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A NEW PREPROCESSING ALGORITHM FOR THE COMPUTATION OF THE GENERALIZED SINGULAR VALUE DECOMPOSITION*

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Abstract. In this note a new algorithm is proposed for the preprocessing phase of Paige's algorithm for computing the generalized singular value decomposition (GSVD). This new algorithm substantially reduces the complexity of Paige's algorithm and makes it much easier to implement. It is also proved that the preprocessing phase is backward stable and a numerical example is demonstrated.

Key words. generalized singular value decomposition, URV decomposition

AMS subject classification. 65F30

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1. Introduction. This note is concerned with the numerical computation of the generalized singular value decomposition (GSVD) of two matrices having the same number of columns. The GSVD was first proposed by Van Loan [9]. Like the singular value decomposition (SVD) of one matrix, the GSVD of matrix pairs is a very useful tool in many numerical linear algebra problems. The following formulation of the GSVD is due to Paige and Saunders [5], and is more suitable for numerical computation.

THEOREM 1.1. *Given a matrix pair (A, B) with $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{p\times n}$, there exist orthogonal matrices U, V, and Q such that*

$$U^TAQ = \Sigma_A(\,0\ \ R\,), \qquad V^TBQ = \Sigma_B(\,0\ \ R\,), \tag{1}$$

where R is $k \times k$ nonsingular upper triangular with $k = \operatorname{rank}(A^T, B^T)^T$, and Σ_A and Σ_B are $m \times k$ and $p \times k$ diagonal matrices such that

$$\Sigma_A^T\Sigma_A + \Sigma_B^T\Sigma_B = I.$$

Paige's algorithm for computing the above-mentioned decomposition consists of two phases: (1) reducing the given matrix pairs to upper triangular (or trapezoidal) forms by orthogonal transformations, which is designated as the preprocessing phase; (2) implicitly applying the Kogbetliantz algorithm to find the GSVD of two triangular matrices [6]. The existing preprocessing procedure may result in an *irregular* triangular pair, which gives rise to several different cases in the second phase and makes the numerical implementation quite complicated [2]. In this note the authors propose a new preprocessing algorithm that essentially leaves only one case in the next phase. More precisely, the authors reduce the problem to the computation of the GSVD of a matrix pair (A, B), where A and B are upper triangular and B nonsingular, which is called a *regular* matrix pair.[1] Our current interest in developing algorithms for computing the GSVD stems

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[1]The generalized singular values of a regular matrix pair are all finite.

from Bai's involvement in the linear algebra software package LAPACK [1]. Paige's algorithm for computing the GSVD will be included in the future release of LAPACK. For an alternative GSVD algorithm via the CS decomposition, the reader is referred to [7] and [10].

2. A new preprocessing algorithm. The purpose of the preprocessing phase is to reduce the given matrix pair (A, B) to a condensed form, so that the implicit Kogbetliantz algorithm can be applied. Our approach is to extract a regular matrix pair from (A, B) by applying orthogonal transformations to the individual matrices A and B. A similar idea was also used in [11] for computing the *restricted singular value decomposition* of matrix triplets. The algorithm consists of three steps. The transformation from step k to step $k+1$ is denoted as

$$\begin{pmatrix} A^{(k+1)} \\ B^{(k+1)} \end{pmatrix} = \begin{pmatrix} (U^{(k)})^T A^{(k)} (Q^{(k)}) \\ (V^{(k)})^T B^{(k)} (Q^{(k)}) \end{pmatrix},$$

where $U^{(k)}$, $V^{(k)}$, and $Q^{(k)}$ are orthogonal; $A^{(k)}$ and $B^{(k)}$ are the transformed A and B at step k with initial values

$$A^{(0)} = A, \qquad B^{(0)} = B.$$

For brevity, in the following description of the algorithm, we only specify the transformed A and B at each step; the corresponding orthogonal transformation matrices can be easily constructed.

Before we proceed, we need to recall a matrix decomposition, which will be the building block of our preprocessing algorithm: for any $m \times n$ matrix A, there exist orthogonal matrices U and V such that A can be decomposed as

$$A = U \begin{pmatrix} 0 & R \\ 0 & 0 \end{pmatrix} V^T,$$

where R is a nonsingular upper triangular matrix. The decomposition is called the *complete orthogonal decomposition*, or simply the *URV decomposition* [3]. Now we are ready to present the preprocessing algorithm.

Step 1. Compute the URV decomposition of B such that

$$\begin{pmatrix} A^{(1)} \\ B^{(1)} \end{pmatrix} = \left(\begin{array}{cc} A_{11}^{(1)} & A_{12}^{(1)} \\ \hline 0 & B_{12}^{(1)} \\ 0 & 0 \end{array}\right),$$

where $B_{12}^{(1)}$ is upper triangular and nonsingular.

Step 2. Compute the URV decomposition of $A_{11}^{(1)}$ (if $A_{11}^{(1)}$ is not empty) and update $A_{12}^{(1)}$, so that we have

$$\begin{pmatrix} A^{(2)} \\ B^{(2)} \end{pmatrix} = \left(\begin{array}{ccc} 0 & A_{12}^{(2)} & A_{13}^{(2)} \\ 0 & 0 & A_{23}^{(2)} \\ \hline 0 & 0 & B_{13}^{(2)} \\ 0 & 0 & 0 \end{array}\right),$$

where $A_{12}^{(2)}$ is upper triangular and nonsingular, and $B_{13}^{(2)} = B_{12}^{(1)}$.

Step 3. Compute the QR decomposition of $A_{23}^{(2)}$, such that

$$\begin{pmatrix} A^{(3)} \\ B^{(3)} \end{pmatrix} = \left(\begin{array}{ccc} 0 & A_{12}^{(3)} & A_{13}^{(3)} \\ 0 & 0 & A_{23}^{(3)} \\ \hline 0 & 0 & B_{13}^{(3)} \\ 0 & 0 & 0 \end{array}\right),$$

where $A_{12}^{(3)} = A_{12}^{(2)}$, $A_{13}^{(3)} = A_{13}^{(2)}$, and $B_{13}^{(3)} = B_{13}^{(2)}$. For $A_{23}^{(3)}$, we need to distinguish two cases. Let $A_{23}^{(3)} \in R^{s\times r}$.

1. If $s \geq r$, then

$$A_{23}^{(3)} = \begin{pmatrix} \tilde{A}_{23}^{(3)} \\ 0 \end{pmatrix},$$

where $\tilde{A}_{23}^{(3)}$ is $r \times r$ upper triangular.

2. If $s < r$, then the first s columns of $A_{23}^{(3)}$ is an upper triangular matrix. We append $r - s$ rows of zeros to $A_{23}^{(3)}$ and denote the resulting matrix $\tilde{A}_{23}^{(3)}$, which is also an upper triangular matrix.

In either case, we end up with a matrix pair $(\tilde{A}_{23}^{(3)}, B_{13}^{(3)})$, where $\tilde{A}_{23}^{(3)}$ and $B_{13}^{(3)}$ are square upper triangular and of the same size; moreover, $B_{13}^{(3)}$ is nonsingular. Therefore, computing the GSVD of $(\tilde{A}_{23}^{(3)}, B_{13}^{(3)})$ is equivalent to computing the SVD of $\tilde{A}_{23}^{(3)}(B_{13}^{(3)})^{-1}$. Using the implicit Kogbetliantz algorithm [6], [2], we can find three orthogonal matrices U_1, V_1, and Q_1 such that

$$U_1^T \tilde{A}_{23}^{(3)} (B_{13}^{(3)})^{-1} V_1 = \text{diagonal},$$

and

$$U_1^T \tilde{A}_{23}^{(3)} Q_1 = \Sigma_1 R_1, \qquad V_1^T B_{13}^{(3)} Q_1 = \Sigma_2 R_1, \tag{2}$$

where Σ_1 and Σ_2 are diagonal, R_1 is upper triangular, and

$$\Sigma_1^T \Sigma_1 + \Sigma_2^T \Sigma_2 = I.$$

Combining Steps 1–3 and the results from the implicit Kogbetliantz algorithm (2), and accumulating the corresponding orthogonal transformations, we have

$$U^T A Q = \Sigma_A \begin{pmatrix} 0 & R \end{pmatrix} \quad \text{and} \quad V^T B Q = \Sigma_B \begin{pmatrix} 0 & R \end{pmatrix}, \tag{3}$$

where

$$\Sigma_A = \begin{pmatrix} I & 0 \\ 0 & \Sigma_1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \Sigma_B = \begin{pmatrix} 0 & \Sigma_2 \\ 0 & 0 \end{pmatrix},$$

and the upper triangular matrix R is given by

$$R = \begin{pmatrix} A_{12}^{(3)} & A_{13}^{(3)} Q_1 \\ 0 & R_1 \end{pmatrix}.$$

Equation (3) gives the desired GSVD of A and B in Theorem 1.1.

3. Backward stability and numerical example. In this section, we first discuss the numerical stability of the new preprocessing algorithm and then present one example as a demonstration. The crux of the numerical stability of the new preprocessing algorithm is how to stably compute the URV decomposition. In the current implementation, this is done by first applying the QR decomposition with column pivoting, and then squeezing the resulting trapezoidal form into upper triangular form by applying a sequence of Householder transformations. Let quantities with an overbar denote computed quantities. From the standard backward error analysis of the QR decomposition [3], we know that for the above preprocessing algorithm, the computed $\bar{A}^{(3)}$ and $\bar{B}^{(3)}$ satisfy

$$\bar{U}^T(A+E)\bar{Q} = \bar{A}^{(3)}, \qquad \bar{V}^T(B+F)\bar{Q} = \bar{B}^{(3)},$$

where

$$\|E\|_F \le \tau\|A\|_2, \qquad \|F\|_F \le \tau\|B\|_2,$$

and where τ is a user-specified tolerance value, which is used in the QR decomposition with column pivoting to determine the effective numerical rank of the matrix. We also mention that there exist more sophisticated algorithms for computing the URV decomposition, for example, the one proposed by Hanson and Lawson [4] and Stewart [8].

To conclude this note, we apply the new preprocessing algorithm and the implicit Kogbetliantz algorithm to a numerical example.[2] Our emphasis here is the backward stability of the preprocessing algorithm. The matrix pair (A, B) is given as follows:

$$A = \begin{pmatrix} 1 & 2 & 3 & 1 & 5 \\ 0 & 3 & 2 & 0 & 2 \\ 1 & 0 & 2 & 1 & 0 \\ 0 & 2 & 3 & 0 & -1 \\ 1 & 0 & 2 & 1 & 1 \\ 0 & 2 & 1 & 0 & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & -2 & 2 & 1 & 1 \\ 0 & 3 & 0 & 0 & 0 \\ 1 & -2 & 2 & 1 & 1 \\ 0 & 2 & 0 & 0 & 0 \\ 2 & -4 & 4 & 2 & 2 \\ 1 & 3 & 2 & 1 & 1 \end{pmatrix}.$$

After the three steps of preprocessing algorithm with the tolerance value set as $\epsilon_M\|A\|_F$ and $\epsilon_M\|B\|_F$ for the matrices A and B, respectively, we have

$$\bar{A}^{(3)} = \left(\begin{array}{c|cc|cc} 0 & 3.6017\mathrm{E}+00 & -1.7136\mathrm{E}+00 & 3.3819\mathrm{E}-01 & 1.8012\mathrm{E}+00 \\ 0 & 0 & -2.6088\mathrm{E}+00 & 4.4448\mathrm{E}+00 & 4.9805\mathrm{E}+00 \\ \hline 0 & 0 & 0 & -1.0628\mathrm{E}+00 & 6.4454\mathrm{E}-02 \\ 0 & 0 & 0 & 0 & 4.2699\mathrm{E}+00 \\ \hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right),$$

[2]For brevity, only five decimal digits are displayed for all the data, though all the results are obtained using our FORTRAN routines run in double precision on an HP Apollo workstation with machine precision $\epsilon_M \approx 2.2204 \times 10^{-16}$.

$$\bar{B}^{(3)} = \left(\begin{array}{c|cc|cc} 0 & 0 & 0 & -6.7823\mathrm{E}+00 & 3.5109\mathrm{E}+00 \\ 0 & 0 & 0 & 0 & 6.0559\mathrm{E}+00 \\ \hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right),$$

where the partitioning of the matrix pair $(\bar{A}^{(3)}, \bar{B}^{(3)})$ corresponds to that in Step 3 of the preprocessing algorithm. At the second phase, we use the scheme proposed by Bai and Demmel [2] to compute the GSVD of the (2,3) block of $\bar{A}^{(3)}$ and the (1,3) block of $\bar{B}^{(3)}$; we obtain

$$\begin{pmatrix} -1.0628\mathrm{E}+00 & 6.4454\mathrm{E}-02 \\ 0 & 4.2699\mathrm{E}+00 \end{pmatrix} = \begin{pmatrix} 1.5379\mathrm{E}-01 & 0 \\ 0 & 5.7885\mathrm{E}-01 \end{pmatrix} \bar{R}_1$$

and

$$\begin{pmatrix} -6.7823\mathrm{E}+00 & 3.5109\mathrm{E}+00 \\ 0 & 6.0559\mathrm{E}+00 \end{pmatrix} = \begin{pmatrix} 9.8810\mathrm{E}-01 & 0 \\ 0 & 8.1544\mathrm{E}-01 \end{pmatrix} \bar{R}_1,$$

where

$$\bar{R}_1 = \begin{pmatrix} -6.9692\mathrm{E}+00 & 3.5064\mathrm{E}+00 \\ 0 & 7.3144\mathrm{E}+00 \end{pmatrix}.$$

Combining the above two phases, we have

$$\bar{U}^T(A+E)\bar{Q} = \bar{\Sigma}_A(0 \;\; \bar{R}), \qquad \bar{V}^T(B+F)\bar{Q} = \bar{\Sigma}_B(0 \;\; \bar{R}), \tag{4}$$

where

$$\bar{\Sigma}_A = \begin{pmatrix} 1.0000\mathrm{E}+00 & 0 & 0 & 0 \\ 0 & 1.0000\mathrm{E}+00 & 0 & 0 \\ 0 & 0 & 1.5379\mathrm{E}-01 & 0 \\ 0 & 0 & 0 & 5.7885\mathrm{E}-01 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\bar{\Sigma}_B = \begin{pmatrix} 0 & 0 & 9.8810\mathrm{E}-01 & 0 \\ 0 & 0 & 0 & 8.1544\mathrm{E}-01 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

and

$$\bar{R} = \begin{pmatrix} 3.6017\text{E}+00 & -1.7136\text{E}+00 & 2.8436\text{E}-01 & 1.8104\text{E}+00 \\ 0 & -2.6088\text{E}+00 & 4.2944\text{E}+00 & 5.1107\text{E}+00 \\ 0 & 0 & -6.9692\text{E}+00 & 3.5064\text{E}+00 \\ 0 & 0 & 0 & 7.3144\text{E}+00 \end{pmatrix},$$

with the backward errors of the computed decomposition

$$\|E\|_F = \|\bar{U}^{\mathrm{T}} A \bar{Q} - \bar{\Sigma}_A \bar{R}\|_F = 4.5118\text{E}-15 \approx \epsilon_{\mathrm{M}} \|\mathrm{A}\|_{\mathrm{F}},$$

$$\|F\|_F = \|\bar{V}^{\mathrm{T}} B \bar{Q} - \bar{\Sigma}_B \bar{R}\|_F = 5.6621\text{E}-15 \approx \epsilon_{\mathrm{M}} \|\mathrm{B}\|_{\mathrm{F}}.$$

The computed orthogonal matrices $\bar{U}$, $\bar{V}$, and $\bar{Q}$ are orthogonal within machine precision. The decomposition in (4) gives the desired GSVD of A and B in Theorem 1.1.

REFERENCES

[1] E. ANDERSON, Z. BAI, C. BISCHOF, J. DEMMEL, J. DONGARRA, J. DU CROZ, A. GREENBAUM, S. HAMMARLING, A. MCKENNEY, S. OSTROUCHOV, AND D. SORENSEN, *LAPACK Users' Guide*, Society for Industrial and Applied Mathematics, Philadelphia, PA, 1992.

[2] Z. BAI AND J. W. DEMMEL, *Computing the generalized singular value decomposition*, Report UCB/CSD 91/645, Computer Science Division, University of California, Berkeley, 1991.

[3] G. H. GOLUB AND C. F. VAN LOAN, *Matrix Computations*, 2nd ed., The Johns Hopkins University Press, Baltimore, MD, 1989.

[4] R. J. HANSON AND C. L. LAWSON, *Extensions and applications of the Householder algorithm for solving linear least squares problems*, Math. Comp., 22 (1969), pp. 787–812.

[5] C. C. PAIGE AND M. A. SAUNDERS, *Towards a generalized singular value decomposition*, SIAM J. Numer. Anal., 18 (1981), pp. 398–405.

[6] C. C. PAIGE, *Computing the generalized singular value decomposition*, SIAM J. Sci. Statist. Comput., 7 (1986), pp. 1126–1146.

[7] G. W. STEWART, *Computing the CS-decomposition of a partitioned orthonormal matrix*, Numer. Math., 40 (1982), pp. 297–306.

[8] ———, *An updating algorithm for subspace tracking*, CS-TR 2494, Department of Computer Science, Univ. of Maryland, College Park, 1990; IEEE Trans. on Signal Process, to appear.

[9] C. F. VAN LOAN, *Generalizing the singular value decomposition*, SIAM J. Numer. Anal., 13 (1976), pp. 76–83.

[10] ———, *Computing the CS and the generalized singular value decomposition*, Numer. Math., 46 (1985), pp. 479–491.

[11] H. ZHA, *A numerical algorithm for computing restricted singular value decomposition of matrix triplets*, Linear Algebra Appl., 168 (1992), pp. 1–25.