Numerical Linear Algebra for Computational Science and Information Engineering

Introduction

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Outline I

Numerical linear algebra: The "Why?", the "What?" and "What's next?"

Why do we need numerical linear algebra?

Prevalence of linear algebra in research and industry:

- Scientific computing (often explicitly related to problems of linear algebra)
- Simulations (e.g., discretized PDEs, ODEs, DAEs, ...)
- Machine learning (e.g., PCA, RKHS, ...)
- Optimization

Methods taught in linear algebra:

- Solving linear systems: Cramer's rule and Gaussian elimination
- Matrix factorizations: Cholesky, LU and QR
- Eigenvalue problems: Root-finding of characteristic polynomials

Limitations of methods taught in linear algebra:

- **No general exact method for eigenvalues of matrices** larger than 4x4
- **Computational infeasibility** of analytical methods **for large systems**
- **Numerical instability** leading to significant **errors**
- **Inability to handle special structures** (e.g., sparsity, implicitness)

Need for methods to solve challenging problems efficiently

What is numerical linear algebra?

What does numerical numerical linear algebra (NLA) address:

- Efficient algorithms for large-scale problems of linear algebra
- Techniques for maintaining numerical stability and accuracy
- Methods for exploiting matrix structure (e.g., sparsity, symmetry, low-rank)
- Matrix-free formulations for implicit operators
- Error analysis and conditioning

Scope of NLA:

- Focuses on both theoretical analysis (e.g., convergence, conditioning and stability) and practical implementation.
- Incorporates aspects of performance and computer architecture for method development, e.g.,
  - Repurposing solvers into preconditioners for higher performance.
  - Designing sparse data structures and BLAS kernels to optimize memory usage.

Key branches of NLA:

- **Direct methods** vs **iterative methods** (stationary vs Krylov)
- **Dense matrices** vs **sparse matrices** and **matrix-free operators**

What's coming next in numerical linear algebra?

Recent developments in NLA research show promise for significant performance improvements, but face challenges in widespread adoption:

- **Randomization**: Randomly reduces problem dimensions while preserving inherent structure with high probability. Associated challenges are
  - Ensuring convergence and assessing stability.
  - Defining and implementing reliably amortized sketching procedures.
- **Communication avoidance**: Redesigns algorithms to minimize data movement between processors or memory hierarchies. Challenges are
  - Maintaining numerical stability with reduced communication.
- **Mixed precision**: Utilizes different numerical precisions within a single algorithm to optimize performance. Associated challenges are
  - Ensuring overall stability and accuracy with lower precision components.
  - Developing adaptive strategies for precision selection.
- **Extension of state-of-the art methods to tensor data**: Assessing convergence and stability when using low-rank approximation of tensor data, e.g., Tucker and Tensor-Train formats.

Computational mathematics @ TUM

Computational mathematics @ TUM, Campus Heilbronn

- Chair of COmputational MAthematics (COMA) @ TUM: Prof. **Hartwig Anzt**
  - Professor @ TUM since 01/2024
  - Director of the Innovative Computing Lab @ University of Tennessee (2022-23)
  - Junior Professor @ KIT (2021-22)
- Recent and ongoing PhD theses directed by Hartwig:
  - Symbolic LU factorizations on GPUs (**Tobias Ribizel**, ongoing)
  - Scalable domain decomposition on GPUs (**Fritz Göbel**, ongoing)
  - Numerical compression in scientific computing (**Thomas Grützmacher**, ongoing)
  - Mixed precision algebraic multigrids on GPUs (**Yu-Hsiang Mike Tsai**, 2024)
  - Asynchronous and batched iterative solvers on GPUs (**Pratik Nayak**, 2023)
- Ongoing projects in COMA:
  - **Ginkgo**: Portable high-performance numerical linear algebra library
  - **Sparse BLAS**: Basic linear algebra subprograms for sparse matrices
  - **ICON**: Large legacy codebase for climate modeling
  - **OGL/OpenFOAM**: Large legacy codebase for computational fluid dynamics
  - **MicroCARD**: Numerical modeling of cardiac electrophysiology
  - **PDExa**: Optimized software methods and technologies for PDEs
  - **nekRS**: Fast and scaleable computational fluid dynamics software package

Computational mathematics @ TUM, Campus Heilbronn, cont'd$_1$

- Course Instructor:

Nicolas Venkovic, Postdoc. in COMA @ TUM

- Postdoctoral Researcher @ TUM since 07/2024
- PhD in Applied Mathematics & Scientific Computing @ Cerfacs (09/2023)
- MSE in Applied Mathematics & Statistics @ Johns Hopkins University (2018)

- Recent and ongoing research efforts (see venkovic.github.io/research):
  - **Fast Convolution Kernels** (**Fourier**, **Walsh-Hadamard**, ...)
  - **Locally Optimal Iterative Methods for**:
    - **Strucutred Matrix Inverses**, **Eigenpairs**, **Low-Rank** and **Non-Negative Factorizations**
  - **Applications**:
    - **Stochastic Preconditioning**, **Matrix Recovery**, **Parallelization**, ...

Computational mathematics @ TUM, Campus Heilbronn, cont'd$_2$

- Teaching Assistant:

Amir Bouslama, Master student @ TUM
- Master student in Information Engineering @ TUM since Winter 2025/26
- BSc in Information Engineering @ TUM (Summer 2025)

- Responsibilities:
  - **Exercise** (Problem Sets) Sessions + **Practice** (Julia) Sessions

    1 Session per 3 Meetings
  - **Grading**
- Research interests:
  - **Numerical Methods** and **Simulation Software**

Class overview

Objectives

Upon completion of the class, students should:

- Understand why numerical linear algebra (NLA) is essential in practice, and what it encompasses.
- Be familiar with the challenges of the main problems and procedures of NLA, such as orthogonalization, least-squares solving, factorization, linear solving, preconditioning, eigenvalue solving, ...
- Understand the definitions, implementations and main properties of the methods presented in class for solving these problems.
- Recognize some pathological behaviors of these methods and be able to explain unwanted numerical behaviors.
- Know the strengths and limits of the presented methods, and know when to use them in practice.
- Have the foundational background to explore methods for solving NLA problems beyond those covered in class.

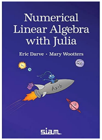
Content

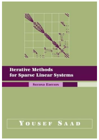
- We will cover the following core topics:
  - `Lecture 01`: Essentials of linear algebra
  - `Lecture 02`: Essentials of the Julia language
  - `Lecture 03`: Floating-point arithmetic and error analysis
  - `Lecture 04`: Direct methods for dense linear systems
  - `Lecture 05`: Sparse data structures and basic linear algebra subprograms
  - `Lecture 06`: Introduction to direct methods for sparse linear systems
  - `Lecture 07`: Orthogonalization and least-squares problems
  - `Lecture 08`: Basic iterative methods for linear systems
  - `Lecture 09`: Basic iterative methods for eigenvalue problems
  - `Lecture 10`: Locally optimal block preconditioned conjugate gradient
  - `Lecture 11`: Arnoldi and Lanczos procedures
  - `Lecture 12`: Jacobi-Davidson method
  - `Lecture 13`: Krylov subspace methods for linear systems
  - `Lecture 14`: Preconditioned iterative methods for linear systems
  - `Lecture 15`: Restarted Krylov subspace methods
  - `Lecture 16`: Elements of randomized numerical linear algebra
  - `Lecture 17`: Introduction to communication-avoiding algorithms

Content, cont'd

- If time permits, additional lectures may be picked among the following based on students' interests:
  - `Lecture E1`: Multigrid methods and domain decomposition
  - `Lecture E2`: Multilinear algebra and tensor decompositions
  - `Lecture E3`: Introduction to mixed precision algorithms
  - `Lecture E4`: Matrix function evaluation
- The duration of a lecture is not tied to a single class period. Some lectures will span less than one class, while others will cover multiple meetings. Several lectures can be covered within one meeting.
- Most lectures will begin by establishing formal foundations, and some will be followed by practice sessions using **Julia notebooks** and/or **problem sets** to test, visualize, and deepen your understanding of the methods and concepts introduced.

Reading material

- **Main references**:
  - **Lecture slides**, **Julia notebooks** and **problem sets** uploaded gradually on Moodle, throughout the semester.
    Content also uploaded at venkovic.github.io/NLA-for-CS-and-IE.
  - 

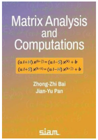
    Darve, E., & Wootters, M. (2021). Numerical Linear Algebra with Julia. Society for Industrial and Applied Mathematics (SIAM).†
  - GitHub repository:
    `https://github.com/EricDarve/numerical_linear_algebra`
- **Most used supplemental reference #1**:
  - 

    Saad, Y. (2003). Iterative Methods for Sparse Linear Systems. Society for Industrial and Applied Mathematics (SIAM).†

† SIAM members get 30% off book prices. SIAM membership is free for students.

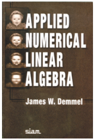
Reading material, cont'd$_1$

- **Most used supplemental reference #2**

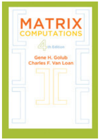
  - 

    Bai, Z. Z., & Pan, J.-Y. (2021). Matrix Analysis and Computations. Society for Industrial and Applied Mathematics (SIAM).†

- **Other useful supplemental references**:

  - 

    Demmel, J. W. (1997). Applied Numerical Linear Algebra. Society for Industrial and Applied Mathematics (SIAM).†

  - 

    Golub, G. H., & Van Loan, C. F. (2013). Matrix Computations. JHU press.

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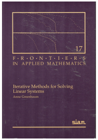
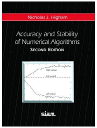
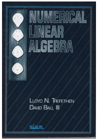
Reading material, cont'd$_2$

- 

  Greenbaum, A. (1997). Iterative Methods for Solving Linear Systems. Society for Industrial and Applied Mathematics (SIAM).†

- 

  Higham, N. J. (2002). Accuracy and Stability of Numerical Algorithms. Society for Industrial and Applied Mathematics (SIAM).†

- 

  Trefethen, L. N., & Bau, D. (2022). Numerical Linear Algebra. Society for Industrial and Applied Mathematics (SIAM).†

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Course evaluation

- **Final exam (determines base grade)**:

> **14:00 - 15:30**
> **Monday, 16 February 2025**
> **Campus Heilbronn**

  - Questions in relation to the homework problems, material presented in class, and practice sessions.
- **Homework policy**:
  - Submit your solution to one problem per lecture.
  - Deadline: 2 weeks after the end of the lecture.
  - Regular submissions upgrade the final grade by one step.
    - Example: 2.0 becomes 1.7.
    - Notes: This upgrade applies to passing grades only.
      1.0 remains the highest possible grade.

Course evaluation

- **Retake exam**:

14:00 - 15:30 **Wednesday, 1 April 2025** **Campus Heilbronn**

  - Questions in relation to the homework problems, material presented in class, and practice sessions.

- **Homework policy**:
  - Submit your solution to one problem per lecture.
  - Deadline: 2 weeks after the end of the lecture.
  - Regular submissions upgrade the final grade by one step.
    - Example: 2.0 becomes 1.7.
    - Notes: This upgrade applies to passing grades only.
1.0 remains the highest possible grade.

Homework assignment

Homework assignment

Send an email to me with the subject line `NLA-YourLastName` addressing the following points:

1. Briefly describe your background, if any, in numerical linear algebra, e.g.,
   - Courses taken, practical experience, self-study, ...
2. Identify a specific area of interest in numerical linear algebra:
   - A problem, method or concept you either work on, want to understand better, or are curious about.
3. Regarding the course syllabus:
   - List 2-3 topics you're most excited to learn about.
   - Mention any topics you feel you already have a strong grasp of, or simply would not mind skipping.
4. Suggest elective topics, listed in the slides or not, that you'd like to see covered, in case time permits.

Note: Your responses could help adapt certain aspects of the course to the class's needs and interests.