NUMERICAL BEHAVIOR of INDEFINITE ORTHOGONALIZATION

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Abstract

For a real symmetric nonsingular matrix $B \in \mathcal{R}^{m,m}$ and for a full column rank matrix $A \in \mathcal{R}^{m,n}$ ($m \geq n$) we look for the decomposition $A = QR$, where the columns of $Q \in \mathcal{R}^{m,n}$ are mutually orthogonal with respect to the bilinear form induced by the matrix B so that $Q^T BQ = \Omega = \text{diag}(\pm 1)$ and where $R \in \mathcal{R}^{n,n}$ is upper triangular with positive diagonal elements. Such problems appear explicitly or implicitly in many applications such as eigenvalue problems, matrix pencils and structure-preserving algorithms, interior-point methods or indefinite least squares problems. It is clear that for $B = I$ or $B = -I$ we get the standard QR decomposition of the matrix A. If B is positive and diagonal then the problem is equivalent to the standard decomposition of the row-scaled matrix $\text{diag}^{1/2}(B)A$. For a general but still symmetric positive definite B, the factors can be obtained from the QR factorization in the form $B^{1/2}A = (B^{1/2}Q)R$. The indefinite case of $B \in \text{diag}(\pm 1)$ has been studied extensively by several authors. It appears that under assumption on nonzero principal minors of $A^T BA$ each nonsingular square A can be decomposed into a product $A = QR$ with $Q^T BQ \in \text{diag}(\pm 1)$ and R being upper triangular. These concepts can be extended also to the case of a full column rank A and a general indefinite (but nonsingular) matrix B.

Although all orthogonalization schemes are mathematically equivalent, their numerical behavior can be significantly different. The numerical behavior of orthogonalization techniques with the standard inner product $B = I$ has been studied extensively over last several decades including the Householder, Givens QR and modified Gram-Schmidt. The classical Gram-Schmidt (CGS) and its reorthogonalized version have been studied much later in [1, 4, 5]. It is also known that the weighted Gram-Schmidt with diagonal B is numerically similar to the standard process applied to the row-scaled matrix $\text{diag}^{1/2}(B)A$. Several orthogonalization schemes with a non-standard inner product have been studied including the analysis of the effect of conditioning of B on the factorization error and on the loss of B-orthogonality between the computed vectors [2].

In this contribution we consider the case of symmetric indefinite B and assume that $A^T BA$ is strongly nonsingular (i.e. that each principal submatrix $A_j^T BA_j$ is nonsingular for $j = 1, \ldots, n$, where A_j denotes the matrix with the first j columns of A). Then the Cholesky-like decomposition of indefinite $A^T BA$ exists and the triangular factor R can be recovered from $A^T BA = R^T \Omega R$. We first analyze the conditioning of factors Q and R. It is clear that if B is positive definite then $\|R\| = \|B^{1/2}A\|$, $\|R^{-1}\| = 1/\sigma_{min}(B^{1/2}A)$ and $\|Q\| \leq \|B^{-1}\|^{1/2}$, $\sigma_{min}(Q) \geq 1/\|B\|^{1/2}$. Therefore $\kappa(R) = \kappa(B^{1/2}A) = \kappa^{1/2}(A^T BA)$ and $\kappa(Q) \leq \kappa^{1/2}(B)$. However, for B indefinite we have only $\|A^T BA\| \leq \|\Omega\|\|R\|^2$ and $\|(A^T BA)^{-1}\| \leq \|\Omega^{-1}\|\|R^{-1}\|^2$ and so the square root of the condition number of $A^T BA$ is just a lower bound for the condition number of the factor R, i.e. $\kappa^{1/2}(A^T BA) \leq \kappa(R)$. The upper bound for $\kappa(R)$ seems more difficult to obtain. One must look at its principal submatrices R_j and derive bounds for the norm of their inverses $\|R_j^{-1}\|$ considering

$$(R_j^T R_j)^{-1} = \begin{pmatrix} (R_{j-1}^T R_{j-1})^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \omega_j \left[(A_j^T BA_j)^{-1} - \begin{pmatrix} (A_{j-1}^T BA_{j-1})^{-1} & 0 \\ 0 & 0 \end{pmatrix} \right].$$

This identity provides the basic insight into relation between the minimum singular value of the factor R and the minimum singular values of some principal submatrices of $A_j^T BA_j$. Observe that its recursive use leads to the expansion of the matrix $(R^T R)^{-1}$ in terms of $(A^T BA)^{-1}$ and in terms of only those inverses of principal submatrices $(A_j^T BA_j)^{-1}$ where there is a change of the sign in the factor $\Omega = diag(\omega_1, \ldots, \omega_n)$, i.e. for such $j = 1, \ldots, n-1$ where $\omega_{j+1} \neq \omega_j$. It follows then that $|\omega_{j+1} - \omega_j| = 2$ and therefore we have the bound

$$\|R^{-1}\|^2 \leq \|(A^T BA)^{-1}\| + 2 \sum_{j;\ \omega_{j+1} \neq \omega_j} \|(A_j^T BA_j)^{-1}\|. \tag{1}$$

The norm of the factor R can be either bounded as $\|R\| \leq \|A^T BA\| \|R^{-T}\|$ or one can consider similar identity for $R^T R$ and get the bound for $\|R\|$ in terms of the Schur complements corresponding only to those principal submatrices $A_j^T BA_j$ (subject to $A^T BA$) where $\omega_{j+1} \neq \omega_j$, i.e.

$$\|R\|^2 \leq \|A^T BA\| + 2 \sum_{j;\ \omega_{j+1} \neq \omega_j} \|(A^T BA) \backslash (A_j^T BA_j)\|. \tag{2}$$

The bounds (1) and (2) can be reformulated also for quasi-definite matrices $A^T BA$, where the factor Ω has a particular structure $\Omega = diag(I; -I)$ with appropriate dimensions. The only nonzero term in the sum over principal submatrices corresponds to the biggest positive definite principal submatrix of $A^T BA$. The singular values of the factor Q can be bounded from $Q = AR^{-1}$.

Here we analyze two types of important schemes used for orthogonalization with respect to the bilinear form induced by B. We give the worst-case bounds for quantities computed in finite precision arithmetic and formulate our results on the loss of orthogonality and on the factorization error (measured by $\|\bar{Q}^T B\bar{Q} - I\|$ and $\|A - \bar{Q}\bar{R}\|$) in terms of quantities proportional to the roundoff unit u, in terms of $\|A\|$ and $\|B\|$ and in terms of the extremal singular values of factors $\bar{Q}$ and $\bar{R}$. Based on previous discussion the latter depend on the extremal singular values of the matrix $A^T BA$ and principal submatrices $A_j^T BA_j$ with the change of the sign $\bar{\omega}_{j+1} \neq \bar{\omega}_j$ during the orthogonalization. First we analyze the QR implementation based on the Cholesky-like decomposition of indefinite $A^T BA$. We show that assuming $\mathcal{O}(u)\kappa(A^T BA)\|A\|^2\|B\| \max_{j,\ \bar{\omega}_{j+1} \neq \bar{\omega}_j} \|(A_j^T BA_j)^{-1}\| < 1$ such decomposition runs to completion and the computed factors $\bar{R}$ and $\bar{\Omega}$ satisfy $A^T BA + \Delta B = \bar{R}^T \bar{\Omega} \bar{R}$ with $\|\Delta B\| \leq \mathcal{O}(u)[\|\bar{R}\|^2 + \|B\|\|A\|^2]$. For the computed orthogonal factor $\bar{Q}$ it follows then that $\|\bar{Q}^T B\bar{Q} - \bar{\Omega}\| \leq \mathcal{O}(u)\kappa(\bar{R}) \left[\kappa(\bar{R}) + 2\|B\bar{Q}\|\|\bar{Q}\|\right]$. The accuracy of these factors can be improved by one step of iterative refinement when we apply the same decomposition to the actual $\bar{Q}^T A\bar{Q}$ and get the bound $\|\bar{Q}^T B\bar{Q} - \bar{\Omega}\| \leq \mathcal{O}(u)\|B\|\|\bar{Q}\|^2$. We consider also the B-CGS algorithm and its version with reorthogonalization and show that their behavior is similar to Cholesky-like QR decomposition and its variant with refinement, respectively. The details can be found in [3].

References

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