Computation of matrix functions with fully automatic Schur-Parlett and Rational Krylov methods

Federico Poloni [1] and Roberto Zanotto[2]

[1] *Department of Computer Science, University of Pisa.* fpoloni@di.unipi.it
[2] *Department of Computer Science, University of Pisa.* robyzan8@gmail.com

We present MatFun, a Julia package for computing dense and sparse matrix functions fully automatically (no user input required, other than the code to compute the function f and the matrix A themselves). This is achieved by combining specifically chosen algorithms and some peculiar feature of Julia. For dense matrices, the Schur-Parlett algorithm [1] has been implemented, leveraging Julia's automatic differentiation capabilities. The algorithm has also been improved from a performance standpoint, making the Parlett recurrence cache-oblivious and enabling the whole procedure to work mostly in real arithmetic, for real inputs. For sparse matrices, we implemented a Rational Krylov method [2], alongside the AAA Rational Approximation [3]. Given a function's samples, AAA is often able to accurately identify its poles, which can then be used by the Rational Krylov method itself for the approximation of $f(A)b$. The accuracy and performance of the algorithms are evaluated, in comparison with already existing specialized methods.

References

[1] Philip I. Davies and Nicholas J. Higham, *A Schur-Parlett Algorithm for Computing Matrix Functions*, SIAM Journal on Matrix Analysis and Applications, 25 (2003) 464-485.

[2] Stefan Güttel, *Rational Krylov approximation of matrix functions: Numerical methods and optimal pole selection*, GAMM-Mitteilungen, 36 (2013) 8-31.

[3] Nakatsukasa Yuji, Sète Olivier and Trefethen Lloyd N., *The AAA algorithm for rational approximation*, ArXiv e-prints, print 1612.00337 (2016).