A REORTHOGONALIZATION PROCEDURE FOR MGS APPLIED TO A LOW RANK DEFICIENT MATRIX

Julien Langou, Luc Giraud and Serge Gratton
CERFACS,
42, Avenue Gaspard Coriolis, 31057 Toulouse Cedex 01, France,
e-mail: langou@cerfacs.fr

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Abstract

We consider the Modified Gram-Schmidt orthogonalization applied to a matrix $\mathbf{A} \in \mathcal{R}^{m \times n}$. This corresponds to a QR factorization : $\mathbf{A} = \mathbf{QR}$. We study this algorithm in finite precision computation when the matrix $\mathbf{A}$ has a numerical rank deficiency k. This subject has already been dealt with success by Björck and Paige in 1992 [1]. They give useful bounds in term of norms. We extend their results to provide bounds on singular values. In order to make it more clear, we present our results in term of numerical rank. In particular, we show that if, $\text{Rank}(\mathbf{A}) = n - k$, then

$$\exists \mathbf{E} \text{ so that } \begin{cases} 0 \leq \text{ Rank}(\mathbf{E}) \leq k \\ \hat{\mathbf{Q}} = \mathbf{Q} - \mathbf{E}, \quad \hat{\mathbf{Q}}^T \hat{\mathbf{Q}} = \mathbf{I}, \quad \mathbf{A} = \hat{\mathbf{Q}}\mathbf{R}. \end{cases}$$

This result says that in finite precision computation, $\mathbf{Q}$ looses orthogonality in just a few directions that are given by $\mathbf{E}$, we can also control the magnitude in each of these directions by the associated singular values of $\mathbf{A}$.

Based on these results, we have developed some applications. The one that we present here is a reorthogonalization process of $\mathbf{Q}$. We have designed an algorithm that computes $\hat{\mathbf{Q}}$ from $\mathbf{Q}$ by exploiting the low rank k of the matrix $\mathbf{E}$. One advantage of this approach is that we can monitor the orthogonality of $\mathbf{Q}$ characterized by $\|\mathbf{I} - \mathbf{Q}^T\mathbf{Q}\|_2$.

We present experimental results in the context of Seed-GMRES. For each "seed", we used the internal reorthogonalization scheme MGS. The stability of this choice is justified by Greenbaum, Rozložník and Strakoš [2]. We then used our reorthogonalization process in order to build an orthogonal basis of the constructed Krylov subspace. This strategy enables us to use Classical Gram-Schmidt and to exploit parallelization in the code when dealing with the other right hand sides.

References

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