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Accuracy of the Kogbetliantz method for scaled diagonally dominant triangular matrices ☆

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ABSTRACT

The paper proves that Kogbetliantz method computes all singular values of a scaled diagonally dominant triangular matrix, which can be well scaled from both sides symmetrically, to high relative accuracy. Special attention is paid to deriving sharp accuracy bounds for one step, one batch and one sweep of the method. By a simple numerical test it is shown that the methods based on bidiagonalization are generally not accurate on that class of well-behaved matrices.

1. Introduction

In this paper we prove a relative accuracy result for the Kogbetliantz method. The result is proved for scaled diagonally dominant (s.d.d.) triangular matrices which can be well scaled from both sides symmetrically. In [1] it has been proved that such triangular matrices are well-behaved for computing the singular values. But until now, no relative accuracy proof of any method for that class has been proposed. A matrix can be well scaled if after the appropriate scaling it has small condition number. If that condition number enters into the perturbation bounds for the singular values (vectors), then the matrix belongs to the class of well-behaved matrices for computing the singular values (vectors). Well-behaved matrices allow for accurate computation of the target data (see [2,3]).

It is known that QR, Divide and Conquer and other methods based on bidiagonalization are generally not relatively accurate for computing the SVD of well-behaved matrices. One-sided Jacobi method and the Kogbetliantz method have better relative accuracy properties. One-sided Jacobi method is relatively accurate provided that the matrix can be well scaled from the right or left side (see [2]). In [4,5] it has been shown that one-sided Jacobi method can be improved by making first one or two QR factorizations of the initial rectangular matrix. After that pre-processing, the obtained triangular matrix becomes even more well-behaved and the method becomes very fast (faster than the QR method), reliable and remains relatively accurate.

The Kogbetliantz method is a known two-sided Jacobi method for computing the SVD of a square matrix. Its algorithm [6–14], the global [8,9,15,11,16] and the asymptotic [10,13,17–21] convergence are well understood. Its implementation details and adaptation for different computer architectures can be found in [12,22–24] and the references cited therein.

In [11,19] it has been shown that on triangular matrices the algorithm simplifies and the method becomes quadratically convergent under the serial strategies. In [14] the core algorithm of the method has been slightly modified to become more accurate. So far, no proof of relative accuracy for that method has been proposed.

The Kogbetliantz method is an important tool in numerical linear algebra since it is the method of choice for the solution of the subspace tracking problem [25–27]. It is an important part of some parallel implementations of the block-Jacobi SVD

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algorithms as is presented in [23,28] and in the references cited therein. Hence its significance might increase by future development of both CPU and GPU implementations of block Jacobi methods. This could yield an improvement for dense SVD diagonalization algorithms.

The Kogbetliantz method is less known because it is generally considered less efficient and less understood than the competitor methods. So, let us make a brief comparison with one-sided Jacobi method. The both methods become more efficient after the same pre-processing of the initial matrix by one or two QR factorizations. Let G denote the so obtained triangular matrix of order n, the starting matrix for the both methods.

One-sided Jacobi method has the following favorable properties: it is very accurate and fairly simple, very fast (provided all tricks from [29,30,4,5] are used), very amenable to parallel processing (even for distributed memory computing) and requires less memory than QR, DC and DQD methods. It can be used with any pivot strategy, it can be generalized to work with block-columns and it can fully exploit vectorization. Its shortcomings are the following. It destroys the initial almost diagonality and triangularity of G. In the final stage of the process, huge cancelations occur in computing the rotation parameters. Dot products of large almost orthogonal vectors have to be computed. This results in uncertainty linked with stopping of the process. And each checking of stoping criterion is very expensive (costs around $n^3/2$ flops).

The nice properties of the Kogbetliantz method include the following. It further diagonalizes the starting almost diagonal triangular matrix G. It even preserves the triangular form in certain way (see [11]). It has very cheap and sound stopping criterion. The method can be parallelized using special pivot strategies and block versions (BLAS 3 algorithms) of the method can be designed (see [24]). Almost all tricks from [29,30,4,5] can be used to accelerate and improve it. The global and the asymptotic convergence have been proved. In numerical tests, it is observed to be relatively accurate. As we prove it here, this is indeed so for a certain class of s.d.d. matrices. But the method also has some imperfections. It is two-sided, and when coding in FORTRAN, row operations are several times slower than the corresponding column operations. In contrast to one-sided Jacobi method, the nice properties of Kogbetliantz method depend on some very special pivot strategies. So, Kogbetliantz has much less freedom in choosing the pivot strategy. A bit more working memory ($n^2/2$ more cells) is required than for the one-sided method.

Here we prove the first accuracy result for the Kogbetliantz method. The proof is based on the perturbation result [1, Theorem 4.1] whose essential part reads as follows (see Theorem 1):

Let σ_i and σ_i', $1 \leqslant i \leqslant n$ be the singular values of the square matrices G and $G + \delta G$ respectively, and let $\|D^{-1}\delta G D^{-1}\|_F \leqslant \eta$, $\|D^{-1}GD^{-1} - \mathrm{diag}(D^{-1}GD^{-1})\|_F \leqslant \alpha$ where $D = |\mathrm{diag}(G)|^{1/2}$. If $\eta + \sqrt{2}\alpha < 1$, then $|\sigma_i'/\sigma_i - 1| \leqslant \eta/(1 - \alpha\sqrt{2})$.

In the paper, we first derive the perturbation δG which comes from applying the Kogbetliantz method in finite arithmetic. To this end we use a detailed error analysis which has already been used in [14,31]. After that we seek for η, an upper bound for the norm of the scaled perturbation $D^{-1}\delta\, GD^{-1}$, which is the measure for the relative perturbation of the singular values. We separately derive δG and estimate η for a single step of the method (Theorem 2) and for several steps which make one batch (Theorem 3). The result for the whole cycle of the method (Corollary 4) is obtained from the result for one batch. All these results are summarized in the main accuracy result, Theorem 6.

The new result poses some questions: is one-sided Jacobi method accurate on that class of well-behaved s.d.d. matrices? Can [1, Theorem 4.1] be used to obtain an additional accuracy result for one-sided Jacobi method? A short remark concerning the first question is given at the end of the paper.

The paper is organized as follows. In Section 2, we give a detailed description of the Kogbetliantz method. We consider two core algorithms for diagonalizing 2×2 triangular matrices, which then define two algorithms: KOGB and KLASV2 for $n \times n$ triangular matrices. In Section 3, we derive sharp estimates for the symmetrically scaled backward errors arising from one step, one batch and one sweep of the method. These estimates are partly based on the results from [14,31]. The only assumption that we use is that the scaled pivot elements are not larger than one. Finally, in Section 4, we combine those results with recently published relative error estimates for the singular values of symmetrically scaled s.d.d. matrices [1]. We also provide some results of numerical tests. They confirm our theoretical claims and also prove that the methods based on bidiagonalization are generally not relatively accurate on that class of matrices. We have moved some details concerning the algorithms and the lengthy proof of the backward error estimate to the Appendix A.

2. The serial Kogbetliantz method

Here, we consider this method under the *column-cyclic* pivot strategy. Recall that the column- and the equivalent *row-cyclic* strategy are commonly called *serial pivot strategies* and they belong to the class of *wavefront* cyclic strategies (see [32–34]). For an initial $n \times n$ triangular matrix G, the Kogbetliantz method repeatedly applies a set of $N = n(n-1)/2$ steps. Each step consists of the two-sided orthogonal transformation by plane rotations, where the both rotations are defined by the same pair of pivot indices. The *pivot pair* runs through the set $\{(l,m): 1 \leqslant l < m \leqslant n\}$ using the "column-wise" ordering:

$$(1,2);\ (1,3),(2,3);\ (1,4),(2,4),(3,4);\ \ldots;\ (1,n),(2,n),\ldots,(n-1,n).$$

After applying the set of N successive orthogonal transformations, one says that one sweep (or cycle) of the method has been completed. If $G^{(k)}$ denotes the matrix obtained at the end of step k, then the method can be described as the iterative process

$$G^{(k+1)} = [U^{(k)}]^* G^{(k)} V^{(k)}, \quad k \geqslant 0; \quad G^{(0)} = G. \tag{2.1}$$