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Rounding error analysis of the classical Gram-Schmidt process and its applications

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In many applications it is important to compute an orthogonal basis $Q = (q_1, \dots, q_n)$ of $\text{span}(A)$, where $A = (a_1, \dots, a_n)$ be a real $m \times n$ matrix ($m \geq n$) with full column rank ($\text{rank}(A) = n$). In this contribution we focus on the Gram-Schmidt (GS) orthogonalization process which also produces a QR factorization of A . Two basic computational variants of the Gram-Schmidt process exist: the classical Gram-Schmidt (CGS) algorithm and the modified Gram-Schmidt (MGS) algorithm (see e.g. [2, 12]). From a numerical point of view, both these techniques may produce a set of vectors which is far from orthogonal and sometimes the orthogonality can be lost completely [1, 11]. Generally accepted view is that the CGS algorithm is unreliable while the MGS algorithm has much better numerical properties [11, 13]. Björck [1] has shown that for a numerically nonsingular matrix A the loss of orthogonality in MGS occurs in a predictable way and it can be bounded by a term proportional to the condition number $\kappa(A)$ and to the roundoff unit u . Therefore, the loss of orthogonality of computed vectors is close to roundoff unit level only for well-conditioned matrices, while for ill-conditioned matrices it can be much larger leading to complete loss (the loss of linear independence) for numerically singular or rank-deficient problems. The results on MGS were reinforced and extended by Paige and Björck [3] who showed that despite the loss of orthogonality in Q the computed upper triangular factor R in MGS is numerically as good as the computed R from the Householder or Givens QR factorization [2, 8]. These results indicate that the loss of orthogonality in Q does not necessarily imply the superiority of orthogonalization techniques which deliver almost orthogonal set of vectors (like Householder or Givens QR orthogonalization) over the MGS scheme when applied to some problems. Indeed there exist applications, where the orthogonality of computed vectors does not play a crucial role. E.g., it was shown by Björck (see e.g. [2, 8]) that the MGS method can be used to solve least squares problems and that the algorithm is backward-stable. Another example of this type is the GMRES method used together with the MGS Arnoldi implementation. Surprisingly, it was shown in [7] that the linear independence of the computed (Arnoldi) basis vectors, not their orthogonality, is important for the convergence of GMRES and that the MGS GMRES performs as well as GMRES with the Householder implementation of the Arnoldi process [7].

Although the rumor is that for some problems the classical Gram-Schmidt algorithm may dramatically fail in producing orthogonal vectors, the relation between CGS and MGS is more

delicate and it deserves more attention. Many textbooks (see e.g. [2, 8, 12]) give examples, where the orthogonality of vectors computed in CGS is lost completely after a few or even two orthogonalization steps, but the connection to the (ill-)conditioning of the problem has not been analyzed. The bad reputation of the algorithm also comes from the fact that, with the exception of $n = 2$ for which are CGS and MGS identical, up to now there was no bound available for the loss of orthogonality of computed vectors in the CGS process. As far as we could check, there was only one attempt to give a bound for the CGS algorithm by Kielbasinski and Schwetlick (published unfortunately without proof only in the Polish version of the 2nd edition of their book [9]). This has led to rather general statements on its poor numerical properties. The mechanism of the loss of orthogonality, however, was not fully understood and detailed analysis of its behavior has been missing so far.

It appears, however, that there exists a bound for the loss of orthogonality of the vectors computed by the CGS algorithm, which was given recently in [6]. Indeed, provided that the matrix $A^T A$ is numerically nonsingular, the loss of orthogonality of the vectors \bar{Q} (measured by the norm of the matrix $I - \bar{Q}^T \bar{Q}$) can be bounded by a term proportional to the square of the condition number $\kappa^2(A)$ times the unit roundoff u . The bound is based on the fact that the computed upper triangular factor \bar{R} is the exact Cholesky factor of a matrix relatively close to the matrix $A^T A$, i.e. there exists a perturbation matrix E of relative small norm such that $A^T A + E = \bar{R}^T \bar{R}$. These results fill the gap in understanding the behaviour of the CGS algorithm, confirm the connection to the Cholesky QR algorithm [2] and clarify also the difference between MGS and CGS. While in the MGS process the computed vectors may lose their orthogonality completely (i.e., they become linearly dependent) only for rank-deficient (numerically singular) problems with $\kappa(A) \geq 1/u$, the CGS algorithm may fail in a same manner already when the condition number $\kappa(A)$ exceeds the level $1/\sqrt{u}$. This is probably the main reason, why CGS was considered unreliable. It is not true, however, that the vectors computed in CGS on a well-conditioned matrix may depart from orthogonality to an almost arbitrary extent. Indeed, provided that the associated system of normal equations is numerically nonsingular, the loss of orthogonality for CGS is proportional to $\kappa^2(A)$ and it can be preserved on certain level, although higher than that for MGS.

In addition, as we have already mentioned, it may be misleading to put too much emphasis on the orthogonality of computed vectors in some applications. E.g., in the GMRES context, it seems that the Arnoldi vectors computed with the CGS process will lose 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).

From a practical point of view, the CGS algorithm is a better candidate for parallel implementation than the MGS 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 because it takes advantage of BLAS2 (e.g. in the GMRES context [5], in the GCR context [4] or in the eigenvalue computation [10]). 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.

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