

KRYLOV SUBSPACE METHODS: THEORY AND APPLICATIONS

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Keywords: Krylov subspace approximation, Krylov projection method, complex polynomial approximation, linear system of algebraic equations, matrix function

Abstract

Most tasks in scientific computing ultimately boil down to the solution of systems of linear equations. Discretizations of differential or integral equations usually result in systems of algebraic equations. When these equations are nonlinear they have to be linearized, e.g., by Newton's method, and finally we face the question: What is the solution of $A\mathbf{x} = \mathbf{b}$?

Many linear systems that arise in practical problems (especially those which result from finite element or finite difference discretizations of partial differential equations) can be so huge that limited storage space as well as limited computing time generally prohibit the application of direct solvers such as Gaussian elimination. Fortunately, large 'real-life' matrices are often sparse, i.e., they have only a few nonzero entries. For practical purposes this means that matrix-vector products with A can be computed cheaply. Iterative methods generate a sequence of approximate solutions, where the main computational effort for constructing the m -th approximant from the previous one consists in one or a few matrix-vector multiplications with A , and this is why large and sparse systems are usually solved iteratively.

Krylov subspace methods, the topic of these lectures, form the most important class of iterative solution method. In the past three decades research on Krylov subspace techniques has brought forth a variety of algorithms and methods so large that even specialists in matrix computations have difficulties keeping up.

It is our objective to develop the theory and algorithms on which all Krylov subspace methods are based in a unified way, to emphasize their connections to other fields of applied mathematics (such as polynomial approximation), but to treat also problems one encounters in practise, e.g., their behavior in finite precision arithmetic and how their convergence can be accelerated using preconditioners. In addition, we shortly describe how Krylov subspace methods help to solve other large linear algebra problems such as finding a few eigenpairs of a matrix, reducing the dimension of a linear model or evaluating a matrix function.

1. **Introduction.** Model problems. Sparse matrices and iterative methods. Krylov subspace methods and preconditioning. The method of successive approximation and other classical iterative methods.
2. **Projection methods on expanding subspaces.** Minimal residual (MR) and orthogonal residual (OR) subspace correction. Projections and angles. Projections onto nested subspaces. MR and OR approximations on nested subspaces. Relations between nested MR and OR approximations.
3. **Coordinate representation and algorithms.** Working with coordinates. The orthogonalization process. Angles and the QR-factorization. The Paige-Saunders basis. Using arbitrary bases. Quasi-minimal and quasi-orthogonal approximations. Multiple subspace correction.
4. **Krylov subspaces.** Why Krylov subspaces? Shift operator, orthogonal and kernel polynomials, Gaussian quadrature. Parameterization of the Arnoldi process. Short recurrences.
5. **Arnoldi-based Krylov subspace methods.** A minimal residual method (GMRES). The full orthogonalization method (FOM). Restarted and truncated variants. GMRES for Hermitian systems: MINRES.
6. **The conjugate gradient (CG) method.** Some remarks on the history of CG. Different views on CG. Gaussian quadrature and the CG method. CG convergence. CG and normal equations.
7. **Lanczos-based Krylov subspace methods.** The nonsymmetric Lanczos process and look-ahead strategies. Lanczos-based equation solvers. The quasi-minimal residual methods (QMR). The biconjugate gradient method (BiCG). BiCGStab and other product methods.
8. **Convergence.** Linear versus superlinear convergence. Bounds based on angles between subspaces. Convergence analysis for the normal case. Convergence results based on potential theory. Convergence analysis for the nonnormal case. Bounds based on the field of values. Bounds based on pseudospectra.
9. **Practical issues.** Krylov subspace methods in finite precision. Error estimates and stopping criteria. Choice of the initial approximation. Preconditioning.
10. **Krylov methods for singular problems.** The minimal polynomial and the Drazin inverse. Termination of Krylov subspace methods. Least-squares solutions in Krylov spaces. Krylov subspace methods for the Drazin inverse solution.
11. **Krylov methods for matrix functions.** The definition of matrix functions. Krylov subspace approximations for matrix functions. Algorithms. Convergence.