Numerical stability of Gram-Schmidt process

M. Rozložník, L. Giraud, J. Langou and J. van den Eshof

Institute of Computer Science Academy of Sciences of the Czech Republic, Prague

In this contribution we study the numerical properties of the classical Gram-Schmidt (CGS) orthogonalization process. Generally accepted view is that due to rounding errors the orthogonality of computed vectors can be lost very quickly or may be even lost totally. The textbooks usually contain examples with progressive deterioration in the orthogonality without any bound relating it to the condition number of initial vectors. We will show, however, that one can derive a bound for the loss of orthogonality in the CGS algorithm. This bound depends only quadratically on the condition number of the system. This result sounds very well with all examples used for demonstrating the unreliability of the CGS process, what will be also illustrated on examples.

From a practical point of view, the CGS algorithm is a better candidate for parallel implementation than the MGS variant of the same algorithm and this aspect could not be overlooked in certain computing environments. Moreover, a new trend is emerging nowadays, several experiments are reporting that even if performing twice as much operations as MGS, the CGS algorithm with one (complete) reorthogonalization may be faster. This indicates that such results to certain extent may lead to reinstating of the CGS algorithm as a suitable alternative for parallel implementation of the Gram-Schmidt orthogonalization process.

E.g., in the GMRES context, it seems that the Arnoldi vectors computed with the CGS process will loose their orthogonality completely only after the residual of the computed approximate solution has been reduced close to its final accuracy (which is, however, different and worse than for the MGS GMRES, but still rather acceptable). Similarly, using the bound for the loss of orthogonality one can analyze also the CGS algorithm used for solving the least squares problems (it is known to be not backward stable, but its accuracy may be quite satisfactory in some applications).

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References

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