SF2524 - Matrix computations for large-scale systems

SF3580 - Numerical linear algebra (PhD level course)

Intro lecture, November 2, 2015

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 (TU Hamburg, TCD - Dublin)
- PhD: TU Braunschweig, Germany
- Topic: Mathematics (applied & computational mathematics)
  Specialization: Numerical linear algebra

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Countries

Sweden, Germany, Belgium, USA, Ireland

Awards / grants

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

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.

KTH - SCI

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

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Large-scale matrix computations

- Algorithms and methods that involve matrices of large size
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Applications / motivation

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 course is about the methods, 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)

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Not-so-serious answers:

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

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- Answer 1: Elias thinks they are full of 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 methods used in industry/companies will be based on these.

Practicalities

Course webpage

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

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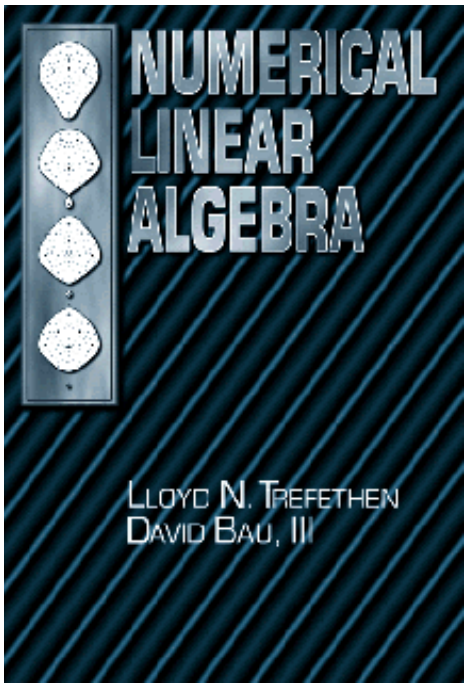
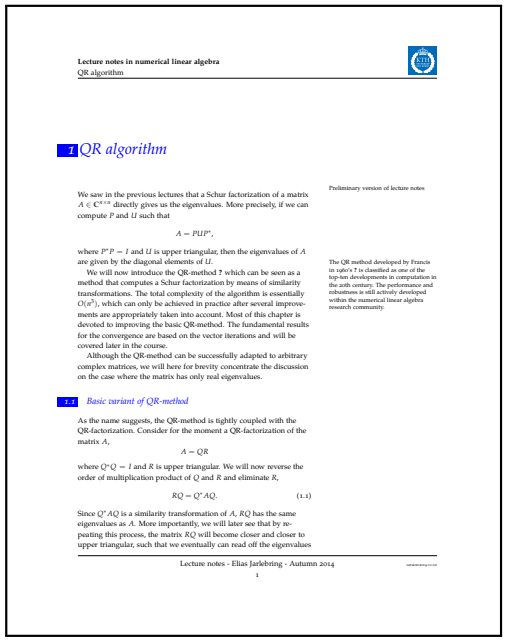
Homework

- 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 $\Rightarrow$ bonus points for exam. One report per group.

Literature

- *Numerical Linear Algebra* by Lloyd N. Trefethen and David Bau, available in kårbokhandeln
- Lecture notes PDFs online
  - Lecture notes on the convergence of the Arnoldi method
  - Lecture notes on the QR-method
  - Lecture notes 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.

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.

The QR method developed by Francis in 1961/62 ? 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.

1.1 Basic variant of QR-method

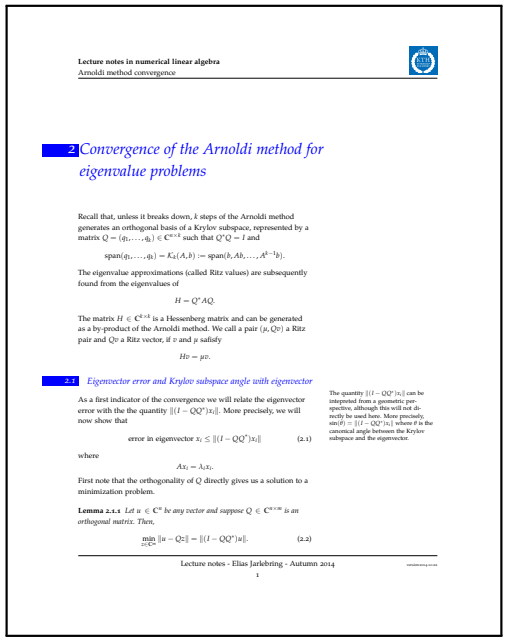
As the name suggests, the QR-method is tightly coupled with the QR-factorization. Consider for the moment a QR-factorization of the matrix A,

$$A = QR$$

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,

$$RQ = Q^*AQ. \tag{1.1}$$

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



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

$$\text{span}(q_1, \ldots, q_k) = K_k(A, b) := \text{span}(b, Ab, \ldots, A^{k-1}b).$$

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 satisfy

$$Hv = \mu v.$$

2.1 Eigenvector error and Krylov subspace angle with eigenvector

The quantity $\|(I - QQ^*)x_i\|$ can be interpreted 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.

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

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

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,*

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

Greetings from "older" students

- **"Take notes during lectures. The proofs in the book are sometimes incomplete."**
- "For me, 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"**
- "The homework are designed to check understanding of the actual contents of the course."
- "Elias är en klippa"
- "High attendence in the lectures is important"
- "I would have liked to learn more about topic XYZ"
- "After the second lecture, I thought, wow this is totally different"

Lecture overview (preliminary)

- Lecture 1-4: Eigenvalue algorithms (part 1)
  - Power method, Rayleigh qoutient iteration
  - Krylov methods
- Lecture 4-8: Linear systems of equations
  - Krylov methods: GMRES, CG, BiCGstab
- Lecture 8-10: Eigenvalue algorithms (part 2): QR-method
- Lecture 11-14: Functions of matrices
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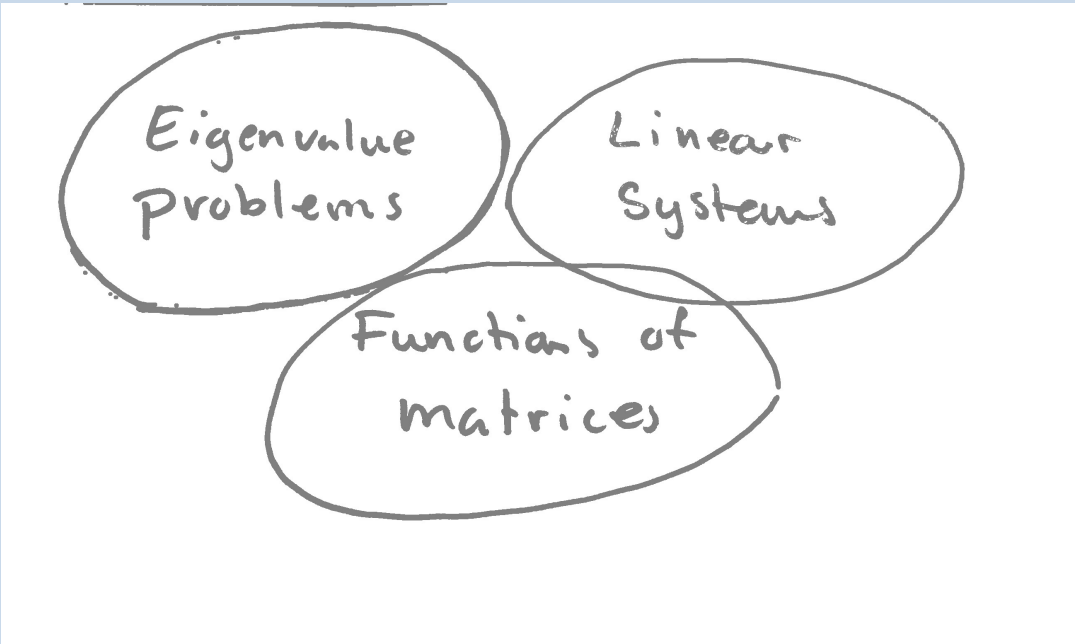

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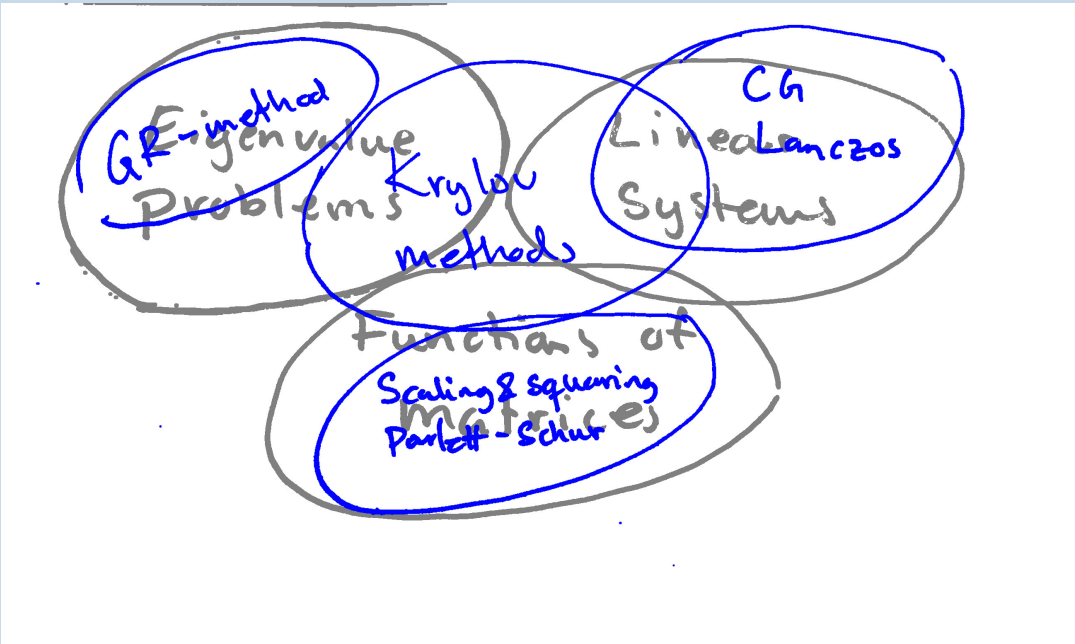

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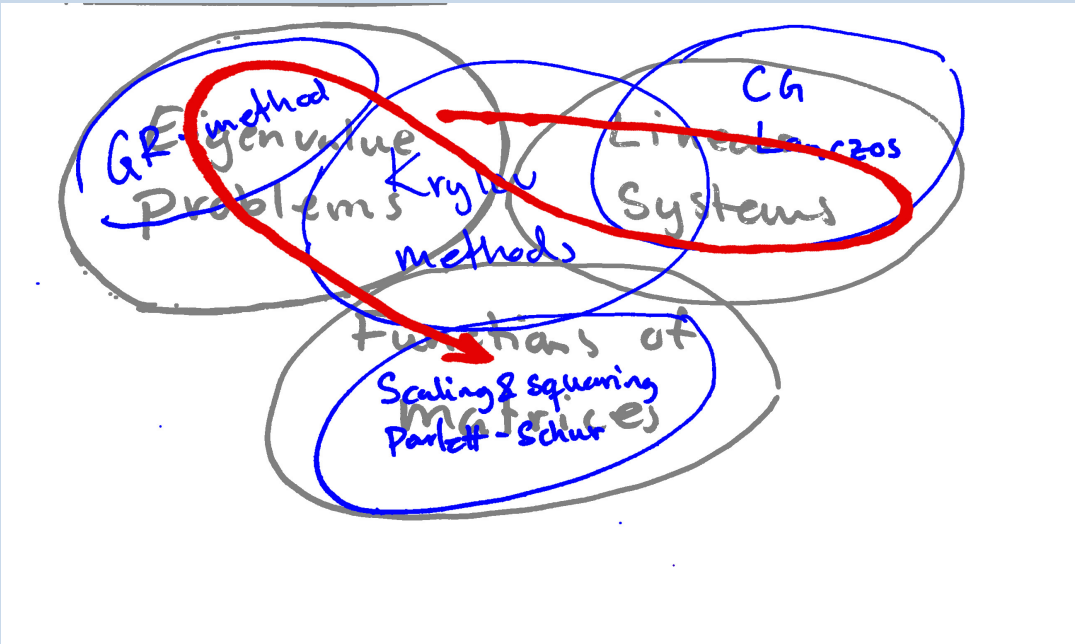

This lecture: Funtamental eigenvalue techniques.

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