Numerical Methods of Linear Algebra for Sparse Matrices

Course for Bachelor Degree students in Southern Federal University

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Outline

- Overview of the course: description, aims and learning outcomes
- Prerequisites and study materials, workload and assessment
- Course map
- Course structure in detail:
  - Lectures
  - Practical assignments
  - Individual project

Description of the course

- **Course title:** Numerical Methods of Linear Algebra for Sparse Matrices
- **Specialty:** FI&IT
- **Language of instruction**: English
- **Status of the subject:** major subject, compulsory module
- **Period:** one semester (winter-spring)
- **Workload: 5 ECTS**
  - 180 hours total, including 34 hours of lectures and 34 hours of practice
  - Lectures: 2 hours per week
  - Practice: 2 hours per week

Aims of the course

- Learn effective solution methods for linear sparse systems of large and extralarge dimension
- Learn different storage schemes for sparse matrices and algorithms for basic sparse matrix operations
- Study direct and **iterative solution methods** for linear systems with sparse matrices
  - Direct solution methods
  - Projection methods
  - **Krylov subspace methods**
- Understand preconditioning techniques and use different types of preconditioners

Learning outcomes: knowledge

On successful completion of the course, students are expected to expected to have the following knowledge, skills and abilities:

- Knowledge of
  - main sparse storage formats for large sparse matrices;
  - direct solution methods for large sparse linear systems;
  - classic iterative and projection solution methods for linear systems;
  - Krylov subspace solution methods for large sparse linear systems;
  - Preconditioning methods

Learning outcomes: skills

On successful completion of the course, students are expected to expected to have the following knowledge, skills and abilities:

- Skills
  - applying sparse matrix technology to investigate modern numerical problems of large size;
  - use of numerical algorithms to solve large sparse linear systems;
  - writing programs in modern mathematical software packages to work with sparse matrices.

Learning outcomes: abilities

On successful completion of the course, students are expected to expected to have the following knowledge, skills and abilities:

- Abilities
  - use technology of sparse matrices for solving discretized problems of mathematical physics;
  - apply a suitable numerical solution method for a given sparse linear system and justify its suitability both theoretically and practically;
  - employ preconditioning techniques to precondition a given sparse linear system by selecting appropriate type of preconditioner;
  - implement direct and iterative algorithms for solving sparse linear systems in the form of program code;
  - use modern mathematical software (Matlab) for programming numerical solution methods for sparse linear systems.

Prerequisites for the course

- Calculus
- Linear Algebra
- Numerical Analysis
- Ordinary Differential Equations
- Partial Differential Equations
- Scientific Computing (knowledge of Matlab or Maple)

Study materials

Course textbook

Yousef Saad. Iterative Methods for Sparse Linear Systems, 2nd edition. SIAM, 2003. 528 p.

Download from https://www-users.cs.umn.edu/~saad/IterMethBook_2ndEd.pdf

Yousef Saad webpage:

https://www-users.cs.umn.edu/~saad/

Study materials

Additional reading

1. Gene H. Golub, Charles F. Van Loan. Matrix Computations. The Johns Hopkins University Press; 3rd edition, 1996. 728 p.
2. James W. Demmel. Applied Numerical Linear Algebra. SIAM, 1997. 184 p.
3. Ole Osterby, Zahari Zlatev. Direct Methods for Sparse Matrices. Springer-Verlag, 1983.
4. Sergio Pissanetzky. Sparse Matrix Technology. Academic Press, 1984. 312 p.

Course structure: lectures

- Lecture 1. **Basic concepts of linear algebra and matrix theory.** Types and structures of square matrices.
- Lecture 2. Vector and matrix norms. Range and kernel. Existence of Solution. Orthonormal vectors. Gram-Schmidt process.
- Lecture 3. Eigenvalues and their multiplicities. **Matrix factorizations and canonical forms**: QR, diagonal form, Jordan form, Schur form.
- Lecture 4. Matrix factorizations: SVD, LU, Cholessky. Properties of normal, Hermittian matrices and positive definite matrices
- Lecture 5. Existence of solution. Perturbation analysis and condition number. Errors and costs.
- Lectures 6. **Discretization of partial differential equations.** Finite difference method. Examples of 1D and 2D Poisson's equation. Overview of Finite element method. Assembly process in FEM.

Course structure: lectures (continues)

- Lecture 7. Structures and graph representations of sparse matrices. Storage formats for sparse matrices.
- Lecture 8. **Direct and iterative methods: comparison.** Direct solution methods (Gaussian elimination with partial pivoting). Direct sparse methods.
- Lecture 9**. Iterative methods**: general idea and convergence criterion. **Classic iterative methods**: Jacobi, Gauss-Seidel, Successive Over Relaxation (SOR), Symmetric Successive Over Relaxation (SSOR). Convergence criteria for classic iterative methods.
- Lecture 10. **Projection methods**: derivation and general formulation of a projection method.

Course structure: lectures (continues)

- Lecture 11. **One-dimensional projection methods**: Steepest Descent method, Minimal Residual Iteration method, Residual Norm Steepest Descent method.
- Lecture 12. **Krylov subspace methods.** Definition of Krylov suspace. General formulation of a Krylov subspace method. **Process of Arnoldi orthogonalization** to form a basis for Krylov subspace. Arnoldi relation and its properties.
- Lecture 13. **Methods based on Arnoldi process:** Full Orthogonalization method (FOM). Derivation of FOM, restarted FOM.
- Lecture 14. Methods based on Arnoldi process: Generalized Minimal Residual method (GMRES). Givens rotations in GRMRES. Calculation of residual in FOM and GMRES. Residual polynomials. Comparison on FOM and GRMRES.

Course structure : lectures (continues)

- Lecture 15. **Lanczos orthogonalization** for symmetric systems. **Methods based on Lacnzos orthogonalization.** Lanczos methods for symmetric systems: classic and direct. Derivation of Direct Lanczos method. Derivation of Conjugate Gradient method (CG). Generalization for nonsymmetric systems: Conjugate Residual (CR), Generalized Conjugate Residual (GCR).
- Lecture 16. **Lanczos biorthogonalization** for nonsymmetric systems. **Methods based on Lacnzos biorthogonalization**. Classic Lanczos method for nonsymmetric systems. Derivation of Biconjugate Gradient method (BiCG). Overview and comparison of efficient and optimal methods.
- Lecture 17. **Basic ideas of preconditioning technique**. Examples of preconditioners: Jacobi, Gauss-Seidel, SOR, SSOR, and incomplete LU preconditioners. **Preconditioned Krylov Subspace methods:** Preconditioned CG, Split Preconditioned CG, Preconditioned GRMES with left and right preconditioning.

Course structure: practice

Module 1. Background in sparse linear systems	
PA 1	Getting started with Matlab
PA 2	Matrix norms. Matrix factorizations
PA 3	Solving linear systems in Matlab, computation time, conditioning of the problem.
PA 4	Discretization of PDEs. Permutations and reordering. Sparse formats.
Module 2. Direct, iterative and projection methods for sparse linear systems	
PA 5	Comparison of direct and iterative methods for different sparse systems
PA 6	Classic iterative methods and 1D projection methods • simple iteration, Jacobi, GaussSeidel, SOR, SSOR • SDM, MRIM, RNSD
Module 3. Krylov subspace methods for sparse linear systems and preconditioning techniques	
PA 7	Arnoldi process, FOM, restarted FOM
PA 8	GMRES. Convergence of GMRES and eigenvalue distribution
PA 9	Understanding preconditioning. Effects of preconditioning when solving the system with symmetric and nonsymmetric matrices