Numerical Methods of Linear Algebra for Sparse Matrices

Course for Master 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:** MSc. in Applied Mathematics and Informatics
- **Master Degree programme:** Mathematical Modeling and Information Technologies
- **Language of instruction**: English
- **Status of the subject:** major subject, compulsory module
- **Period:** one semester (autumn-winter)
- **Workload: 5 ECTS**
  - 180 hours total, including 34 hours of lectures, 52 hours of practice, 58 hours of independent study, and 36 hours to prepare for exam
  - Lectures: 2 hours per week
  - Practice: 3 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.

Workload and assessment

Workload

- Lectures: 34 hours
- Practice (work on practical assignments): 52 hours
- Independent study (work on individual project): 58 hours

Assessment

- Total score: 100 points
  - Practical assignments: **60 points**
  - Individual project or Final written exam : **40 points**

Grading: 2-5 (60-100 points) are pass grades

Grade scale in Southern Federal University

Score	SFedU grades	ECTS grades
85-100	5 (excellent)	A (excellent): 95-100 B (very good): 85-94
71-84	4 (good)	C (good)
60-70	3 (satisfactory)	D (satisfactory): 65-70 E (sufficient): 60-64
<60	2 (fail)	FX (some further work required): 31-59 F (re-study of the discipline required): <31

Lectures

- Lecture 1**. Basic concepts of linear algebra and matrix theory.** Types and structures of square matrices. Vector and matrix norms.
- Lecture 2. Range and kernel. Existence of Solution. Orthonormal vectors. Gram-Schmidt process. Thin and full QR-factorization.
- Lecture 3. Eigenvalues and their multiplicities. Canonical forms by similarity transformation: diagonal form, Jordan form, Schur form. Other matrix factorizations: SVD, LU, Cholessky. Positive definite matrices.
- Lecture 4. Properties of normal and Hermittian matrices. Powers of matrices. Perturbation analysis and condition number. Errors and costs.
- Lecture 5. Structures and graphs representations of sparse matrices.
- Lectures 6. Storage schemes for sparse matrices. Algorithms for matrix by vector multiplication.

Lectures (continues)

- Lecture 7. **Direct and iterative methods: comparison**. Overview of direct solution methods. Direct sparse methods (Gaussian elimination with partial pivoting).
- Lecture 8. 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.
- 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. One-dimensional projection methods: Steepest Descent method, Minimal Residual Iteration method, Residual Norm Steepest Descent method.

Lectures (continues)

- Lecture 11. **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. **Methods based on Arnoldi process:** Full Orthogonalization method (FOM). Derivation of FOM, restarted FOM.
- Lecture 12. **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.
- Lecture 13. **Lanczos orthogonalization** for symmetric systems. **Methods based on Lacnzos orthogonalization**: Direct Lanczos, Conjugate Gradient method (CG). Generalization for nonsymmetric systems: Conjugate Residual (CR), Generalized Conjugate Residual (GCR). **Lanczos biorthogonalization** for nonsymmetric systems. **Methods based on Lacnzos biorthogonalization:** Classic Lanczos, Biconjugate Gradient method (BiCG). Overview and comparison of efficient and optimal methods. **Basic ideas of preconditioning technique**. Examples of preconditioners: Jacobi, Gauss-Seidel, SOR, SSOR, and incomplete LU preconditioners.

Individual project (40 points)

- **Description of individual project**
  - Perform a discretization of a given boundary-value problem and obtain a linear system with varied size
  - Study the properties of the matrix in the resulting system, write the code for the given sparse format
  - Solve the system using given classic iterative methods, 1D projection methods, Krylov subspace methods
  - Solve the system applying preconditioning
  - Compare the results for different system size and make conclusions
- Individual project is a part of final control together with oral exam. It can be done in a group of maximum two students. Students are expected to prepare a report containing the results of all project assignments.
- Formal presentation and defense of an individual project can be regarded as taking exam. In this case it will include oral discussion with each student about theoretical aspects of the used methods and approaches.

Practical assignments (60 points)

No	Brief description of practical assignment	Max points
Module 1. Background in matrix theory and sparse linear systems		
PA 1	Getting started with Matlab	2
PA 2	Matrix fundamentals: types and structures	3
PA 3	Vector and matrix norms. Existence of solution, solving linear system in Matlab.	4
PA 4	Gram-Schmidt and QR-factorization	4
PA 5	Eigenvalues and their multiplicities, matrix factorizations, Hermitian and positive definite matrices	4
PA 6	Schur, LU- and Cholessky factorizations of Hermitian positive definite matrices. Solving linear systems using LU- and Cholessky factorizations.	5
PA 7	Condition number, computational costs, well- and ill-conditioned problems	3
PA 8	Permutations, reordering and fill-ins	5
PA 9	Sparse storage and sparse formats	5
Module 2. Krylov subspace methods for sparse linear systems and preconditioning techniques		
PA 10	Comparison of direct and iterative methods for different sparse systems	5
PA 11	Classic iterative methods	4
PA 12	Arnoldi process and FOM	8
PA 13	Givens rotations and GMRES	8