we will here for brevity concentrate the discussion on the case where the matrix has only real eigenvalues.

1.1 Basic variant of QR-method

As the name suggests, the QR-method is tightly coupled with the QR-factorization. Consider for the moment a QR-factorization of the matrix A,

$$A = QR$$

where $Q^*Q = I$ and R is upper triangular. We will now reverse the order of multiplication product of Q and R and eliminate R,

$$RQ = Q^*AQ. \quad (1.1)$$

Since Q^*AQ is a similarity transformation of A, RQ has the same eigenvalues as A. More importantly, we will later see that by repeating this process, the matrix RQ will become closer and closer to upper triangular, such that we eventually can read off the eigenvalues

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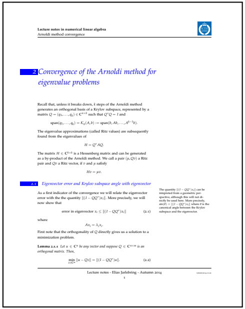
1



Lecture notes in numerical linear algebra
Arnoldi method convergence

2 Convergence of the Arnoldi method for eigenvalue problems

Recall that, unless it breaks down, k steps of the Arnoldi method generates an orthogonal basis of a Krylov subspace, represented by a matrix $Q = (q_1,\ldots,q_k) \in \mathbb{C}^{n\times k}$ such that $Q^*Q = I$ and

$$\operatorname{span}(q_1,\ldots,q_k) = \mathcal{K}_k(A,b) := \operatorname{span}(b, Ab, \ldots, A^{k-1}b).$$

The eigenvalue approximations (called Ritz values) are subsequently found from the eigenvalues of

$$H = Q^*AQ.$$

The matrix $H \in \mathbb{C}^{k\times k}$ is a Hessenberg matrix and can be generated as a by-product of the Arnoldi method. We call a pair (μ, Qv) a Ritz pair and Qv a Ritz vector, if v and μ safisfy

$$Hv = \mu v.$$

2.1 Eigenvector error and Krylov subspace angle with eigenvector

As a first indicator of the convergence we will relate the eigenvector error with the the quantity $\|(I - QQ^*)x_i\|$. More precisely, we will now show that

$$\text{error in eigenvector } x_i \le \|(I - QQ^*)x_i\| \quad (2.1)$$

The quantity $\|(I - QQ^*)x_i\|$ can be intepreted from a geometric perspective, although this will not directly be used here. More precisely, $\sin(\theta) = \|(I - QQ^*)x_i\|$ where θ is the canonical angle between the Krylov subspace and the eigenvector.

where

$$Ax_i = \lambda_i x_i.$$

First note that the orthogonality of Q directly gives us a solution to a minimization problem.

Lemma 2.1.1 *Let $u \in \mathbb{C}^n$ be any vector and suppose $Q \in \mathbb{C}^{n\times m}$ is an orthogonal matrix. Then,*

$$\min_{z\in\mathbb{C}^m} \|u - Qz\| = \|(I - QQ^*)u\|. \quad (2.2)$$

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Greetings from "older" students

Feedback in similar courses given by the lecturer:

- "The lectures are pre-cooking so I can read the material easier myself"
- **"I first looked at the home-work and thought, this will be so much work..., and then we actually started and the tasks in the homework were quite specific so it went fast"**
- "High attendence in the lectures is important"
- "I would have liked to learn more about XYZ"

Lecture overview (preliminary)

- Lecture 1-3: Eigenvalue algorithms (part 1)
  - Power method, Rayleigh qoutient iteration
  - Krylov methods
- Lecture 4-8: Linear systems of equations
  - Krylov methods: GMRES, CG, BiCGstab
- Lecture 8-9: Eigenvalue algorithms (part 2): QR-method
- Lecture 10-13: Functions of matrices
  - Scaling-and-squaring, Krylov methods

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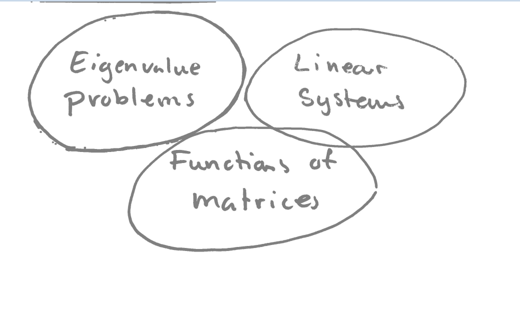

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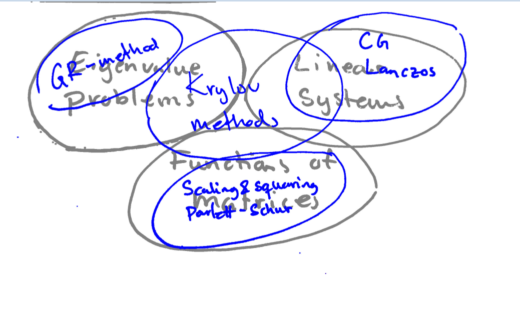

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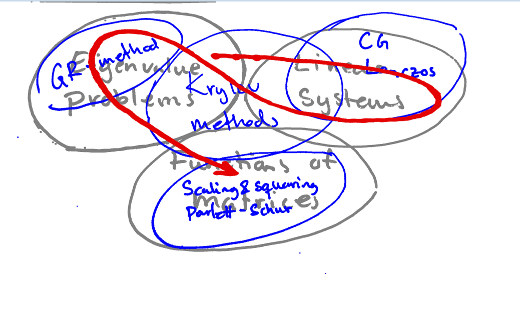

Funtamental eigenvalue techniques:

- Rayleigh qoutient
- Power method = power iteration
- Inverse iteration
- Rayleigh qoutient iteration