Distributed Matrix Exponentiation in R

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Matrix exponentiation is an important matrix function which is useful in a wide variety of domains and applications. Formally, matrix exponentiation is an easily understood power series; but efficient, numerically stable algorithms for computing this function have been debated for over 30 years. There are several serial implementations of the matrix exponential available to *R*, including those found in the **Matrix** and **rexpokit** packages. We introduce a relatively new algorithm for computing the matrix exponential due to Al-Mohy and Higham, implemented in the **pbdDMAT** package. Our implementation includes both serial and distributed versions of this algorithm, the latter of which fully integrates with the pbdR framework for high performance computing with *R*. Finally, we will conclude by demonstrating the scalability of the implementation with benchmarks on University of Tennessee supercomputing resources.

References

[1] Al-Mohy, A. H. and N. J. Higham (2009). A New Scaling and Squaring Algorithm for the Matrix Exponential.

[2] Blackford, L. S., J. Choi, A. Cleary, E. D'Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet, K. Stanley, D. Walker, and R. C. Whaley (1997). *ScaLAPACK Users' Guide*. Philadelphia, PA: Society for Industrial and Applied Mathematics.

[3] Matzke, N. J., R. B. Sidje, and D. Schmidt. *rexpokit: R wrappers for EXPOKIT; other matrix functions*. R package.

[4] Moler, C. and C. Van Loan (2003). Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later. *SIAM Review 45*(1), 3–49.

[5] Ostrouchov, G., W.-C. Chen, D. Schmidt, and P. Patel. Programming with Big Data in R,.

[6] Schmidt, D., W.-C. Chen, G. Ostrouchov, and P. Patel (2012). pbdDMAT: Distributed Matrix Algebra Computation. R Package, URL http://cran.r-project.org/package=pbdDMAT.

[7] Sidje, R. B. (1998, March). Expokit: A Software Package for Computing Matrix Exponentials. *ACM Trans. Math. Softw. 24*(1), 130–156.