Numerics of the Gram-Schmidt process and its relation to the SR decomposition

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Abstract

In this contribution we first consider the most important schemes used for orthogonalization with respect to the standard and non-standard inner product and briefly review the main results on their behavior in finite recision arithmetic. We treat separately the particular case of the standard inner product and show that similar results hold also for the case when the inner product is induced by a positive diagonal matrix. We will show that in the general case of non-standard inner product the conditioning of computed factors depends not only on the conditioning of initial vectors but it depends also on the condition number of the matrix that induces the non-standard inner product.

We also study the orthogonalization schemes for computing vectors that are mutually orthogonal with respect to the bilinear form induced by a symmetric nonsingular but indefinite matrix. Under assumption on strong nonsingularity of this matrix we develop bounds for the extremal singular values of the triangular factor that comes from is symmetric indefinite factorization. It appears that they depend on the the extremal singular values of the matrix and of only those principal submatrices where there is a change of sign in the associated subminors. Using these results we analyze two types of schemes used for orthogonalization and we give the worst-case bounds for quantities computed in finite precision arithmetic. In particular, we consider Cholesky QR implementation based on the Cholesky-like factorization and the Gram-Schmidt process with respect to this bilinear form. We consider also their versions with reorthogonalization and with one step of iterative refinement.

Finally we discuss the extension of this theory to the case of skew-symmetric bilinear forms used in the context of various structure-preserving transformations. We analyze the freedom of choice in the symplectic and the triangular factors and review several existing suggestions on how to choose the free parameters in the SR decomposition.

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Keywords

Orthogonalization, Gram-Schmidt process, indefinite inner product, skew-symmetric bilinear form, SR decomposition.

References

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