THE NUMERICAL APPROXIMATION OF MATRIX FUNCTIONS

Michael Eiermann
Institut für Numerische Mathematik und Optimierung,
Technische Universität Bergakademie Freiberg, D-09596 Freiberg, Germany,
e-mail: eiermann@math.tu-freiberg.de

Keywords: matrix function, Krylov subspace approximation, Krylov projection method, complex polynomial approximation, potential theory

Abstract

The evaluation of $f(A)\boldsymbol{b}$, where $A \in \mathbb{C}^{n\times n}$, $\boldsymbol{b} \in \mathbb{C}^n$ and $f : \mathbb{C} \supset D \to \mathbb{C}$ is a function for which $f(A)$ is defined, is a common computational task. Besides the solution of linear systems of equations, which involves the reciprocal function $f(\zeta) = 1/\zeta$, by far the most important application is the time evolution of a system under a linear operator, in which case $f(\zeta) = f_t(\zeta) = e^{t\zeta}$ and time acts as a parameter t. Other applications arising in the context of solving differential equations require the evaluation of $f(A)\boldsymbol{b}$ for the square root and trigonometric functions. Further applications include identification problems for semigroups involving the logarithm and lattice quantum chromodynamics simulations requiring the evaluation of the matrix sign function.

In this overview talk, we first discuss the definition, some basic properties and the main applications of matrix functions (see, e.g., [3, Chapter 9]). We then review a few old and new numerical algorithms for computing $f(A)$ (cf. [1]). The main emphasis however is put on Krylov subspace approximations to $f(A)\boldsymbol{b}$ (cf. [4]) which have to be used in many of the applications mentioned above. The reason is that the matrices A arising there are so large that evaluating $f(A)\boldsymbol{b}$ by first computing $f(A)$ is generally unfeasible. We discuss implementation issues of these methods (involving restarts, preconditioning and stopping criteria, see [2]) as well as their convergence behavior whose analysis is based on results from complex polynomial approximation and potential theory.

References

[1] P. I. Davies and N. J. Higham. A Schur-Parlett algorithm for computing matrix functions, SIAM J. Matrix Anal. Appl., **25** (2003), 464-485.

[2] M. Eiermann and O. G. Ernst. A restarted Krylov subspace method for the evaluation of matrix functions, SIAM J. Numer. Anal., **44** (2006), 2481–2504.

[3] P. Lancaster and M. Tismenetsky. The Theory of Matrices With Applications, 2nd ed., Academic Press, San Diego (CA) 1985.

[4] Y. Saad, Analysis of some Krylov subspace approximations to the matrix exponential operator, SIAM J. Numer. Anal., 29 (1992), 209-228.