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Near instance optimality of the Lanczos method for Stieltjes and related matrix functions

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Polynomial Krylov subspace methods are among the most widely used methods for approximating $f(A)b$, the action of a matrix function on a vector, in particular when A is large and sparse. When A is Hermitian positive definite, the Lanczos method is the standard choice of Krylov method, and despite being very simplistic in nature, it often outperforms other, more sophisticated methods. In fact, one often observes that the error of the Lanczos method behaves almost exactly as the error of the best possible approximation from the Krylov space (which is in general not efficiently computable). However, theoretical guarantees for the deviation of the Lanczos error from the optimal error are mostly lacking so far (except for linear systems and a few other special cases). We prove a rigorous bound for this deviation when f belongs to the important class of Stieltjes functions (which, e.g., includes inverse fractional powers as special cases) and a related class (which contains, e.g., the square root and the shifted logarithm), thus providing a *near instance optimality* guarantee.

The proof of this result crucially relies on exploting low-rank update relations between the tridiagonal matrices generated by the Lanczos process.

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