Computing dense matrix factorizations to high relative accuracy

Zlatko Drmač[1]

Department of Mathematics, University of Zagreb, Croatia
drmac@math.hr,
WWW home page: http://www.math.hr/~drmac

Abstract. We outline the principles behind the design of the new Jacobi–type algorithm for accurate computation of the SVD, and its applications as kernel procedure in computation of various generalizations of the SVD (PSVD, QSVD, (H,K)-SVD, canonical correlations) as well as for diagonalization of positive definite matrices and matrix pencils. New LAPACK style software, and future plans are presented.

1 Introduction

Our contribution presents the current state of affairs in the development of LAPACK style software for computation of the SVD and its generalizations to high relative accuracy. From the numerical point of view, our codes have important property: the backward error is structured, which means that the forward error is governed by better condition number. All singular values and eigenvalues are computed to the level of relative accuracy warranted by the data.

We discuss the main principles and ideas of recent development, as well as future development toward reliable and efficient numerical software.

2 Dense SVD

The new Jacobi–type (serial) SVD algorithm [4], [5] outperforms the best previous implementations of the Jacobi SVD algorithm with factor as big as ten! In case of computing the full SVD it outperforms the QR algorithm (SGESVD from LAPACK) and, depending on the distribution of the spectrum, it comes close the currently fastest *divide and conquer* SGESDD code from LAPACK.

It is important to note that this efficiency is not traded for numerical accuracy: If the input matrix A can be factored as $A = BD$ (or $A = D_1CD_2$) with diagonal D (D_1, D_2) and well–conditioned B (C), then our algorithm (its variant following [1]) computes the SVD of A to high relative accuracy, independent of the scaling diagonal matrices. This high level of accuracy cannot be guaranteed by the methods which first bidiagonalize A.

This means that the new algorithm is currently the fastest known SVD algorithm capable of reaching numerical stability guaranteed by the state of the

art perturbation theory. If applied to the Cholesky factor of symmetric positive definite H, then it delivers the eigenvalues and eigenvectors of $H + \delta H$ with $\max_{i,j} |\delta H_{ij}|/\sqrt{H_{ii}H_{jj}} \leq O(n)\epsilon$. (For tridiagonalization-based methods, the backward error can be bounded only in norm, $\|\delta H\|/\|H\| \leq O(n)\epsilon$.)

The results of numerical testing of our new software give us reasons to believe that the barrier between accuracy and speed is not unbreakable. We know that our algorithm has even more potential for speedup, while retaining high relative accuracy properties. For instance, in our current LAPACK style code, the most expensive part are Jacobi iterations for SVD computation of a preconditioned lower triangular matrix. We expect to have much more efficient code, using the fast scaled block Jacobi rotations and ideas of Hari [6].

Further, the initial preprocessing/preconditioning is a rank revealing decomposition based on pivoted QR factorization(s). This stage is open for improvements, and will benefit from any advance in QR factorization software. We explore some new objective functions for pivot strategies in the QRF.

Moreover, the new algorithm can run in the "classical mode" of accuracy and in the cases of matrices with low numerical rank, for which only the dominant singular triplets are of interest (which is very often the case in applications of the SVD), it can even outperform the SGESDD procedure from LAPACK.

3 Generalized decompositions

This efficiency of the kernel procedure is basis for accurate and efficient computation of the generalized SVD decompositions (PSVD, QSVD, (H,K)-SVD, canonical correlations). Let us illustrate the power of this approach:

We already know that e.g. SVD of the product AB can be computed with high relative accuracy via reduction to the SVD of a single matrix, see [2], [3]. This reduction, combined with the new Jacobi SVD procedure, results in numerically reliable, efficient, and simple software. A modification of the algorithm computes the eigenvalues of $HM - \lambda I$ (H, M positive definite) with entry–wise small backward errors $|\delta H_{ij}| \leq \epsilon\sqrt{H_{ii}H_{jj}}$, $|\delta M_{ij}| \leq \epsilon\sqrt{M_{ii}M_{jj}}$, $1 \leq i, j \leq n$.

Finally, we will present the results of rigorous numerical testing of the new LAPACK–style software for the above mentioned decompositions.

References

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