CONQUERING ROUNDOFF EFFECTS IN THE CONJUGATE GRADIENT AND LANCZOS-TYPE METHODS

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Abstract

Algorithms based on the Lanczos process — these include the celebrated conjugate gradient method — are quite important in many areas of computational science and engineering, both for computing part of the spectrum of a large sparse matrix A and for solving linear systems with such a coefficient matrix. Their main feature is that a three-term (or two coupled two-term) recurrences for building up the Krylov subspace basis exists, which means small computational cost and small memory requirements. As for all Krylov space methods, only a procedure for the product Ay has to be provided; the individual matrix elements need not be available.

While the treatment of Hermitian (that is, selfadjoint) eigenvalue problems and Hermitian linear systems has been well established for quite some time, much development on non-Hermitian problems has taken place in the last twelve years. For linear systems a large number of algorithms have been proposed, including some that converge nearly as fast as ideal GMRES, but at much lower cost. However, roundoff errors may cause serious problems.

Therefore, some of the recent work — even for the Hermitian case — concentrates on making these methods more reliable. This requires, on the one hand, roundoff error analyses for these algorithms, and, on the other hand, well chosen numerical experiments. Both lead to quite remarkable findings and make us reevaluate some of the algorithms.

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