Scaling inverse factorization iterations

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Inverse factors of symmetric positive definite matrices are used in the solution of eigenvalue problems, linear systems of equations, and for congruence transformations in electronic structure calculations. This project is about efficient computation of an inverse factor when an approximate inverse is available or can be cheaply obtained.

1 A sign matrix formulation for the inverse factor

For complex scalar input z with nonzero real part, the sign function is defined as

$$\operatorname{sign}(z) = \begin{cases} 1, & \text{if } \operatorname{Re}(z) > 0, \\ -1, & \text{if } \operatorname{Re}(z) < 0, \end{cases} \tag{1}$$

and is extended to matrix input in the standard sense of primary matrix functions [1].

It was shown recently that if Q is a nonsingular matrix, then

$$\operatorname{sign}\left(\begin{bmatrix} 0 & Q^*S \\ Q & 0 \end{bmatrix}\right) = \begin{bmatrix} 0 & Z^*S \\ Z & 0 \end{bmatrix} \tag{2}$$

where Z is an inverse factor of S, i.e. $ZZ^* = S^{-1}$ [3].

This means that if an approximate inverse factor (Q) is available, iterative methods for the matrix sign function can be used to refine the inverse factor and make it more accurate. The approximate inverse factor can for example come from an update of molecular geometry in electronic structure theory (e.g. due to a molecular dynamics time step) or from a lower level in a hierarchical inverse factorization solver.

2 Tasks

- Study literature and survey general theory on matrix functions and their evaluation.
- Study literature and survey specialized results on iterative methods for the matrix sign function and inverse factorization.
- Implement existing inverse factorization solvers described in ref. [3].

- Develop new inverse factorization solvers based on existing methods for the matrix sign function, and the formulation in (2). In particular, we will investigate if the scaling techniques of ref. [2] can be used to speed up the calculation.

Prerequisites: Basic programming and scientific computing skills and an interest in numerical linear algebra.

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References

[1] Nicholas J. Higham. *Functions of Matrices : Theory and Computation.* SIAM, Philadelphia, 2008.

[2] Emanuel H. Rubensson. Nonmonotonic recursive polynomial expansions for linear scaling calculation of the density matrix. *J. Chem. Theory Comput.*, 7(5):1233–1236, 2011.

[3] Emanuel H Rubensson, Anton G Artemov, Anastasia Kruchinina, and Elias Rudberg. Localized inverse factorization. *IMA J. Numer. Anal.*, 41(1):729–763, 04 2021.