

# Krylov Subspace Methods for the Evaluation of Matrix Functions Applications and Algorithms

Michael Eiermann

Institut für Numerische Mathematik und Optimierung  
Technische Universität Bergakademie Freiberg, Germany

In recent years, interest in the numerical analysis of matrix functions grew rapidly—in particular, the approximation of  $f(A)\mathbf{b}$ , the action of a matrix function on a vector, has become an intensive area of research. We identify the following sources for this development: Novel solution strategies for differential equations which approximate the solution operator directly, such as exponential and trigonometric integrators, require the evaluation of  $f(A)\mathbf{b}$ , where  $f$  is some function (the most prominent example being the exponential function),  $A$  is the discrete version of some differential operator and  $\mathbf{b}$  is a vector, e.g., corresponding to some initial condition or source term. But matrix functions do not play only a role for solving differential equations. Their computation is an important ingredient of more complex numerical algorithms for solving semidefinite programming problems, analysing the transient behavior of time-continuous Markov chains or for solving nonlinear matrix equations (e.g., the algebraic Riccati equation). In addition, matrix functions and their approximation is a field which has connections not only to matrix analysis and numerical linear algebra but to many other mathematical subjects, such as functional analysis, complex variables, approximation and potential theory. Finally, matrix functions are needed in many application areas reaching from Statistics, Theoretical Physics, Chemistry, Plasma Physics, Geophysics to Computer Graphics and the modelling of financial derivatives in Economics.

In many of the applications mentioned above the matrix  $A$  is large and sparse or structured, typically resulting from discretization of an infinite-dimensional operator. In this case evaluating  $f(A)\mathbf{b}$  by first computing  $f(A)$  is usually unfeasible, so that most of the algorithms for the latter task cannot be used. The standard approach for approximating  $f(A)\mathbf{b}$  directly is based on a Krylov subspace of  $A$  with initial vector  $\mathbf{b}$ . The advantage of this approach is that it requires  $A$  only for computing matrix-vector products and that, for smooth functions such as the exponential, it converges superlinearly.

In these lectures, the state of the art of Krylov subspace methods is described both from a theoretical and an algorithmic point of view. Special emphasis is laid on the convergence analysis. More specifically, we cover the following topics:

1. Definitions of  $f(A)$
2. Applications
3. Theory of Matrix Functions
4. Computational Techniques for Special Functions
5. Krylov Subspace Methods
6. Restart Algorithms
7. Error Bounds and Convergence
8. Rational Krylov Techniques