Backward stability of s-step GMRES

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Abstract

Communication, i.e., data movement, is a critical bottleneck for the performance of classical Krylov subspace method solvers on modern computer architectures. Variants of these methods which avoid communication have been introduced, which, while equivalent in exact arithmetic, can be unstable in finite precision. In this work, we address the backward stability of s-step GMRES, also known as communication-avoiding GMRES. We present a framework for simplifying the analysis of s-step GMRES, which includes standard GMRES ($s = 1$) as a special case, by isolating the effects of rounding errors in the QR factorization and the solution of the least squares problem. Using this framework, we analyze s-step GMRES with popular block orthogonalization methods: block modified Gram–Schmidt and reorthogonalized block classical Gram–Schmidt algorithms.

An example illustrates the resulting instability of s-step GMRES when paired with the classical s-step Arnoldi process and shows the limitations of popular strategies for resolving this instability. To address this issue, we propose a modified Arnoldi process that allows for much larger block size s while maintaining satisfactory accuracy, as confirmed by our numerical experiments.

PS: I am a postdoc researcher in Charles University. My interests are about numerical analysis and high performance computing, i.e., mixed precision algorithms, communication-avoiding algorithms, and finite precision analysis.