SF2524 - Matrix computations for large-scale systems

≈ Numerical linear algebra for large-scale systems

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

Lecture 1

- About the teachers
- About the students
- About the topic
- About the course

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

About the Lecturer

Elias Jarlebring - Associate Professor - teacher - researcher

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Background - Elias Jarlebring

- From: Vännäs/Umeå, Sweden
- MSc: KTH, Stockholm (Teknisk fysik)
- MSc thesis: TU Hamburg
- PhD: TU Braunschweig, Germany
- Post-doc: KU Leuven, Belgium
- Dahlquist fellow: KTH, Stockholm
- Assoc. Prof (Lektor): KTH, Stockholm
- Assoc. Prof (Docent): KTH, Stockholm

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  - applied and computational mathematics
  - numerical linear algebra: e.g. Nonlinear eigenvalue problems

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- EU globetrotter: Sweden, Ireland, Germany, Belgium, USA

Teaching portfolio - Elias Jarlebring

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- Experience: All university levels + four countries
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- Germany 2006: Clear explanations
- Sweden ∼2012: Authorative style. Strict. Structured and competent.
- Sweden ∼2016: The best learning experience I have had

About the Teaching Assistant

Teaching assistant: Giampaolo Mele

TA: Giampaolo Mele

- Moderator of Wiki
- Answers questions (email)
- Answers questions office hours
- Substitute lecturer
- Competent: researcher in numerical linear algebra
- Very friendly!

About the students

Who are the students

?

Who are the students

?

Students from countries

Sweden, France, Germany, USA, Denmark, Netherlands, India, South africa, China, UK, Spain, Iceland . . .

Beware: Different student background $\Rightarrow$ Different skill set.

About the topic

Numerical linear algebra in a bigger context

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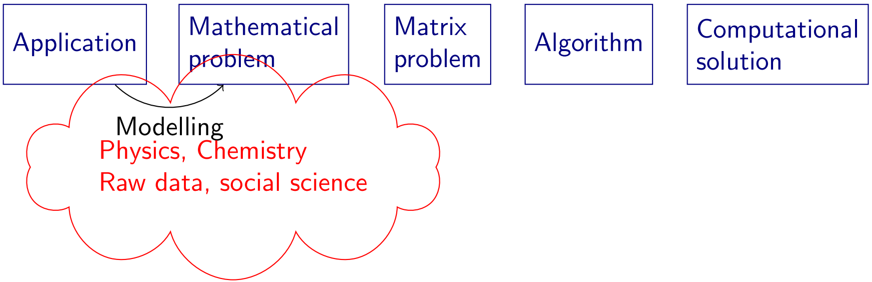

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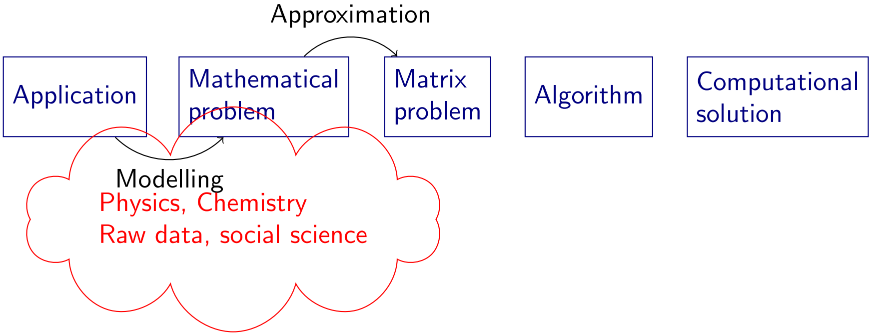

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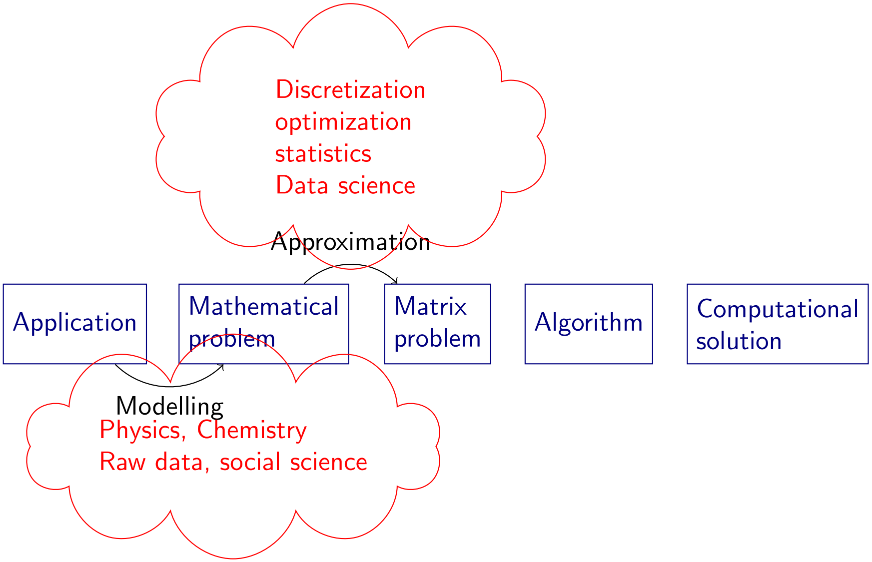

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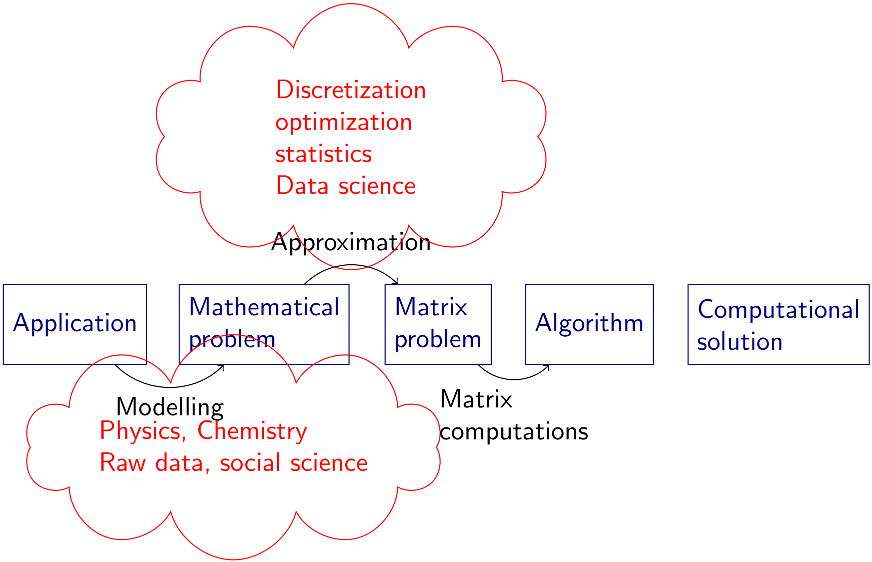

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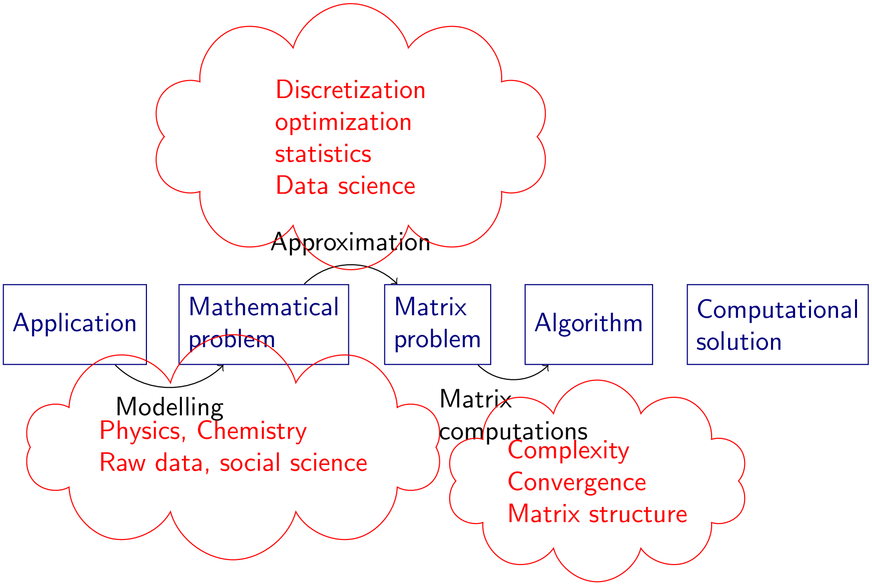

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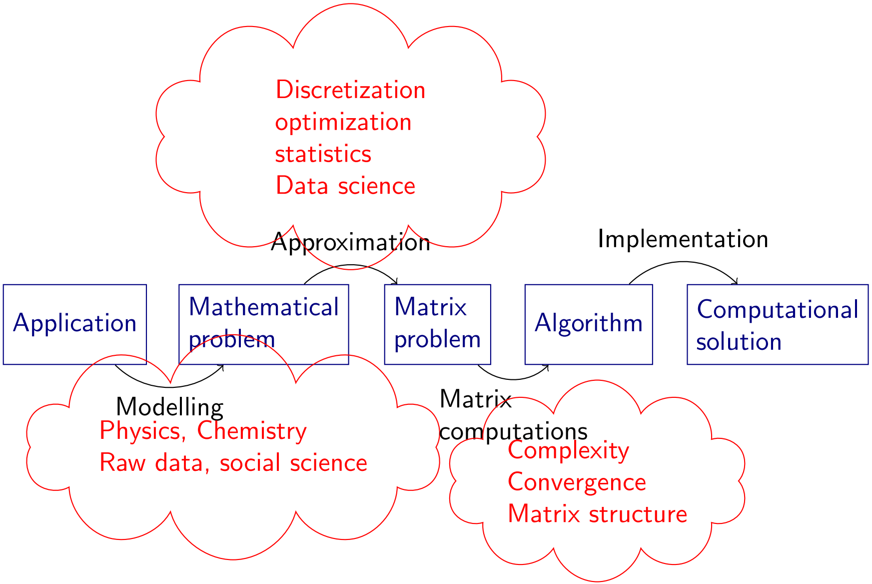

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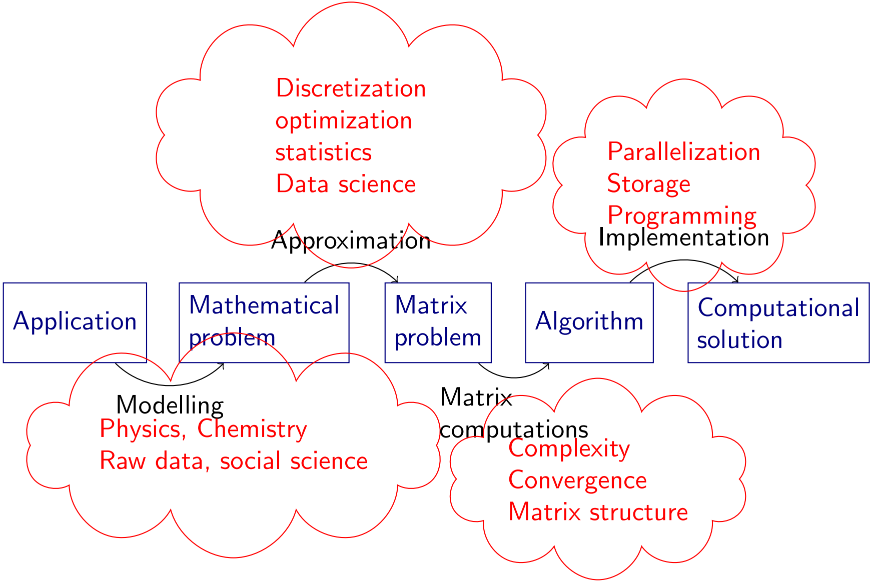

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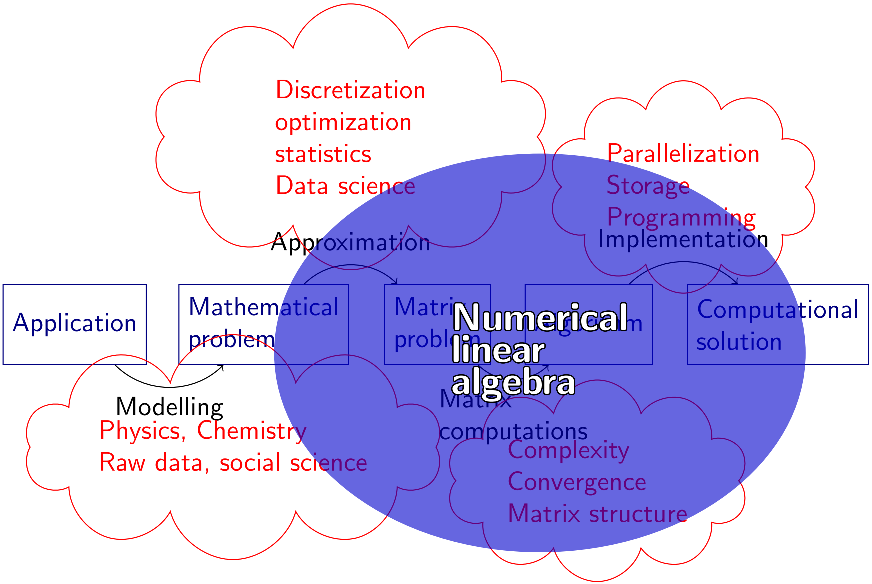

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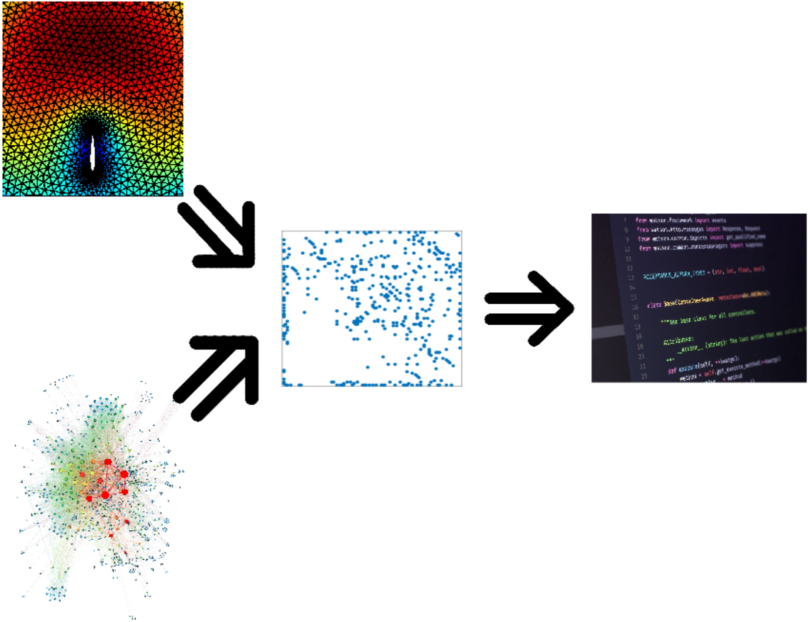

Definition: Numerical linear algebra

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

Large-scale matrix computations

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

Applications / motivation

Applications arise in essentially all scientific fields

- Physics, mechanics, astronomy, etc
- Chemistry, quantum chemistry, biology,
- Data science, data analysis, machine learning
- Discretizations of PDEs
- ...

The predictive power of the model is often limited by the performance of the algorithms. We study the details of the algorithms.

Definition: Numerical linear algebra

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About the course - SF2524

Course contents - SF2524

A selection of topics in numerical linear algebra.
Separated into blocks:

- Background: Orthogonal matrices Jordan decomposition
- Block 1: Large and sparse eigenvalue algorithms
- Block 2: Iterative methods for Linear systems
- Block 3: QR method
- Block 4: Matrix functions
- (Block 5: Matrix equations only PhD students SF3580)

Why these topics?

- Most mature problem classes in research on matrix comp
- Most common matrix problems in applications

Lectures

Lectures: approx 15 lectures

- Introduce you to concepts (pre-cooking)
- Sometimes more details where book not satisfactory
- Learning by watching live programming (+interaction)

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Lecture overview (preliminary)

- Lecture 1-4: Block 1: Eigenvalue algorithms (part 1)
- Lecture 4-9: Block 2: Linear systems of equations
- Lecture 10-11: Block 3: Eigenvalue algorithms (part 2): QR-method
- Lecture 12-15: Block 4: Functions of matrices

Practicalities

Course webpage

- Online learning platform: CANVAS
- Course registration necessary to obtain complete access.
- Most course material online
- Mandatory quizzes
- Optional quiz: background

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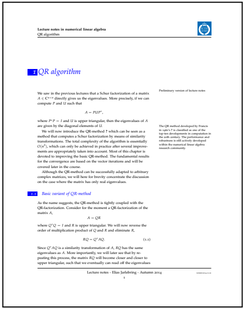
Literature

- Lecture notes PDFs online (block$X$.pdf $X = 1, 2, 3, 4, 5$). References to pages in [TB].
- *Numerical Linear Algebra* by Lloyd N. Trefethen and David Bau [TB], available in kårbokhandeln



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,

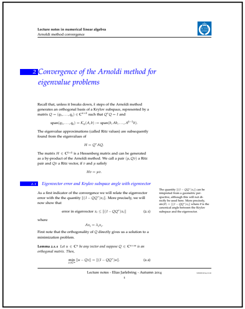
$$A = QR$$

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

Lecture notes - Elias Jarlebring - Autumn 2014
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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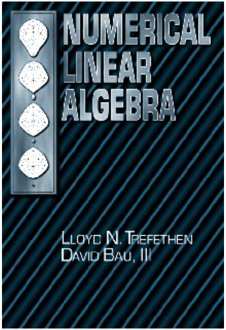

MATLAB julia

Programming language

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SF2524: Select between

- MATLAB; or
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SF3580:

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- Live programming in lectures will be in MATLAB.

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Homework

- 3× homework sets: theory and hands-on practice of the methods
- Work in groups of at most two

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Two types of bonus points

- Regular bonus points.
- Wiki bonus points: Reduces limits for grade A and B.

Elias: More info on CANVAS web and hw1.pdf

Course wiki: active learning

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- Students create problems and solutions

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- Think out of the box! Help each other! Don't be afraid to pose easy problems! Don't be afrait make mistakes! It's fun!

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Course analysis and development

Course analysis and development

Greetings from "older" students:

Messages from students of previous year(s)

- "Take notes during lectures. The proofs in the book are sometimes incomplete."
- "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 specific so it went fast"
- "The homework are designed to check understanding of the actual contents of the course."
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[width=]FFF-Rose-87-year-old-student-150x150.jpg Greetings from old student

Course development HT19 (see course analysis)

- New parts in homeworks
- More written material in blockX.pdf
- More video material

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Time to start the lecture ...

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Fundamental eigenvalue techniques (block 1)

- Examples: Large and sparse eigenvalue problems
- Rayleigh quotient
- Power method = power iteration
- Inverse iteration
- Rayleigh qoutient iteration

Large eigenproblem example: Structural mechanics

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Structural mechanics + Finite Element Method ⇒

$$Ax = \lambda x$$

- A is a large and sparse matrix (stiffness matrix)
- (λ, x) determines vibrations

Large eigenproblem example: Data science

Facebook network:

[width=0.45]facebook-network.png

Graph of representing interconnectedness of data $\Rightarrow$

$$Ax = \lambda x$$

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Large eigenproblem example: Data science

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Graph of representing interconnectedness of data $\Rightarrow$

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Learn more in SF2526 - Numerics for data science

Algorithm 27.1. Power Iteration

$v^{(0)}$ = some vector with $\|v^{(0)}\| = 1$
for $k = 1, 2, \ldots$
  $w = Av^{(k-1)}$ — apply A
  $v^{(k)} = w/\|w\|$ — normalize
  $\lambda^{(k)} = (v^{(k)})^T A v^{(k)}$ — Rayleigh quotient

In this and the algorithms to follow, we give no attention to termination conditions, describing the loop only by the suggestive expression "**for** $k = 1, 2, \ldots$." Of course, in practice, termination conditions are very important, and this is one of the points where top-quality software such as can be found in LAPACK or MATLAB is likely to be superior to a program an individual might write.

We can analyze power iteration easily. Write $v^{(0)}$ as a linear combination of the orthonormal eigenvectors q_i:

$$v^{(0)} = a_1 q_1 + a_2 q_2 + \cdots + a_m q_m.$$

Since $v^{(k)}$ is a multiple of $A^k v^{(0)}$, we have for some constants c_k

$$\begin{aligned} v^{(k)} &= c_k A^k v^{(0)} \\ &= c_k(a_1\lambda_1^k q_1 + a_2\lambda_2^k q_2 + \cdots + a_m\lambda_m^k q_m) \\ &= c_k\lambda_1^k\left(a_1 q_1 + a_2(\lambda_2/\lambda_1)^k q_2 + \cdots + a_m(\lambda_m/\lambda_1)^k q_m\right). \end{aligned} \quad (27.4)$$

From here we obtain the following conclusion.

Theorem 27.1. *Suppose $|\lambda_1| > |\lambda_2| \geq \cdots \geq |\lambda_m| \geq 0$ and $q_1^T v^{(0)} \neq 0$. Then the iterates of Algorithm 27.1 satisfy*

$$\|v^{(k)} - (\pm q_1)\| = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right), \qquad |\lambda^{(k)} - \lambda_1| = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^{2k}\right) \quad (27.5)$$

as $k \to \infty$. The $\pm$ sign means that at each step k, one or the other choice of sign is to be taken, and then the indicated bound holds.

Proof. The first equation follows from (27.4), since $a_1 = q_1^T v^{(0)} \neq 0$ by assumption. The second follows from this and (27.3). If $\lambda_1 > 0$, then the $\pm$ signs are all + or all −, whereas if $\lambda_1 < 0$, they alternate. □

The $\pm$ signs in (27.5) and in similar equations below are not very appealing. There is an elegant way to avoid these complications, which is to speak of convergence of subspaces, not vectors—to say that $\langle v^{(k)}\rangle$ converges to $\langle q_1\rangle$, for

example. However, we shall not do this, in order to avoid getting into the details of how convergence of subspaces can be made precise.

On its own, power iteration is of limited use, for several reasons. First, it can find only the eigenvector corresponding to the largest eigenvalue. Second, the convergence is linear, reducing the error only by a constant factor $\approx |\lambda_2/\lambda_1|$ at each iteration. Finally, the quality of this factor depends on having a largest eigenvalue that is significantly larger than the others. If the largest two eigenvalues are close in magnitude, the convergence will be very slow.

Fortunately, there is a way to amplify the differences between eigenvalues.

Inverse Iteration

For any $\mu \in \mathbb{R}$ that is not an eigenvalue of A, the eigenvectors of $(A - \mu I)^{-1}$ are the same as the eigenvectors of A, and the corresponding eigenvalues are $\{(\lambda_j - \mu)^{-1}\}$, where $\{\lambda_j\}$ are the eigenvalues of A. This suggests an idea. Suppose μ is close to an eigenvalue λ_J of A. Then $(\lambda_J - \mu)^{-1}$ may be much larger than $(\lambda_j - \mu)^{-1}$ for all $j \neq J$. Thus, if we apply power iteration to $(A - \mu I)^{-1}$, the process will converge rapidly to q_J. This idea is called *inverse iteration*.

Algorithm 27.2. Inverse Iteration

$v^{(0)}$ = some vector with $\|v^{(0)}\| = 1$
for $k = 1, 2, \ldots$
  Solve $(A - \mu I)w = v^{(k-1)}$ for w — apply $(A - \mu I)^{-1}$
  $v^{(k)} = w/\|w\|$ — normalize
  $\lambda^{(k)} = (v^{(k)})^T A v^{(k)}$ — Rayleigh quotient

What if μ is an eigenvalue of A, so that $A - \mu I$ is singular? What if it is nearly an eigenvalue, so that $A - \mu I$ is so ill-conditioned that an accurate solution of $(A - \mu I)w = v^{(k-1)}$ cannot be expected? These apparent pitfalls of inverse iteration cause no trouble at all; see Exercise 27.5.

Like power iteration, inverse iteration exhibits only linear convergence. Unlike power iteration, however, we can choose the eigenvector that will be found by supplying an estimate μ of the corresponding eigenvalue. Furthermore, the rate of linear convergence can be controlled, for it depends on the quality of μ. If μ is much closer to one eigenvalue of A than to the others, then the largest eigenvalue of $(A - \mu I)^{-1}$ will be much larger than the rest. Using the same reasoning as with power iteration, we obtain the following theorem.

Theorem 27.2. *Suppose λ_J is the closest eigenvalue to μ and λ_K is the second closest, that is, $|\mu - \lambda_J| < |\mu - \lambda_K| \leq |\mu - \lambda_j|$ for each $j \neq J$. Furthermore,*

suppose $q_J^T v^{(0)} \neq 0$. Then the iterates of Algorithm 27.2 satisfy

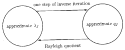
$$\|v^{(k)} - (\pm q_J)\| = O\left(\left|\frac{\mu - \lambda_J}{\mu - \lambda_K}\right|^k\right), \qquad |\lambda^{(k)} - \lambda_J| = O\left(\left|\frac{\mu - \lambda_J}{\mu - \lambda_K}\right|^{2k}\right)$$

as $k \to \infty$, where the $\pm$ sign has the same meaning as in Theorem 27.1.

Inverse iteration is one of the most valuable tools of numerical linear algebra, for it is the standard method of calculating one or more eigenvectors of a matrix if the eigenvalues are already known. In this case Algorithm 27.2 is applied as written, except that the calculation of the Rayleigh quotient is dispensed with.

Rayleigh Quotient Iteration

So far in this lecture, we have presented one method for obtaining an eigenvalue estimate from an eigenvector estimate (the Rayleigh quotient), and another method for obtaining an eigenvector estimate from an eigenvalue estimate (inverse iteration). The possibility of combining these ideas is irresistible:



(The figure is oversimplified; to get from an approximate λ_J to an approximate q_J by a step of inverse iteration, one also needs a preliminary approximation to q_J.) The idea is to use continually improving eigenvalue estimates to increase the rate of convergence of inverse iteration at every step. This algorithm is called *Rayleigh quotient iteration*.

Algorithm 27.3. Rayleigh Quotient Iteration

$v^{(0)}$ = some vector with $\|v^{(0)}\| = 1$
$\lambda^{(0)} = (v^{(0)})^T A v^{(0)}$ = corresponding Rayleigh quotient
for $k = 1, 2, \ldots$
  Solve $(A - \lambda^{(k-1)} I)w = v^{(k-1)}$ for w — apply $(A - \lambda^{(k-1)} I)^{-1}$
  $v^{(k)} = w/\|w\|$ — normalize
  $\lambda^{(k)} = (v^{(k)})^T A v^{(k)}$ — Rayleigh quotient