

Computing the Generalized Singular Value Decomposition*

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Abstract

We present a variation of Paige’s algorithm for computing the generalized singular value decomposition (GSVD) of two matrices A and B . There are two innovations. The first is a new preprocessing step which reduces A and B to upper triangular forms satisfying certain rank conditions. The second is a new 2 by 2 triangular GSVD algorithm, which constitutes the inner loop of Paige’s algorithm. We present proofs of stability and high accuracy of the 2 by 2 GSVD algorithm, and demonstrate it using examples on which all previous algorithms fail.

Key words: generalized singular value decomposition, CS decomposition, matrix decomposition, Jacobi algorithm, Kogbetliantz algorithm.

Subject classifications: AMS(MOS): 65F30; CR:G1.3

1 Introduction

The purpose of this paper is to describe a variation of Paige’s algorithm [28] for computing the following generalized singular value decomposition (GSVD) introduced by Van Loan [33], and Paige and Saunders [25]. This is also called the quotient singular value decomposition (QSVD) in [8].

Theorem *Let $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{p \times n}$ have $\text{rank}(A^T, B^T) = n$.¹ Then there are orthogonal matrices U , V and Q such that*

$$U^T A Q = \Sigma_1 R, \quad V^T B Q = \Sigma_2 R, \quad (1.1)$$

where R is a $n \times n$ upper triangular and nonsingular, and

$$\Sigma_1 = \begin{matrix} l & k & n-l-k \\ \begin{matrix} I_1 & & \\ & D_1 & \\ & & O_1 \end{matrix} \end{matrix}, \quad \Sigma_2 = \begin{matrix} l & k & n-l-k \\ \begin{matrix} O_2 & & \\ & D_2 & \\ & & I_2 \end{matrix} \end{matrix}, \quad (1.2)$$

$I_1 \in \mathbb{R}^{l \times l}$ and $I_2 \in \mathbb{R}^{(n-l-k) \times (n-l-k)}$ are identity matrices, $Q \in \mathbb{R}^{(m-l-k) \times (n-l-k)}$ and $O_2 \in \mathbb{R}^{(p-n+l) \times l}$ are zero matrices,

$$D_1 = \text{diag}(\alpha_{l+1}, \dots, \alpha_{l+k}), \quad D_2 = \text{diag}(\beta_{l+1}, \dots, \beta_{l+k}), \quad (1.3)$$

$$1 > \alpha_{l+1} \geq \dots \geq \alpha_{l+k} > 0, \quad 0 < \beta_{l+1} \leq \dots \leq \beta_{l+k} < 1, \quad \alpha_i^2 + \beta_i^2 = 1. \quad (1.4)$$

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¹The assumption that $\text{rank}(A^T, B^T) = n$ is not essential but simplifies exposition.

The GSVD is a generalization of the singular value decomposition (SVD) in the sense that if B is the identity matrix, then the GSVD of A and B is the SVD of A . Moreover, if B is nonsingular, then the GSVD of A and B reduces to the SVD of AB^{-1} . If $(A^T, B^T)^T$ has orthonormal columns, then the GSVD of A and B is the GS decomposition [31]. The pairs (α_i, β_i) defined by the diagonal elements of Σ_1 and Σ_2 are called the *generalized singular value pairs (GSVPs)*. The quotient $\lambda_i = \alpha_i/\beta_i$ is called a *generalized singular value (GSV)*. Note that the λ_i are the square roots of the eigenvalues of the symmetric pencil $A^T A - \lambda B^T B$.

The GSVD of two matrices A and B is a tool used in many applications, such as the Kronecker canonical form of a general matrix pencil [22], the linearly constrained least-squares problem [35, 5], the general Gauss-Markov linear model [27, 3], the generalized total least squares problem [21], and real time signal processing [30]. As a further generalization of the SVD, Everbring and Luk [13], Zha [36] proposed a generalized SVD for matrix triplets, and De Moor, Golub and Zha [8, 9] have generalized the SVD into a factorization of any number of matrices. For all these applications and multi-matrix generalization of the SVD the development of a stable and efficient algorithm for computing the GSVD of two matrices is a basic problem.

Stewart [31] and Van Loan [34] proposed two algorithms for computing the GSVD. Their algorithms have two phases: The first phase is to compute the QR decomposition (or the SVD if necessary) of $(A^T, B^T)^T$. The second phase is to compute the GS decomposition. Paige's algorithm is a Jacobi-Kogbetliantz approach [28], which applies orthogonal transformations to A and B separately without the GS decomposition. It also has two phases:

- (1) Reduce matrices A and B to the following form

$$U^T A P = \begin{matrix} & r & q & n-t \\ \begin{matrix} r \\ q \\ m-t \end{matrix} & \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{matrix}, \quad V^T B P = \begin{matrix} & r & q & n-t \\ \begin{matrix} r \\ q \\ p-t \end{matrix} & \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ 0 & B_{22} & B_{23} \\ 0 & 0 & 0 \end{pmatrix} \end{matrix}, \quad (1.5)$$

where $m \times m$ matrix U and $p \times p$ matrix V are orthogonal, P is a $n \times n$ permutation matrix, $A_{11} \in \mathbb{R}^{r \times r}$ is nonsingular upper triangular, $B_{11} \in \mathbb{R}^{r \times r}$ is upper triangular, $t = r + q$, and if $q > 0$, $B_{22} \in \mathbb{R}^{q \times q}$ is nonsingular upper triangular.

- (2) Compute the GSVD of two $n \times n$ upper triangular matrices of form (1.5) by a generalized Kogbetliantz algorithm².

Phase 1 can be done first by the QR factorization with column pivoting [17] of matrix A and determine the rank r of A , meanwhile permuting the columns of matrix B in the same way, and then applying the QR factorization with column pivoting to the block of the last $p - r$ rows and $n - r$ columns of B and obtain the rank q of the block; this yields the form (1.5) [4]. Phase 2 is iterative.

In this paper, we will present a variation of Paige's algorithm for computing the GSVD. There are two innovations. The first is as follows: in [28], it is assumed (without providing detail) that in (1.5) the nonzero part of $V^T B P$ has full rowrank. It is known that it is complicated to choose V to guarantee this condition and P may not be a permutation matrix. However in the preprocessing step (1.5), we do not require this condition, and so we can simply use conventional QR factorization with column pivoting. Moreover, note that the GSVD is independent of column scaling of A and B . The form (1.5) preserve this property.

The second innovation is a new 2 by 2 triangular GSVD algorithm which constitutes the inner loop of Paige's algorithm. We will present proofs of stability and high accuracy of our method, and demonstrate it using examples on which all previous algorithms fail. Hereafter, we assume that A and B have been preprocessed to the upper trapezoidal form (1.5).

²We may need to add zero rows or columns to get square matrices. This is not essential but it simplifies the description.

The numerical technique developed in this paper can be extended to deal with the numerical computation of other closely related decompositions such as the GS decomposition and the product SVD of two matrices [20, 15]. We will not go into the details.

The rest of the paper is organized as follows: § 2 reviews the Kogbetliantz algorithm for computing the SVD of a triangular matrix, and Paige’s generalization of the Kogbetliantz algorithm for computing the GSVD § 3 explores the inner loop of Paige’s algorithm which includes the GSVD of a 2×2 matrix in terms of exact and floating point arithmetic. In § 4, we describe the overall algorithm. The last section reports the results of numerical experiments. In the appendix, we include Demal and Kahan’s 2×2 triangular SVD code, which has not been published in its entirety before, and plays an important role in our algorithm.

2 Paige’s GSVD Algorithm

To describe Paige’s algorithm we first review the Kogbetliantz algorithm [23] for computing the SVD of an upper triangular matrix A . Then we describe Paige’s algorithm for computing the GSVD of A and B with B nonsingular. Finally, we discuss how to generalize the idea to the case where B is ill-conditioned or singular.

2.1 Kogbetliantz algorithm for the SVD of a triangular matrix

The Kogbetliantz algorithm [23] is a kind of Jacobi scheme. Assume that the k th transformation of the algorithm operates on the rows and columns i and j of A . Let A_{ij} be the 2×2 submatrix subtended by rows and columns i and j of A . Let the rotation matrices $U_k = \text{rot}(c_u, s_u)$ and $V_k = \text{rot}(c_v, s_v)$ be chosen³ so that

$$U_k^T A_{ij} V_k = \text{diag}(\gamma_{ii}, \gamma_{jj})$$

is the SVD of A_{ij} , where $c_u = \cos \phi_k$, $s_u = \sin \phi_k$ and $c_v = \cos \psi_k$, $s_v = \sin \psi_k$. Let \hat{U}_k and \hat{V}_k be identity matrices with (i, i) , (i, j) , (j, i) and (j, j) elements replaced by the $(1, 1)$, $(1, 2)$, $(2, 1)$ and $(2, 2)$ elements of U_k and V_k respectively. Then let

$$A_{k+1} = \hat{U}_k^T A_k \hat{V}_k,$$

where $A_0 = A$. After the first sweep through all the (i, j) in rowcyclic order, an upper triangular matrix A will become lower triangular. The second sweep will restore upper triangular form and so on [20, 19]. There is a literature on the different sweep orders for sequential and parallel computations besides the conventional row and column order, for example [24].

Ersythe and Henri ci [16] considered the convergence of the rowcyclic Kogbetliantz algorithm. Fernando [14] proved a global convergence theorem under the assumption that one of the rotation angles $\{\phi_k, \psi_k\}$ at each (i, j) transformation lies in a closed interval $J \subset (-\pi/2, \pi/2)$, i.e.,

$$\phi_k \in J \text{ or } \psi_k \in J, \quad k = 1, 2, \dots, . \tag{2.1}$$

This is the condition that our algorithm will satisfy. Furthermore, it has been proved that the cyclic Kogbetliantz algorithm multi tly converges quadratically [29, 2, 7].

³Throughout this paper, we use $\text{rot}(c, s)$ to denote the rotation matrix $\begin{pmatrix} c & s \\ -s & c \end{pmatrix}$.

2.2 The Generalization of the Kogbetliantz Algorithm for the GSVD

We begin by computing the SVD of two upper triangular matrices A and B with B nonsingular.

It is known that this is equivalent to computing the SVD of the triangular matrix $C = AB^{-1}$.

Of course, it is unwise to form C explicitly. We note that a sweep of the Kogbetliantz algorithm

applied to C will make it lower triangular. This means that there are orthogonal matrices U

V_1 such that

$$U_1^T C V_1 = C_{-1}, \quad (2.2)$$

where C_{-1} is lower triangular. Recasting (2.2) as $U_1^T A = C_{-1} V_1^T B$, we see that if we can determine an orthogonal matrix Q_{-1} satisfying

$$U_1^T A Q_{-1} = A_{-1}, \quad V_1^T B Q_{-1} = B_{-1},$$

where A_{-1} and B_{-1} are lower triangular, then $C_{-1} = A_{-1} B_{-1}^{-1}$. This means that using a sweep of the

Kogbetliantz algorithm on the upper triangular C to get the lower triangular C_{-1} is equivalent to

the problem of finding orthogonal matrices U_{-1} , V_1 and Q_{-1} so that $U_{-1}^T A Q_{-1}$ and $V_1^T B Q_{-1}$ are lower

triangular. Heath *et al* [20], Paige [28] and Hari and Veselić [19] have shown that we may take advantage of the triangular structures of A and B and the ordering of sweeps to get the desired

orthogonal transformations U_{-1} , V_1 and Q_{-1} without forming AB^{-1} explicitly. Specifically, at the

(i, j) transformation, the needed 2×2 submatrix C_{ij} of C is given by

$$C_{ij} = A_{ij} B_{ij}^{-1} = \begin{pmatrix} a_{ii} & a_{ij} \\ 0 & a_{jj} \end{pmatrix} \begin{pmatrix} b_{ii} & b_{ij} \\ 0 & b_{jj} \end{pmatrix}^{-1}, \quad (2.3)$$

where a_{ij} and b_{ij} are the elements subtended by the rows and columns i and j of the updated A

and B , respectively. By using the SVD of C_{ij} : $U_{ij}^T C_{ij} V_{ij} = \text{diag}(\tilde{c}_{ii}, \tilde{c}_{jj})$, we have

$$U_{ij}^T A_{ij} = \text{diag}(\tilde{c}_{ii}, \tilde{c}_{jj}) V_{ij}^T B_{ij}.$$

This shows that the corresponding rows of $U_{ij}^T A_{ij}$ and $V_{ij}^T B_{ij}$ are parallel. Hence if we choose

rotation Q_{ij} so that $V_{ij}^T B_{ij} Q_{ij}$ is lower triangular, then $U_{ij}^T A_{ij} Q_{ij}$ must also be lower triangular,

which is just the SVD of the 2×2 triangular matrices A_{ij} and B_{ij} . With this observation,

we see that after completing a sweep in row order, the desired U_{-1} , V_1 and Q_{-1} are the products

$U_{12} U_{13} \cdots U_{n-1,n}$, $V_{12} V_{13} \cdots V_{n-1,n}$ and $Q_{12} Q_{13} \cdots Q_{n-1,n}$, respectively. By the end of the row

cyclic sweep, we obtain lower triangular matrices A_{-1} and B_{-1} .⁴ Then the next sweep consists of

zeroing lower off diagonal elements of $C_{-1} = A_{-1} B_{-1}^{-1}$ in column order to return it to upper triangular

form and so on. Overall, we are actually carrying out the Kogbetliantz algorithm to diagonalize

the implicitly defined matrix C . Upon convergence, this gives $U^T (AB^{-1}) V = \Sigma$, a diagonal matrix.

That is

$$U^T A Q = \Sigma \cdot V^T B Q$$

i.e., the i th rows of $U^T A Q$ and $V^T B Q$ are parallel, which is the desired SVD of A and B .

In general, if B is ill-conditioned with respect to inversion or B is singular after phase 1, then

using B_{ij}^{-1} is not recommended. Paige [28] suggests using

$$C_{ij} = A_{ij} \cdot \text{adj}(B_{ij}) = \begin{pmatrix} a_{ii} & a_{ij} \\ 0 & a_{jj} \end{pmatrix} \begin{pmatrix} b_{jj} & -b_{ij} \\ 0 & b_{ii} \end{pmatrix} \quad (2.4)$$

⁴By incorporating Gentleman's suggested row and column permutations [28] after each transformation, we need only use an upper triangular array to carry out the computation. But for clearer exposition, we will use the entire square array in this paper.

instead of C_{ij} in (2.3), where $\text{adj}(B_{ij})$ stands for the adjugate of B_{ij} . Since $B_{ij} \cdot \text{adj}(B_{ij}) = \det(B_{ij})I$, it seems to be direct and natural to use $\text{adj}(B_{ij})$ instead of B_{ij}^{-1} . The incorporation of (2.4) into the above procedure circumvents the numerical difficulties when B_{ij} is ill-conditioned with respect to inversion or B_{ij} is singular. But it also introduces two questions. First, are there still rotation matrices U_{ij} , V_{ij} and Q_{ij} such that $U_{ij}^T A_{ij} Q_{ij}$ and $V_{ij}^T B_{ij} Q_{ij}$ are the GSVD of 2 by 2 matrices A_{ij} and B_{ij} ? Second, does the scheme converge to our required GSVD form of A and B ? The following section will address these questions.

3 The GSVD of 2 by 2 Triangular Matrices

As we see in § 2, the kernel of computing the GSVD using a generalized Kogbetliantz algorithm is the computation of the GSVD of 2 by 2 matrices. In this section, we first discuss the computation of the 2×2 GSVD for different possible 2×2 matrices A_{ij} and B_{ij} in exact arithmetic, and then we will discuss the computation in the presence of floating point arithmetic.

3.1 The 2×2 GSVD in exact arithmetic

When A and B are processed to have upper trapezoidal form (1.5), we see that at the (i, j) transformation, the 2×2 matrices A and B are of the form

$$A = \begin{pmatrix} a_{11} & a_{12} \\ 0 & a_{22} \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} b_{11} & b_{12} \\ 0 & b_{22} \end{pmatrix}, \tag{3.1}$$

where $a_{11} \neq 0$, if A is nonzero. We have the following lemma:

Lemma 1 *There exist 2×2 rotation matrices U , V and Q such that*

$$\tilde{A} = U^T A Q = \begin{pmatrix} \tilde{a}_{11} & 0 \\ \tilde{a}_{21} & \tilde{a}_{22} \end{pmatrix}, \quad \tilde{B} = V^T B Q = \begin{pmatrix} \tilde{b}_{11} & 0 \\ \tilde{b}_{21} & \tilde{b}_{22} \end{pmatrix}$$

is the GSVD of A and B . Moreover,

- (a) $\tilde{a}_{11} \neq 0$ if A is nonzero,
- (b) $\tilde{b}_{22} \neq 0$ if both A and B are nonzero, except that
- (c) if the first rows of A and B are parallel and the second rows are zero, then $U = V = I$, and Q can be chosen to zero the $(1, 2)$ entries of A and B simultaneously.

Proof. The proof proceeds by considering all possible cases. If B is nonsingular, the lemma follows immediately by § 2.2. If A or B is zero, the results are trivial. The remaining cases are for B singular but not zero. This includes the following three cases, where $C = A \cdot \text{adj}(B)$:

(1) $B = \begin{pmatrix} b_{11} & b_{12} \\ 0 & 0 \end{pmatrix}$ with $b_{11} \neq 0$. In this case, $C = \begin{pmatrix} 0 & a_{12}b_{11} - a_{11}b_{12} \\ 0 & a_{22}b_{11} \end{pmatrix} \equiv \begin{pmatrix} 0 & c_{12} \\ 0 & c_{22} \end{pmatrix}$.

If $c_{12} = 0$, i.e., the first row vectors of A and B are parallel, then if c_{22} is also equal to zero, $U = V = I$. Q_{ij} is chosen to zero $(1, 2)$ entry of A and must also zero the $(1, 2)$ entry of B , yielding the result (c). If $c_{22} \neq 0$, then both U and V are chosen as permutation matrices. Q is chosen to zero the $(1, 2)$ entry of $U^T A$.

If $c_{12} \neq 0$, then U is chosen to zero $(2, 2)$ entry of C and $V = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. $V^T B$ has second row nonzero. The lemma follows by choosing Q to zero $(1, 2)$ entry of $U^T A$.

⁵For simplicity of exposition, we drop the subscript ij from the 2 by 2 triangular matrices A_{ij} and B_{ij} .

(2) $B = \begin{pmatrix} 0 & b_{12} \\ 0 & b_{22} \end{pmatrix}$ with $b_{22} \neq 0$. Hence $C = a_{11} \begin{pmatrix} b_{22} & -b_{12} \\ 0 & 0 \end{pmatrix}$. Then $U = I$, and V is chosen to zero (1,2) entry of C , i.e. to zero the (1,2) entry of B . The lemma follows by choosing Q to zero (1,2) entry of A .

(3) $B = \begin{pmatrix} 0 & b_{12} \\ 0 & 0 \end{pmatrix}$ with $b_{12} \neq 0$. We see that $C = \begin{pmatrix} 0 & -a_{11}b_{12} \\ 0 & 0 \end{pmatrix}$. Then we can choose $U = I$, $V = \text{rot}(0, 1)$. Therefore the second row of $V^T B$ is nonzero. The lemma follows by choosing Q to zero (1,2) entry of $U^T A$. ■

It has been shown by induction (see [28, 4]) that with the properties of Lemma 1, a sweep in row order with possible reordering takes the initial upper trapezoidal form (1.5) of A and B into the form

$$A_1 = U_1^T A Q_1 = \begin{matrix} r & n-r \\ r-r & \end{matrix} \begin{pmatrix} A_{11} & 0 \\ 0 & 0 \end{pmatrix}, \quad B_1 = V_1^T B Q_1 = \begin{matrix} r & n-r \\ n-r & \end{matrix} \begin{pmatrix} B_{11} & 0 \\ B_{21} & B_{22} \end{pmatrix}, \quad (3.2)$$

where A_{11} , B_{11} and B_{22} are lower triangular, and A_{11} , B_{22} are nonsingular. B_{11} may be singular, but there must exist nonzero diagonal elements in the nonzero rows of B_{11} .

From (3.2), we see that at (i, j) transformation in column ordering, the 2×2 matrices A and B are lower triangular matrices, where if A is singular, then A is either the zero matrix or its second row is zero, and moreover, if $b_{22} = 0$, then $b_{21} = 0$. By a similar argument as in Lemma 1, we can show that there are 2×2 orthogonal matrices U , V and Q such that $\tilde{A} = U^T A Q$ and $\tilde{B} = V^T B Q$ both are upper triangular, and the GSVD of A and B . The proof of Lemma 1 suggests the following algorithm where for brevity, we omit the part for lower triangular matrices.

Algorithm 1 (The 2×2 GSVD algorithm).
 form $C = A \cdot \text{adj}(B)$;
 compute the SVD of C : $U^T C V = \text{diag}(\sigma_1, \sigma_2)$;
 form the products $G = U^T A$, $H = V^T B$;
 if A is nonzero, then
 determine Q to zero out (1, 2) entry of G ;
 else
 determine Q to zero out (1, 2) entry of H ;
 end if
 $\tilde{A} = G Q$, $\tilde{B} = H Q$, $\tilde{a}_{12} = 0$; $\tilde{b}_{12} = 0$;

Again, from [28, 4], at the end of the second sweep, we have $A_2 = U_2^T A_1 Q_2$ and $B_2 = V_2^T B_1 Q_2$, such that

$$A_2 = \begin{matrix} r_1 & r_2 & n-r \\ r_1 & r_2 & n-r \\ n-r & & \end{matrix} \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A_{22} & A_{23} \\ 0 & 0 & 0 \end{pmatrix}, \quad B_2 = \begin{matrix} r_1 & r_2 & n-r \\ r_1 & r_2 & n-r \\ n-r & & \end{matrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & B_{22} & B_{23} \\ 0 & 0 & B_{33} \end{pmatrix}, \quad (3.3)$$

where A_{11} , A_{22} , B_{22} and B_{33} are upper triangular matrices and nonsingular, $r_1 + r_2 = r$. Hence there is a unique $(n - r_1) \times (n - r_1)$ upper triangular matrix T such that

$$\begin{pmatrix} A_{22} & A_{23} \\ 0 & 0 \end{pmatrix} = T \begin{pmatrix} B_{22} & B_{23} \\ 0 & B_{33} \end{pmatrix}.$$

This implies that the rest of computation is essentially equivalent to computing the SVD of the implicitly defined matrix T . By the global convergence theory of the cyclic Kogbetliantz algorithm

(see § 2.1), we have

$$T \rightarrow \Sigma, \tag{3.4}$$

where Σ is a diagonal matrix, and the convergence is ultimately quadratic, provided the rotation angles of U and V obey (2.1). (3.4) implies that there exists diagonal matrices Σ_1 and Σ_2 with $\Sigma_1^2 + \Sigma_2^2 = I$, and an upper triangular matrix R , such that

$$A_2 \rightarrow \Sigma_1 R \quad \text{and} \quad B_2 \rightarrow \Sigma_2 R,$$

which gives the desired GSVD of A and B .

3.2 The 2×2 GSVD in Floating Point Arithmetic

In this section, we will use the usual model of floating point arithmetic: barring over/underflow $\text{fl}(x \circ y) = (1 + \delta)(x \circ y)$ where \circ is one of the basic operations $\{+, -, \times, \div\}$ and $|\delta| \leq \epsilon$ where ϵ is the machine roundoff. This model eliminates machines like Crays without guard digits, but with some effort all the results can be extended to these machines as well.

When using floating point arithmetic, roundoff can cause the rowvectors of \tilde{A} and \tilde{B} computed by Algorithm 1 not to be parallel. This means \tilde{A} and \tilde{B} are not the GSVD of the 2×2 matrices A and B , or in short, the algorithm is not convergent. Another possibility is that the computation may not be backward stable, because the entries \tilde{a}_{12} or \tilde{b}_{12} (\tilde{a}_{21} or \tilde{b}_{21}) which are explicitly set to zero by Algorithm 1 may be much larger than $O(\epsilon)\|A\|$ and $O(\epsilon)\|B\|$, respectively.⁶ Thus, the algorithms in [28, 20, 4], which use the SVD of 2 by 2 triangular matrix to guarantee convergence, are potentially numerical unstable. On the other hand, to guarantee numerical stability, it is suggested in [18, 6] that after computing the SVD of the 2×2 triangular matrix C , one uses U (say) to form $G = U^T A$, then determines Q such that GQ is lower triangular, and finally determines \tilde{V} such that $\tilde{V}^T BQ$ is also lower triangular. However, in practice, $U^T C \tilde{V}$ might not be diagonal, which results in divergence. In § 5, we will present numerical examples illustrating the failures of these schemes. In this section, we propose a new algorithm to overcome these shortcomings. We first discuss the two fundamental algorithmic building blocks: SLASV2 and SLARCG.

SLASV2 computes the SVD of a 2×2 upper triangular matrix

$$\begin{pmatrix} c_u & s_u \\ -s_u & c_u \end{pmatrix} \begin{pmatrix} f & g \\ 0 & h \end{pmatrix} \begin{pmatrix} c_v & -s_v \\ s_v & c_v \end{pmatrix} = \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix}.$$

Barring over/underflow SLASV2 computes all of $c_u, s_u, c_v, s_v, \sigma_1$ and σ_2 to nearly full machine precision. This algorithm was described briefly in [10], but not published in its entirety. For completeness, we include a listing of Fortran code in the appendix, and a statement and proof sketch of its error analysis. As discussed in [10], the high accuracy of SLASV2 is based on the fact that the algorithm uses formulas that only contain products, quotients, square roots, sums of terms of like sign, differences of computed quantities only when cancellation is impossible, and the difference $|f| - |h|$ of the input data, which, if cancellation occurs, is exact.⁷

SLARCG(f, g, c, s, r) generates a rotation matrix $\text{rot}(c, s)$ from f and g to zero g , i.e., $c = f/r$ and $s = g/r$, $r = \sqrt{f^2 + g^2}$, but this is subject to spurious over/underflow if we directly compute them from these formulas. A more robust way to compute c, s and r can be found in [17]:

⁶Throughout, $\|\cdot\|$ will denote the matrix 2-norm.

⁷This exact cancellation property, which is essential for the accuracy claim of SLASV2, requires a guard digit and so fails on machines like the Cray. On a Cray we retain backward stability of SLASV2, but lose forward stability. Since the proof uses forward stability of SLASV2 in an important way, it does not apply to Cray. However, there is a more complicated proof which does work on the Cray. The reader is invited to try to find it.

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(handle  $f = 0$  and  $g = 0$  as special cases)
if  $|f| > |g|$  then
     $t = g/f$ ;  $tt = \sqrt{1+tt^2}$ ;  $c = 1/tt$ ;  $s = t * c$ ;  $r = f * tt$ 
else
     $t = f/g$ ;  $tt = \sqrt{1+tt^2}$ ;  $s = 1/tt$ ;  $c = t * s$ ;  $r = g * tt$ ;
endif

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The same techniques used to analyze SLASV2 in the appendix can be straightforwardly used to show that the relative error in the computed c and s is bounded by 6ϵ .

Using SLARTG and SLASV2, we present a high-level description of an algorithm for computing the 2 by 2 GSVD. Later we will show that the proposed algorithm guarantees numerical stability and convergence. We will use the notation $|X| = (|x_{ij}|)$.

Algorithm GSVD22: Let A and B be 2×2 upper triangular matrices. The following algorithm computes the orthogonal matrices $U = \text{rot}(c_u, s_u)$, $V = \text{rot}(c_v, s_v)$ and $Q = \text{rot}(c_q, s_q)$, such that

$$\tilde{A} = U^T A Q = \begin{pmatrix} \tilde{a}_{11} & 0 \\ \tilde{a}_{21} & \tilde{a}_{22} \end{pmatrix}, \quad \tilde{B} = V^T B Q = \begin{pmatrix} \tilde{b}_{11} & 0 \\ \tilde{b}_{21} & \tilde{b}_{22} \end{pmatrix}$$

are the GSVD of A and B . For brevity, we omit the part for lower triangular matrices, which can be described similarly.

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compute  $C = A \text{adj}(B)$ ;
use SLASV2 to compute the SVD of  $C$ :  $U^T C V = \Sigma$ ;
compute  $G = U^T A$ ,  $H = V^T B$ ;
compute  $\hat{G} = |U^T| A$ ;  $\hat{H} = |V^T| B$ ;
/* The angles of  $U$  and  $V$  are chosen to satisfy the convergence condition (3.4). */
if  $|u_1| \geq |u_2|$  or  $|v_1| \geq |v_2|$  then
    /* Choose  $Q$  to zero out (1, 2) entries of  $U^T A$  and  $V^T B$  */
    if  $g_{12}/(|g_1| + |g_2|) \leq h_{12}/(|h_1| + |h_2|)$  then
        call SLARTG( $-g_{11}, g_{12}, c_q, s_q, r$ ) /* Compute  $Q$  from  $U^T A$  */
    else
        call SLARTG( $-h_{11}, h_{12}, c_q, s_q, r$ ) /* Compute  $Q$  from  $V^T B$  */
    end if
     $\tilde{A} = GQ$ ,  $\tilde{B} = HQ$ ,  $\tilde{a}_{12} = 0$ ,  $\tilde{b}_{12} = 0$ .
else
    /* Choose  $Q$  to zero out (2, 2) entries of  $U^T A$  and  $V^T B$  and then swap rows. */
    if  $g_{22}/(|g_1| + |g_2|) \leq h_{22}/(|h_1| + |h_2|)$  then
        call SLARTG( $-g_{21}, g_{22}, c_q, s_q, r$ ) /* Compute  $Q$  from  $U^T A$  */
    else
        call SLARTG( $-h_{21}, h_{22}, c_q, s_q, r$ ) /* Compute  $Q$  from  $V^T B$  */
    end if
     $\tilde{A} = GQ$ ,  $\tilde{B} = HQ$ ,  $\tilde{a}_{22} = 0$ ,  $\tilde{b}_{22} = 0$ .
    /* Swap, where  $P = \text{rot}(0, 1)$  */
     $\tilde{A} \leftarrow P\tilde{A}$ ;  $\tilde{B} \leftarrow P\tilde{B}$ ;
     $U \leftarrow UP$ ;  $V \leftarrow VP$ ;
end if

```

We now present a theorem about the stability and convergence of the above algorithm. Quantities with bars (like \tilde{C}) denote actual computed quantities.

Theorem 2 The \tilde{A} and \tilde{B} computed by Algorithm GSVD22 have the following properties.

- (a) Both are triangular;
- (b) $\bar{U}^T \bar{C} \bar{V}$ is within 132ϵ of being diagonal.
- (c) The rows of \tilde{A} and \tilde{B} are within 87ϵ of being parallel.
- (d) They are computed stably, i.e., there exist δA and δB , where $\|\delta A\| \leq 377\epsilon \|A\|$ and $\|\delta B\| \leq 377\epsilon \|B\|$, and orthogonal U, V and Q such that

$$\tilde{A} = U^T (A + \delta A) Q, \quad \tilde{B} = V^T (B + \delta B) Q.$$

Proof. We only prove a branch of the algorithm where Q is computed from $U^T A$ and used to zero out the (1,2) entries of $U^T A$ and $V^T B$; the proof for the other cases is similar. We will also leave some of the more tedious details of error analysis to the ambitious reader.

We first note the following facts about the algorithm

Fact 1 $\bar{C} = (A + \delta A)^{-1} \cdot \text{adj}(B + \delta B)$ where δA and δB are small componentwise relative perturbations of A and B .

$$\bar{C} = \begin{bmatrix} a_{11} b_{22} (1 + \epsilon_1) & -a_{11} b_{12} (1 + 2\epsilon_2) + a_{12} b_{11} (1 + 2\epsilon_3) \\ 0 & a_{22} b_{11} (1 + \epsilon_4) \end{bmatrix} = \begin{bmatrix} a'_{11} b_{22} & -a'_{11} b'_{12} + a'_{12} b'_{11} \\ 0 & a_{22} b'_{11} \end{bmatrix}$$

where $a'_{11} = a_{11} (1 + \epsilon_1)$, $b'_{11} = b_{11} (1 + \epsilon_4)$, $a'_{12} = a_{12} (1 + 2\epsilon_3) / (1 + \epsilon_4)$ and $b'_{12} = b_{12} (1 + 2\epsilon_2) / (1 + \epsilon_1)$. (The ϵ_i are independent quantities bounded in magnitude by the machine precision ϵ .) So there is at most a 3 ulp perturbation in any entry, and also $\|\delta A\| \leq 4\epsilon \|A\|$ and $\|\delta B\| \leq 4\epsilon \|B\|$.

Fact 2 The computed \bar{U} and \bar{V} from SLAS2 satisfy $\bar{U} = U + \delta U$, $\bar{V} = V + \delta V$, where $U^T \bar{C} \bar{V}$ is the exact SVD of \bar{C} and δU (δV) is a small componentwise relative perturbation of U (V), bounded by 46.5ϵ in each component (see the proposition in the appendix). This also implies $\|\delta U\| \leq \sqrt{2} \cdot 46.5\epsilon < 66\epsilon$ and $\|\delta V\| < 66\epsilon$.

Fact 3 The error in the \bar{g}_{ij} (\bar{h}_{ij}) is bounded by $48.5\epsilon \bar{g}_{ij}$ ($48.5\epsilon \bar{h}_{ij}$). In the factor 48.5, 2 comes from the roundoff in computing $\text{fl}(U^T A)$ or $\text{fl}(V^T B)$, and 46.5 comes from the errors in U and V .

Fact 4 Using simple geometry, one can show that changing f to $f + \delta f$ and g to $g + \delta g$ can change $c = f / \sqrt{f^2 + g^2}$ and $s = g / \sqrt{f^2 + g^2}$ to $c + \delta c$ and $s + \delta s$, respectively, where $\sqrt{\delta c^2 + \delta s^2} \leq 2((\delta f^2 + \delta g^2) / (f^2 + g^2))^{1/2}$.

Fact 5 Subroutine SLARC computes $c = f / \sqrt{f^2 + g^2}$ and $s = g / \sqrt{f^2 + g^2}$ with relative errors bounded by 6ϵ . This means the 2 by 2 matrix $\text{rot}(c, s)$ has an error bounded in norm by $\sqrt{2} \cdot 6\epsilon < 9\epsilon$.

Fact 6 If X and Y are 2-by-2 matrices, then $\|\text{fl}(X \cdot Y) - X \cdot Y\| \leq 4 \cdot \epsilon \cdot \|X\| \cdot \|Y\|$.

We note that triangularity (a) holds by construction. We prove (b) as follows. Near diagonality of $\bar{U}^T \bar{C} \bar{V}$ holds by the high accuracy of \bar{U} and \bar{V} :

$$\bar{U}^T \bar{C} \bar{V} = (U + \delta U)^T \bar{C} (V + \delta V) = U^T \bar{C} V + F_1$$

where Fact 2 tells us that to first order in ϵ

$$\|F_1\| \leq \|\delta \bar{U}^T \bar{C} \bar{V}\| + \|U^T \bar{C} \delta V^T\| \leq 66\epsilon \|\bar{C}\| + 66\epsilon \|\bar{C}\| = 132\epsilon \|\bar{C}\|.$$

Next we prove assertion (c). The top rows of \tilde{A} and \tilde{B} are trivially parallel by construction (their second components are zero), so we only consider the bottom rows. Likewise by construction that the bottom rows of $U^T(A+\delta A_1)$ and $V^T(B+\delta B_1)$ are parallel. Thus the bottom rows of

$$\bar{G} = \text{fl}(\bar{U}^T A) = \bar{U}^T A + F_2 = (U^T + \delta U^T)(A + \delta A_1) + F_2 = U^T(A + \delta A_1) + F_3$$

and $\bar{H} = V^T(B + \delta B_1) + F_4$ are within $\|F_3\| \leq 74\epsilon\|A\|$ and $\|F_4\| \leq 74\epsilon\|B\|$, respectively, of being parallel. Here we have used Facts 1, 2 and 6.

So for any $\bar{Q} = Q + \delta Q$ that is within 9ϵ in norm of an orthogonal matrix Q , the bottom rows of \tilde{A} and \tilde{B} are the same as the bottom rows of

$$\text{fl}(\bar{G}\bar{Q}) = \bar{G}\bar{Q} + F_5 = (U^T(A + \delta A_1) + F_3)(Q + \delta Q) + F_5 = U^T(A + \delta A_1)Q + F_6$$

and $\text{fl}(\bar{H}\bar{Q}) = V^T(B + \delta B_1)Q + F_7$, which are within $\|F_6\| \leq 87\epsilon\|A\|$ and $\|F_7\| \leq 87\epsilon\|B\|$ of being parallel; we have used our bounds on $\|F_3\|$ and $\|F_4\|$, and Facts 5 and 6. This proves assertion (c).

Let $\eta_a = \tilde{g}_{12}\epsilon / (|g_{11}| + |g_{12}|)$, and $\eta_b = \tilde{h}_{12}\epsilon / (|\bar{h}_{11}| + |\bar{h}_{12}|)$. Then η_a (η_b) is an approximate bound on relative error of Q if it is computed from $U^T A$ ($V^T B$). In the branch of the algorithm we consider, $\eta_a \leq \eta_b$, and the algorithm chooses to compute Q from $U^T A$. The remarkable fact is that even if $\epsilon \ll \eta_a$, so that the forward error in Q is large, the backward error in B is small.

To finally prove this assertion (d), we need to show the (1,2) entry of $\text{fl}(\bar{H}\bar{Q})$, which is zeroed out to get \tilde{B} , is at most $286\epsilon\|B\|$. (Q is chosen to accurately zero out the (1,2) entry of $\text{fl}(\bar{G}\bar{Q})$.) Earlier we showed that $\bar{h}_{11} = h_{11} + 74\epsilon\|B\|$ and $\bar{h}_{12} = h_{12} + 74\epsilon\|B\|$, where h_{11} and h_{12} are the exact entries of $V^T(B + \delta B_1)$. Now write $c_q = c_q + \delta c_q$ and $s_q = s_q + \delta s_q$, where c_q and s_q are the exact cosine and sine computed from $U^T(A + \delta A_1)$. Then

$$\begin{aligned} |\text{fl}(\bar{H}\bar{Q})_{12}| &= |(h_{11} + 76\epsilon\|B\|)(s_q + \delta s_q) + (h_{12} + 76\epsilon\|B\|)(c_q + \delta c_q)| \\ &= |(h_{11}s_q + h_{12}c_q) + (h_{11}\delta s_q + h_{12}\delta c_q) + \sqrt{2} \cdot 76\epsilon\|B|| \\ &\leq (|h_{11}| + |h_{12}|)(|s_q| + |c_q|) + 108\epsilon\|B| \end{aligned} \quad (3.5)$$

There are two cases, $\eta_a < \epsilon$ and $\eta_a \geq \epsilon$. In the first case, we will show δs_q and δc_q are both bounded by 175ϵ , and so $|\text{fl}(\bar{H}\bar{Q})_{12}| \leq 286\epsilon$. To see this, use Fact 3 to write

$$(48.5\epsilon\bar{g}_{11})^2 + (48.5\epsilon\bar{g}_{12})^2 = (48.5\epsilon^{-1}g_{11})^2 + (48.5\epsilon\bar{g}_{12})^2 \leq (48.5\epsilon)^2(\bar{g}_{11}^2 + (|\bar{g}_{11}| + |g_{12}|)^2)$$

so by Facts 4 and 5, $\sqrt{|\delta s_q|^2 + |\delta c_q|^2}$ can be at most

$$9\epsilon + 2 \cdot 48.5\epsilon \left(\frac{\bar{g}_{11}^2 + (|\bar{g}_{11}| + |\bar{g}_{12}|)^2}{\bar{g}_{11}^2 + g_{12}^2} \right)^{1/2} \leq 178\epsilon.$$

Now we use this bound in inequality (3.5) to get $|\text{fl}(\bar{H}\bar{Q})_{12}| \leq 286\epsilon$ as desired.

In the second case, we bound $\sqrt{|\delta s_q|^2 + |\delta c_q|^2}$ by

$$9\epsilon + 2 \left(\frac{48.5^2((\epsilon\bar{g}_{11})^2 + (\eta_a(|g_{11}| + |g_{12}|)^2))}{\bar{g}_{11}^2 + g_{12}^2} \right)^{1/2} \leq 178\eta_a.$$

Plugging in to inequality (3.5) and using

$$|\bar{h}_{11}| + |\bar{h}_{12}| = \frac{\epsilon\tilde{h}_{12}}{\eta_b} \leq \frac{\epsilon\|B\|}{\eta_b}$$

yields the upper bound

$$|\mathfrak{f}(\bar{H}\bar{Q})_{12}| \leq (|k_1| + |k_2|) \cdot (178\eta + 108\epsilon) \|B\| \leq \frac{\epsilon \|B\|}{\eta_b} \cdot (178\eta_a + 108\epsilon) \|B\| = 286\epsilon \|B\|$$

as before, since $\eta_b \geq \eta_a$.

This means that we can write the final output

$$\tilde{B} = V^T (B + \delta B_1) Q + F_7 + F_8 = V^T (B + \delta B_1 + V F_7 Q^T + V F_8 Q^T) Q \equiv V^T (B + \delta B) Q$$

where F_8 zeroes out the (1,2) entry of \tilde{B} and leaves the others unchanged. We just showed $\|F_8\| \leq 286\epsilon \|B\|$ and combining this with our earlier bounds of $\|F_7\| \leq 87\epsilon \|B\|$ and $\|\delta B_1\| \leq 4\epsilon \|B\|$ yields the final result $\|\delta B\| \leq 377\epsilon \|B\|$. We can similarly show that $\tilde{A} = U^T (A + \delta A) Q$ with $\|\delta A\| \leq 107\epsilon \|A\|$, using the fact that Q is computed to directly zero out the (1,2) entry of \tilde{A} . This completes the proof of assertion (d). ■

The constants in these error bounds could doubtless be decreased by a more detailed analysis.

4 Summary of the Complete Algorithm

In this section, we present a high-level description of our version of Paige's algorithm for computing the GSVD of two upper triangular matrices A and B of the form (1.5). Let κ be a user chosen parameter specifying the maximum number of cycles the algorithm may perform (say, $\kappa = 20$). Let P_{ij} be the identity matrix with rows i and j interchanged.

Algorithm GSVD

```

/* Initialization */
cycle := 0;
ξ := r + q + 1; /* r and q are defined in (1.5) */
U := I; V := I; Q := I if desired;
/* Main loop */
if nonconvergence and cycle ≤ κ do
  cycle := cycle + 1;
  do (i, j)-loop
    /* 2 × 2 GSVD */
    Use GSVD22 to find Uij, Vij, Qij from aii, ajj and bii, bjj;
    /* Updating */
    A := UijT A Qij;
    B := VijT B Qij;
    U := U Uij; V := V Vij; Q := Q Qij if desired;
    /* reordering */
    if the (j, j) entry of B is nonzero, where j > l, then
      A := A Pξj;
      B := Pξj B Pξj;
      V := V Vξj; Q := Q Pξj if desired;
      ξ := ξ + 1;
    end if
  end of (i, j)-loop
  convergence test if cycle is even
end if
compute αi and βi.

```

The (i, j) -loop can be simply chosen as the standard cyclic pivot sequence. It is natural to use the parallelism (linear dependency) of the corresponding row vectors of A and B at the end of an even cycle as the stopping criterion of the iteration. To measure the parallelism of two k -vectors a and b to high accuracy and despite possible over/underflow we propose the following scheme: first compute the QR factorization of the $k \times 2$ matrix $\begin{pmatrix} a & b \\ \|a\| & \|b\| \end{pmatrix}$:

$$Q^T \begin{pmatrix} a & b \\ \|a\| & \|b\| \end{pmatrix} = \begin{pmatrix} \mu_{11} & \mu_{12} \\ 0 & \mu_{22} \\ 0 & 0 \end{pmatrix},$$

and then compute the singular values $\gamma_1 \geq \gamma_2 \geq 0$ of the 2×2 upper triangular (μ_{ij}) . It is clear that

$$\text{par} \left(\frac{a}{\|a\|}, \frac{b}{\|b\|} \right) \equiv \gamma_2$$

measures the parallelism of these two vectors. Vectors a and b are exactly parallel iff $\gamma_2 = 0$.

Using the above described scheme as the stopping criterion in Algorithm SVD let a_i and b_i be the i -th row vectors of A and B , respectively, at the end of an even cycle. For a given tolerance value τ , we take

$$\text{error} = \sum_{i=1}^n \text{par} \left(\frac{a_i}{\|a_i\|}, \frac{b_i}{\|b_i\|} \right) \leq n\tau.$$

This means that there are perturbations of size at most $n\tau \|a_i\|$ in row a_i and $n\tau \|b_i\|$ in row b_i that makes them exactly parallel. This means that after making these perturbations, there would exist scalars α_i and β_i such that

$$\beta_i a_i = \alpha_i b_i, \quad i = 1, \dots, n, \tag{4.1}$$

where α_i and β_i can be chosen so that $\alpha_i^2 + \beta_i^2 = 1$. From (4.1), it is seen that there is an upper triangular matrix R , such that

$$U^T A Q = \text{diag} (\alpha_i) R, \quad V^T B Q = \text{diag} (\beta_i) R$$

which is the desired GSVD of matrices A and B , where α_i and β_i are the GSVPairs.

5 Numerical Experiments

The numerical experiments we discuss here first compare Algorithm SVD2 with previous algorithms developed by Paige [28], Heath et al [20], Bi [4], Hammarling [18] and Bjanczyk *et al* [6]. Then we will evaluate Algorithm SVD for different cases of random matrices A and B , measuring the backward stability, accuracy, average total number of sweeps, rate of convergence, elapsed time when computing GSVPairs only, or both GSVPairs and transformation matrices.

All tests were performed using FORTRAN 77 on a SUN sparc station 4+. The arithmetic was IEEE standard double precision [1], with a machine precision of $\epsilon = 2^{-53} \approx 10^{-16}$ and over/underflow threshold $10^{\pm 307}$. We use $\tau = 10^{-14}$ as the stopping criterion.

5.1 Backward Stability and Accuracy

Before we proceed, it is appropriate to state what we mean by the *backward stability* and the *accuracy* of Algorithm SVD. The backward stability is defined as follows: Let the computed orthogonal matrices be \bar{U} , \bar{V} and \bar{Q} , the diagonal matrices be $\bar{\Sigma}_1$ and $\bar{\Sigma}_2$, and the upper triangular matrix be \bar{R} . Then the following conditions should be satisfied:

$$\|\bar{U}^T \bar{U} - I\|_F \approx \epsilon; \quad \|\bar{V}^T \bar{V} - I\|_F \approx \epsilon; \quad \|\bar{Q}^T \bar{Q} - I\|_F \approx \epsilon; \tag{5.1}$$

$$\|\bar{U}^T A \bar{Q} - \bar{\Sigma}_1 \bar{R}\|_F \approx n\epsilon \|A\|_F; \quad \|\bar{V}^T B \bar{Q} - \bar{\Sigma}_2 \bar{R}\|_F \approx n\epsilon \|B\|_F, \quad (5.2)$$

where $\|\cdot\|_F$ is Frobenius norm. These assertions say that to within roundoff error, the computed matrices \bar{U} , \bar{V} and \bar{Q} are orthogonal, and the rows of $\bar{U}^T A \bar{Q}$ and $\bar{V}^T B \bar{Q}$ are parallel.

The accuracy test of computed GSV pairs by Algorithm GSVD is based on Sun and Paige's perturbation bound of the GSV pairs [32, 26], which says that: if $\text{rank}(G) = \text{rank}(\tilde{G}) = n$, where $G = (A^T, B^T)^T$, and $\tilde{G} = (\tilde{A}^T, \tilde{B}^T)^T = ((A+E)^T, (B+F)^T)^T$, and the GSV pairs (α_i, β_i) of A and B , and $(\tilde{\alpha}_i, \tilde{\beta}_i)$ of \tilde{A} and \tilde{B} are ordered as in (1.4), respectively, then we have

$$\sqrt{\sum_{i=1}^n [(\alpha_i - \tilde{\alpha}_i)^2 + (\beta_i - \tilde{\beta}_i)^2]} \leq \sqrt{2} \min\{\|G^\dagger\|_2, \|\tilde{G}^\dagger\|_2\} \left\| \begin{pmatrix} E \\ F \end{pmatrix} \right\|_F. \quad (5.3)$$

If we generate the matrices A and B with known GSV pairs, then the above perturbation bound can be used to measure the accuracy of the computed GSV pairs.

5.2 The numerical comparison of different 2×2 GSVD algorithms

Several versions have been proposed for computing the 2 by 2 GSVD. There are essentially two kinds of schemes:

Schem I: First compute the SVD of $C = A \cdot \text{adj}(B)$: $U^T C V = \Sigma$, then form the product of $G = U^T A$ and $H = V^T B$, and finally compute Q from G such that the (1,2) or (2,1) entry of GQ is zero. Mathematically, it is known that the (1,2) or (2,1) entry of HQ is automatically zero. The algorithms proposed by Paige [28], Heath *et al* [20], and Bi [4] fall in this category.

Schem II: First compute the SVD of $C = A \cdot \text{adj}(B)$: $U^T C V = \Sigma$, form the product of $G = U^T A$, compute Q so such the (1,2) or (2,1) entry of GQ is zero, and finally compute V to zero out the (1,2) or (2,1) entry of BQ . The algorithms proposed by Hammarling [18] and Björnczyk *et al* [6] fall in this category.

To demonstrate the failure of the first kind of scheme, the following example shows that in finite precision, the (1,2) or (2,1) entry of the final B may be much larger than $O(\epsilon)\|B\|$:

$$A = \begin{pmatrix} 2 & 0 \\ 1 & 10^{-8} \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 \\ 3 & 1 \end{pmatrix}.$$

With the scheme described by Paige [28], Heath *et al* [20] and Bi [4], for the computed \bar{U} , \bar{V} and \bar{Q} , we have

$$\begin{aligned} \bar{U}^T A \bar{Q} &= \begin{pmatrix} \bar{a}_1 \\ \bar{a}_2 \end{pmatrix} = \begin{pmatrix} 0.707106775090009934\text{E}+00 & 0.21213203455917919\text{E}+01 \\ 0.0000000000000000\text{E}+00 & 0.28284271491319831\text{E}-07 \end{pmatrix}, \\ \bar{V}^T B \bar{Q} &= \begin{pmatrix} \bar{b}_1 \\ \bar{b}_2 \end{pmatrix} = \begin{pmatrix} 0.31622776518779000\text{E}+00 & 0.94868330465141837\text{E}+00 \\ -0.33959487444334968\text{E}-08 & 0.31622776582710133\text{E}+01 \end{pmatrix}. \end{aligned}$$

If we now set the (2,1) entry of $\bar{B} = \bar{V}^T B \bar{Q}$ to zero, the backward stability condition (5.2) is violated for matrix B , even though

$$\bar{U}^T C \bar{V} = \begin{pmatrix} 0.22360679640833827\text{E}+01 & 0.0000000000000000\text{E}+00 \\ 0.17888543605335784\text{E}-16 & 0.89442719636647925\text{E}-08 \end{pmatrix}.$$

To show how Schem II can fail for the same example, using Hammarling's method [18], we have

$$\begin{aligned} \bar{U}^T A \bar{Q} &= \begin{pmatrix} \bar{a}_1 \\ \bar{a}_2 \end{pmatrix} = \begin{pmatrix} 0.707106775090009934\text{E}+00 & 0.21213203455917919\text{E}+01 \\ 0.0000000000000000\text{E}+00 & 0.28284271491319831\text{E}-07 \end{pmatrix}, \\ \bar{V}^T B \bar{Q} &= \begin{pmatrix} \bar{b}_1 \\ \bar{b}_2 \end{pmatrix} = \begin{pmatrix} -0.31622776518778994\text{E}+00 & -0.94868327069193081\text{E}+00 \\ 0.11102230246251565\text{E}-15 & -0.31622776684588585\text{E}+01 \end{pmatrix}. \end{aligned}$$

Thus the stability is achieved, but for the computed \bar{U} and \bar{V} , we have

$$\bar{U}^T C \bar{V} = \begin{pmatrix} -0.22360679640833823\text{E}+01 & -0.24012983681642603\text{E}-07 \\ 0.78163392273857838\text{E}-16 & -0.89442719636647908\text{E}-08 \end{pmatrix}$$

which is not within $O(\epsilon)\|C\|$ of diagonal form. This means that the computed $\bar{A} = \bar{U}^T A \bar{Q}$ and $\bar{B} = \bar{V}^T B \bar{Q}$ are not the SVD of A and B . In fact, $\text{par} \left(\frac{\bar{a}_1}{\|\bar{A}\|}, \frac{\bar{b}_1}{\|\bar{B}\|} \right) \approx \text{par} \left(\frac{\bar{a}_1}{\|\bar{a}_1\|}, \frac{\bar{b}_1}{\|\bar{b}_1\|} \right) \approx 7.59 \times 10^{-9}$.
 But using Algorithm GSVD2 in § 3.2, we have

$$\begin{aligned} \bar{U}^T A \bar{Q} &= \begin{pmatrix} \bar{a}_1 \\ \bar{a}_2 \end{pmatrix} = \begin{pmatrix} 0.70710677736817096\text{E}+00 & 0.21213203448324349\text{E}+01 \\ 0.30374288814267665\text{E}-16 & 0.28284271491319831\text{E}-07 \end{pmatrix}, \\ \bar{V}^T B \bar{Q} &= \begin{pmatrix} \bar{b}_1 \\ \bar{b}_2 \end{pmatrix} = \begin{pmatrix} 0.31622776620657461\text{E}+00 & 0.94868330431182346\text{E}+00 \\ 0.000000000000000\text{E}+00 & 0.31622776582710133\text{E}+01 \end{pmatrix}, \end{aligned}$$

and

$$\bar{U}^T C \bar{V} = \begin{pmatrix} 0.22360679640833827\text{E}+01 & 0.000000000000000\text{E}+00 \\ 0.17888543605335784\text{E}-16 & 0.89442719636647925\text{E}-08 \end{pmatrix}.$$

Thus both stability and convergence conditions are satisfied, where $\text{par} \left(\frac{\bar{a}_1}{\|\bar{A}\|}, \frac{\bar{b}_1}{\|\bar{B}\|} \right) \approx \text{par} \left(\frac{\bar{a}_1}{\|\bar{a}_1\|}, \frac{\bar{b}_1}{\|\bar{b}_1\|} \right) \approx 7.02 \times 10^{-17}$.

Recently, Bjanczyk *et al* [6] proposed a variation of Scheme II, which we refer to as the **HEV** schema. The **HEV** schema was originally designed for treating a matrix triple (A, A_1, A_2, A_3) . It is easy to see that the 2×2 SVD of two matrices is a special case when one of the matrices (say, A_3 is the identity). The **HEV** schema does significantly improve Hammarling's method, but it still suffers from possible nonconvergence. For example, using the **HEV** schema, we see that for the following 2×2 matrices

$$A = \begin{pmatrix} 100000 & 10000 \\ 0 & 0.0001 \end{pmatrix}; \quad B = \begin{pmatrix} 100000 & 10000.0000000001 \\ 0 & 0.003 \end{pmatrix},$$

the computed orthogonal matrices \bar{U} , \bar{V} and \bar{Q} by **HEV** schema satisfy the stability conditions (5.1) and (5.2):

$$\begin{aligned} \bar{U}^T A \bar{Q} &= \begin{pmatrix} \bar{a}_1 \\ \bar{a}_2 \end{pmatrix} = \begin{pmatrix} 0.99503719020998935\text{E}-04 & -0.12189168086858831\text{E}-03 \\ 0.000000000000000\text{E}+00 & 0.10049875621120891\text{E}+06 \end{pmatrix} \\ \bar{V}^T B \bar{Q} &= \begin{pmatrix} \bar{b}_1 \\ \bar{b}_2 \end{pmatrix} = \begin{pmatrix} 0.29851115706299699\text{E}-02 & -0.36499576550546638\text{E}-02 \\ 0.000000000000000\text{E}+00 & 0.10049875621120886\text{E}+06 \end{pmatrix} \end{aligned}$$

However, the computed \bar{U} and \bar{V} do not diagonalize the matrix C :

$$\bar{U}^T C \bar{V} = \begin{pmatrix} 0.9999999999999964\text{E}+01 & -0.67590597725531451\text{E}-09 \\ 0.20277179317658482\text{E}-07 & 0.300000000000023\text{E}+03 \end{pmatrix},$$

since the off-diagonal elements are much larger⁸ than $O(\epsilon)\|C\| \approx 10^{-14}$, $\text{par} \left(\frac{\bar{a}_1}{\|\bar{A}\|}, \frac{\bar{b}_1}{\|\bar{B}\|} \right) = 6.44 \times 10^{-4}$, and even $\text{par} \left(\frac{\bar{a}_1}{\|\bar{a}_1\|}, \frac{\bar{b}_1}{\|\bar{b}_1\|} \right) = 1.43 \times 10^{-12}$, so that the first rows of \bar{A} and \bar{B} are not parallel.

⁸In [6] it is proven that the off-diagonal elements should be $O(\epsilon)\|A\|\|B\| \approx 10^{-6}$, which is attained. Since $\|C\| = \|A \text{adj}(B)\| \ll \|A\|\|B\|$, our bound is much tighter.

But Algorithm(SVD2) yields

$$\begin{aligned} \bar{U}^T A \bar{Q} &= \begin{pmatrix} \bar{a}_1 \\ \bar{a}_2 \end{pmatrix} = \begin{pmatrix} -0.10049875621120894E+06 & 0.0000000000000000E+00 \\ -0.12189168086858835E-03 & -0.99503719020998963E-04 \end{pmatrix} \\ \bar{V}^T B \bar{Q} &= \begin{pmatrix} \bar{b}_1 \\ \bar{b}_2 \end{pmatrix} = \begin{pmatrix} -0.10049875621120886E+06 & -0.18189894035458565E-11 \\ -0.36567504260576521E-02 & -0.29851115706299099E-02 \end{pmatrix} \end{aligned}$$

and

$$\bar{U}^T C \bar{V} = \begin{pmatrix} 0.3000000000000028E+03 & 0.16940658945086007E-20 \\ 0.0000000000000000E+00 & 0.999999999999982E+01 \end{pmatrix}$$

with $\text{par} \left(\frac{\bar{a}_1}{\|\bar{A}\|}, \frac{\bar{b}_1}{\|\bar{B}\|} \right) = \text{par} \left(\frac{\bar{a}_1}{\|\bar{a}_1\|}, \frac{\bar{b}_1}{\|\bar{b}_1\|} \right) = 0$, and $\text{par} \left(\frac{\bar{a}_2}{\|\bar{A}\|}, \frac{\bar{b}_2}{\|\bar{B}\|} \right) < \text{par} \left(\frac{\bar{a}_2}{\|\bar{a}_2\|}, \frac{\bar{b}_2}{\|\bar{b}_2\|} \right) = 1.72 \times 10^{-16}$.

The above examples show that Algorithm(SVD2) is superior to all previous schemes.

5.3 Test matrix generation for testing backward stability

To test the backward stability of Algorithm(SVD) we used the LAPACK test matrix generation suite [11] to generate different types of upper triangular matrices A and B . The conditioning of a generated upper triangular matrix can be controlled by the following parameters:

dist specifies the type of probability distribution to be used to generate the random matrices:

- =U uniform distribution on (0, 1);
- =S uniform distribution on (-1, 1);
- =N normal distribution on (0, 1).

cond specifies the reciprocal of the condition number of generated matrix, $\text{cond} \geq 1$.

mode describes how the singular values d_i of generated matrix are to be distributed:

- =1: sets $d_{i-1} = 1$ and $d_i = 1/\text{cond}$, $i = 2, \dots, n$;
- =2: sets $d_i = 1$, $i = 1, \dots, n-1$ and $d_n = 1/\text{cond}$;
- =3: sets $d_i = \text{cond}^{-(i-1)/(n-1)}$, $i = 1, \dots, n$;
- =4: sets $d_i = 1 - \frac{i-1}{n-1} \left(1 - \frac{1}{\text{cond}} \right)$, $i = 1, \dots, n$;
- =5: sets d_i to random in ($1/\text{cond}$, 1), their logarithms are uniformly distributed;
- =6: sets d_i to random numbers from same distribution as the rest of the matrix.

We generated 12 separate classes of upper triangular matrices A and B according to different choices of parameters **dist**, **cond** and **mode**, since this allows us to form different types of matrices to fairly test the behavior of the algorithm. The 12 classes are listed in Table 5.1. Thus classes 1 to 6 consist of well-conditioned matrices B , and the conditioning of matrix A is changed from well to ill-conditioned. Classes 7 to 10 consist of well-conditioned matrices A and the conditioning of matrix B is changed from moderate to ill-conditioned. Classes 11 and 12 consist of moderately conditioned matrices A and B .

5.4 Test Results

We tested the above 12 classes of matrix pairs of dimension of $n = 5, 10, 20, 50$. In each class of dimension 5 we generated 401 matrix pairs, in each class of dimension 10 we generated 301 matrix pairs, in each class of dimension 20 we generated 201 matrix pairs, and in each class of dimension 50 we generated 101 matrix pairs. This makes a total of 12,048 test matrix pairs.

class	A			B		
	dist	cond	mode	dist	cond	mode
1	U	10	6	U	10	6
2	U	10 ²	2	S	10	6
3	U	10 ⁵	1	N	10	5
4	S	10 ⁸	3	S	10	6
5	S	10 ¹²	4	U	10	5
6	S	10 ¹⁴	4	N	10	6
7	N	10	6	N	10 ⁵	1
8	N	10	6	U	10 ⁸	2
9	N	10	6	S	10 ¹²	2
10	S	10	6	N	10 ¹⁴	4
11	S	10 ⁵	4	N	10 ⁵	4
12	S	10 ³	3	N	10 ⁴	4

Table 5.1: Test matrices

Class		1	2	3	4	5	6	7	8	9	10	11	12
n	5	2.29	2.40	2.02	2.00	2.19	2.18	2.07	2.05	2.00	2.12	2.01	1.93
	10	3.00	3.01	2.99	2.01	3.01	3.00	2.97	3.01	2.00	2.99	3.00	2.00
	20	3.26	3.50	3.07	2.19	3.53	3.30	3.05	3.21	2.98	3.23	3.21	2.20
	50	4.00	4.01	3.99	3.00	4.00	4.00	3.89	4.01	3.00	4.00	4.00	3.00

Table 5.2: Average Number of double sweeps

Table 5.2 illustrates the average number of double sweeps required to converge with the tolerance value $\tau = 10^{-14}$, where a double sweep consists of a sweep of rowordering and a sweep of column ordering. None of 12,048 test matrix pairs failed to converge. The observed largest number of double sweeps required to converge was 5. The backward stability conditions (5.1) and (5.2) held throughout the test. The following quadratic convergence rate of the algorithm is typical of what we observed:

$$\frac{\text{cycle}}{\text{error} = \sum_{i=1}^n \text{par}(a_i, b)} \quad \left| \begin{array}{c|c|c|c} 2 & 4 & 6 & 8 \\ \hline 1.5094 & 1.0252 \cdot 10^{-2} & 9.4356 \cdot 10^{-9} & 6.4874 \cdot 10^{-16} \end{array} \right.$$

where A and B are 50×50 matrices, the condition numbers for both matrices are about 10⁴.

5.5 Test matrix generation for testing accuracy.

To test accuracy of Algorithm(SVD) we generated random matrices A and B with known SVD pairs. Specifically, let $\Sigma_1 = \text{diag}(\alpha_i)$ and $\Sigma_2 = \text{diag}(\beta_i)$ be the given SVD pairs. Then we generated random orthogonal matrices U, V and Q uniformly distributed with respect to Haar measure, and a random upper triangular matrix R with specified smallest singular value, and finally formed

$$A = U \Sigma_1 R Q^T \quad \text{and} \quad B = V \Sigma_2 R Q^T. \tag{5.4}$$

Hence the SVD pairs of A and B are known to be (α_i, β_i) .

Type	α_i, β_i	$\sigma_{\min}(R)$	double sweeps for different n				Δ_1
			5	10	20	40	
1	$U(0,1), U(0,1)$	10	2.28	3.02	3.53	4.02	$1.51 \cdot 10^{-14}$
		10^{-6}	2.02	3.00	3.23	4.00	$1.21 \cdot 10^{-15}$
		10^{-12}	2.07	3.04	3.45	4.21	$8.64 \cdot 10^{-15}$
2	$1/i^2, 1$	10	2.01	2.62	3.00	3.00	$2.56 \cdot 10^{-15}$
		10^{-6}	2.00	2.61	3.00	3.00	$2.65 \cdot 10^{-15}$
		10^{-12}	2.00	2.61	3.00	3.10	$9.99 \cdot 10^{-15}$
3	$i, 1$	10	2.48	3.06	3.99	4.06	$2.52 \cdot 10^{-14}$
		10^{-6}	2.07	3.01	3.99	4.02	$9.71 \cdot 10^{-15}$
		10^{-12}	2.75	3.38	4.01	4.53	$3.89 \cdot 10^{-16}$
4	$1+\text{mod}(i, n/4+1), 1$	10	1.03	2.03	3.00	4.00	$7.33 \cdot 10^{-14}$
		10^{-6}	1.00	2.26	3.04	4.02	$5.11 \cdot 10^{-15}$
		10^{-12}	1.08	3.51	3.50	4.59	$1.95 \cdot 10^{-15}$
5	$1 - \frac{i-1}{n-1}(1 - \frac{1}{\text{cond}}), 1$	10	2.06	3.00	3.55	4.14	$3.29 \cdot 10^{-14}$
		10^{-6}	2.01	3.01	3.62	4.18	$4.23 \cdot 10^{-15}$
		10^{-12}	2.01	3.01	3.62	4.20	$6.05 \cdot 10^{-15}$
6	$1, \text{cond}^{-(i-1)/(n-1)}$	10	2.28	3.00	3.28	4.00	$1.51 \cdot 10^{-14}$
		10^{-6}	2.00	2.77	3.00	3.17	$2.98 \cdot 10^{-16}$
		10^{-12}	2.00	2.00	3.00	3.20	$1.14 \cdot 10^{-15}$

Table 5.3: Average double sweeps and accuracy of computed CSV pairs

In this way we can generate random test matrices having any distribution of the CSV pairs, and

$$\|G\|_2^{-1} = \sigma_{\min}(G) = \sigma_{\min}(R).$$

Hence $\sigma_{\min}(R)$ (the smallest singular value) gives the conditioning of the designed test matrix pair. If $\bar{\alpha}_i$ and $\bar{\beta}_i$ are computed the CSV pairs by Algorithm(SVD) then the quantity

$$\Delta_1 \equiv \left\{ \sum_{i=1}^n [(\alpha_i - \bar{\alpha}_i)^2 + (\beta_i - \bar{\beta}_i)^2] \right\}^{1/2} \sigma_{\min}(R) \quad (5.5)$$

should be $O(\tau)$, where $\tau = 10^{-14}$ is our stopping criterion.

We designed six different distributions of the CSV pairs as illustrated in the second column of Table 5.3, where α_i and β_i are normalized so that $\alpha_i^2 + \beta_i^2 = 1$ for $i = 1, \dots, n$ if necessary. $(U(0,1), U(0,1))$ means that CSV pairs (α_i, β_i) comes from the normalization of a pair of random numbers from a uniform distribution on the interval (0,1). cond is the reciprocal of the smallest singular value of the matrix R in (5.4). Note that some of the distributions of CSV are well separated, some of them are highly clustered or multiple.

5.6 Test Results

We generated several categories of matrix pairs according to three parameters: the dimension n , the smallest singular value of R ($\sigma_{\min}(R)$), and the type of distribution of CSV. We first separated test matrices with three possible values of $\sigma_{\min}(R) = 1, 10^{-6}, 10^{-12}$, i.e., corresponding to well,

moderately, and ill-conditioned GSVD problems. For each $\kappa(R)$, we tested matrices of dimension $n = 5, 10, 20, 40$ with six different distributions of GSVD pairs as showed in table 1. This makes a total of $3 \times 4 \times 6 = 72$ different classes of matrices. In each class of dimension 5 we generated 301 matrices, in each class of dimension 10 we generated 201 matrices, in each class of dimension 20 we generated 101 matrices, and in each class of dimension 40 we generated 51 matrices, for a total of 10,772 test matrix pairs.

Table 5.3 illustrates the average number of double sweeps and accuracy of the algorithm for different size of matrices. The preprocessing orthogonal transformations of A and B to upper trapezoidal forms (1.5) are performed using LINPACK QR decomposition subroutine DQRDC [12]. In all tests, the backward stability conditions (5.1) and (5.2) are satisfied, so we do not report the details here. Given the backward stability, we can assume that the backward errors E of A and F of B satisfy $O(\|E\|, \|F\|) = O(4)0$. For each type of GSVD distribution, we let the conditioning (i.e. $\kappa(R)$) of the GSVD problems vary from well to moderate to ill-conditioned, as indicated in column 3 of Table 5.3. The numbers in column 4 to 7 are the average numbers of double sweeps needed for convergence. The last column of the table is the largest value of Δ computed from the formula (5.5). We see that all computed results are as accurate as predicted.

Finally, we briefly report timing results. The codes have not been polished intensively in order to reduce the execution time. The following table illustrates the required time for a 50 by 50 matrix pair A and B with 5 double sweeps to satisfy the stopping criterion.

Timing in seconds with $\tau = 10^{-14}$		
	without U, V, Q	with U, V, Q
preprocessing	0.28	1.11
iteration	13.11	20.99

Appendix: The SVD of 2 2 Triangular Matrix

In this appendix, for the convenience of the reader, we include Demmel and Kahan's 2 by 2 triangular SVD algorithm. The algorithm was used in their high relative accuracy bidiagonal SVD algorithm [10], but the algorithm details were not presented there.

It is known that the singular values of the 2 by 2 upper triangular matrix $\begin{pmatrix} f & g \\ 0 & h \end{pmatrix}$ are the values of the unobvious expression $\frac{1}{2}|\sqrt{(f+h)^2 + g^2} \pm \sqrt{(f-h)^2 + g^2}|$, of which the bigger is γ_1 and the smaller is $\gamma_2 = |fh|/\gamma_1$. The right singular vector $\text{row}(-s_v, c_v)$ turns out to be parallel to $(f^2 - \gamma_1^2, fg)$. After computing a right singular vector, the corresponding left singular vector is determined by $(c_u, s_u) = (fc_v + gs_v, hs_v)/\gamma_1$. But computing the singular values/vectors directly from these expressions is unwise because roundoff can destroy all relative accuracy, and they can suffer from over/underflow in the squared subexpressions even when the singular values/vectors are far from over/underflow thresholds. Demmel and Kahan have carefully reorganized the computation as described in the following so that barring over/underflow and assuring a guard digit in subtraction, all output quantities are correct to within a few units in the last place (ulps). In IEEE arithmetic [1], the code works correctly even if one matrix entry is infinite. Overflow is impossible unless the largest singular value itself overflows, or is within a few ulps of overflow (On machines with partial overflow like the Cray, overflow may occur if the largest singular value is within a factor of 2 of overflow) Underflow is harmless if underflow is gradual. Otherwise, results may correspond to a matrix modified by perturbations of size near the underflow threshold.

The error analysis of the main path of the code depends on the fact that all the operations except two are

multiplication and division, where the relative error of the result is at most 1 ulp larger than the sum of the relative errors of the inputs,
 addition of positive quantities, where the relative error of the result is at most 1 ulp larger than the maximum of the relative errors of the inputs, and
 square root, where the relative error of the result is at most 1 ulp more than half the relative error of the input.

There are also two subtractions in the main code path. The first subtracts original data $D=FAHA$, and so has a 1 ulp error. In the second, $T \approx L$ with $0 \leq \epsilon \leq 1$, the relative error in T can only be 1 ulp larger than the relative error in L . These rules are sufficient to straightforwardly bound the error in the main code path, provided we ignore second order terms. There is another path corresponding to the case where the offdiagonal g is much larger than the other two matrix entries, which is analyzed much more easily. Summarizing all these considerations we can easily prove the

Proposition. *Barring over/underflow, and assuming there is a guard digit in subtraction relative errors in the computed singular values are at most 7 ulps, and the computed singular vectors are at most 46.5 ulps in each component.*

The comments in the following code indicate the error bound in ulp of each computed quantity.

```

SUBROUTINE SLAEV2( F, G, H, SSMIN, SSMAX, SNR, CSR, SNL, CSL )
REAL CSL, CSR, F, G, H, SNL, SNR, SSMAX, SSMIN
C
C Computes singular value decomposition of 2 by 2 triangular matrix:
C [ CSL SNL ] . [ F G ] . [ CSR SNR ] = [ SSMAX 0 ]
C [ -SNL CSL ] [ 0 H ] [ SNR CSR ] [ 0 SSMIN ]
C Absolute value of SSMAX is larger singular value, Absolute value of SSMIN
C is smaller singular value. Both CSR**2+SNR**2=1 and CSL**2+SNL**2=1.
C
C .. Parameters ..
REAL ZERO, HALF, ONE, TWO, FOUR
PARAMETER( ZERO=0.0, HALF=0.5, ONE=1.0, TWO=2.0, FOUR=4.0 )
C .. Local Scalars ..
LOGICAL GSMML, SWP
INTEGER PMAX
REAL A, CLT, CRT, D, FA, FT, GA, GF, HA, HT, L, M
REAL MM, R, S, SLT, SRT, T, TEMP, TSIGN, TT
C .. Intrinsic Functions ..
INTRINSIC ABS, SIGN, SQRT
C
FT = F
FA = ABS( FT )
HT = H
HA = ABS( H )
PMAX = 1 /* PMAX points to maximum absolute entry of matrix */
SWP = ( HA GT FA )
IF ( SWP ) THEN
    PMAX = 3
    TEMP = FT
    FT = HT
    HT = TEMP
    TEMP = FA
    FA = HA
    HA = TEMP
ENDIF /* Now FA .ge. HA */
GT = G
GA = ABS( GF )
IF ( GA EQ ZERO ) THEN /* Diagonal matrix */
    SSMIN = FA
    SSMAX = FA
    CLT = ONE
    CRT = ONE
    SLT = ZERO
    SRT = ZERO
ELSE
    GSMML = .TRUE.
    IF ( GA GT FA ) THEN
        PMAX = 2
        IF ( ABS( FA / GA ) .LE. EPS ) THEN /* Case of very large GA, EPS is machine epsilon */
            GSMML = .FALSE.
            SSMAX = GA /* 1 ulp error */
            IF ( HA GT ONE ) THEN /* 2 ulps error */
                SSMIN = FA / ( GA / HA )
            ELSE /* 2 ulps error */
                SSMIN = ( FA / GA ) * HA
            ENDIF
            CLT = ONE /* 1 ulp error */
            SLT = HT / CRT /* 1 ulp error */
            SRT = ONE /* 1 ulp error */
            CRT = FT / GF /* 1 ulp error */
        ENDIF
    ENDIF
ENDIF

```

```

END IF
IF (GASMA) THEN
    D = FA - HA
    IF (DEQ, FA) THEN
        L = ONE
    ELSE
        L = D / FA
    ENDIF
    M = GF / FT
    T = TWO - L
    MM = MM
    TT = TT
    S = SQRT(TT - MM)
    IF (LEQ, ZERO) THEN
        R = ABS(M)
    ELSE
        R = SQRT(L * L + MM)
    ENDIF
    A = HPLP(S * R)
    SSMIN = HA / A
    SSMAX = FA * A
    IF (NLEQ, ZERO) THEN
        IF (LEQ, ZERO) THEN
            T = SIGN(TWO, FT) * SIGN(ONE, GF)
        ELSE
            T = GF / SIGN(D, FT) + M / T
        ENDIF
    ELSE
        T = (M / (S * T) + M / (R * L)) * ONE
    ENDIF
    L = SQRT(TT - FOUR)
    CRT = TWO / L
    SRT = T / L
    CLT = (CRT * SRT * M) / A
    SLT = (HF / FT) * SRT / A
ENDIF
ENDIF
IF (SWP) THEN
    CSL = SRT
    SNL = CRT
    CSR = SLT
    SNR = CLT
ELSE
    CSL = CLT
    SNL = SLT
    CSR = CRT
    SNR = SRT
ENDIF
C Correct the signs of SSMAX and SSMIN
IF (PAKEQ, 1) THEN
    T1GN = SIGN(ONE, CSR) * SIGN(ONE, CSL) * SIGN(ONE, F)
IF (PAKEQ, 2) THEN
    T2GN = SIGN(ONE, SNR) * SIGN(ONE, CSL) * SIGN(ONE, G)
IF (PAKEQ, 3) THEN
    T3GN = SIGN(ONE, SNR) * SIGN(ONE, SNL) * SIGN(ONE, H)
SSMAX = SIGN(SSMAX, T1GN)
SSMIN = SIGN(SSMIN, T2GN * SIGN(ONE, F) * SIGN(ONE, H))
RETURN
END

```

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