

# GSVD in Julia

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December 21, 2020

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# 1 Definitions

## 1.1 GSVD in LAPACK and JuliaX.X

**Definition.** According to LAPACK [1, pp. 23–24], the generalized singular value decomposition (GSVD) of an  $m$ -by- $n$  matrix  $A$  and a  $p$ -by- $n$  matrix  $B$  is given by the pair of factorizations:

$$A = UC \begin{bmatrix} 0 & R \end{bmatrix} Q^T, \quad B = VS \begin{bmatrix} 0 & R \end{bmatrix} Q^T \quad (1.1)$$

where

- $U$  is  $m$ -by- $m$ ,  $V$  is  $p$ -by- $p$ ,  $Q$  is  $n$ -by- $n$  and all three matrices are orthogonal.
- $R$  is a  $(k + \ell)$ -by- $(k + \ell)$ , upper triangular and nonsingular,  $\begin{bmatrix} 0 & R \end{bmatrix}$  is  $k + \ell$ -by- $n$ .
- $C$  is  $m$ -by- $(k + \ell)$  and  $S$  is  $p$ -by- $(k + \ell)$ , both are real non-negative diagonal (returned in the arrays  $\alpha$  and  $\beta$ ), and  $C^T C + S^T S = I_{k+\ell}$ .  $C$  and  $S$  have the following detailed structures:

(1) Case  $m \geq k + \ell$ :

$$C = \begin{matrix} & k & \ell \\ & \begin{matrix} I & 0 \\ 0 & \Sigma_1 \\ 0 & 0 \end{matrix} \\ \begin{matrix} k \\ \ell \\ m - k - \ell \end{matrix} & \end{matrix}, \quad S = \begin{matrix} & k & \ell \\ & \begin{matrix} 0 & \Sigma_2 \\ 0 & 0 \end{matrix} \\ \begin{matrix} \ell \\ p - \ell \end{matrix} & \end{matrix},$$

where  $\Sigma_1$  and  $\Sigma_2$  are diagonal matrices. and  $\Sigma_1^2 + \Sigma_2^2 = I_\ell$  and  $\Sigma_2$  is nonsingular. In this case,

$$\alpha_1 = \cdots = \alpha_k = 1, \quad (\Sigma_1)_{ii} = \alpha_{k+i} \text{ for } i = 1, \dots, \ell, \\ \beta_1 = \cdots = \beta_k = 0, \quad (\Sigma_2)_{ii} = \beta_{k+i} \text{ for } i = 1, \dots, \ell.$$

(2) Case  $m < k + \ell$ :

$$C = \begin{matrix} & k & m - k & k + \ell - m \\ & \begin{matrix} I & 0 & 0 \\ 0 & \Sigma_1 & 0 \end{matrix} \\ \begin{matrix} k \\ m - k \end{matrix} & \end{matrix}, \quad S = \begin{matrix} & k & m - k & k + \ell - m \\ & \begin{matrix} 0 & \Sigma_2 & 0 \\ 0 & 0 & I \\ 0 & 0 & 0 \end{matrix} \\ \begin{matrix} m - k \\ k + \ell - m \\ p - \ell \end{matrix} & \end{matrix},$$

where  $\Sigma_1$  and  $\Sigma_2$  are diagonal matrices and  $\Sigma_1^2 + \Sigma_2^2 = I$ , and  $\Sigma_2$  is nonsingular.

In this case,

$$\alpha_1 = \cdots = \alpha_k = 1, \quad (\Sigma_1)_{ii} = \alpha_{k+i} \text{ for } i = 1, \dots, m - k, \quad \alpha_{m+1} = \cdots = \alpha_{k+\ell} = 0. \\ \beta_1 = \cdots = \beta_k = 0, \quad (\Sigma_2)_{ii} = \beta_{k+i} \text{ for } i = 1, \dots, m - k, \quad \beta_{m+1} = \cdots = \beta_{k+\ell} = 1.$$

**Q:** can two cases be consolidated into one as the definition by Edelman (1.6)?

**Essential properties.**

*Property 1.*  $k + \ell = \text{rank}([A; B])$  and  $\ell = \text{rank}(B)$ .

*Property 2.*  $\alpha_i, \beta_i \in [0, 1]$  for  $i = 1, \dots, k + \ell$ . The ratios

$$\sigma_i \equiv \alpha_i / \beta_i \quad (1.2)$$

are called the **generalized singular values** of the pair  $(A, B)$ , and are in non-increasing order. The first  $k$  values are infinite, the remaining  $\ell$  values are finite.

*Property 3.* If we rewrite the GSVD (1.1) as

$$A \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} = UC \begin{bmatrix} 0 & R_0 \end{bmatrix}, \quad B \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} = VS \begin{bmatrix} 0 & R_0 \end{bmatrix} \quad (1.3)$$

where  $Q_1$  is  $n$ -by- $(n-k-\ell)$ ,  $Q_2$  is  $n$ -by- $(k+\ell)$  and  $R_0$  is  $(k+\ell)$ -by- $(k+\ell)$ . Then,

$$\text{null}(A) \cap \text{null}(B) = \text{span}(Q_1),$$

i.e.,  $Q_1$  is an orthonormal basis of the common nullspace of  $A$  and  $B$ .

*Property 4.* Let

$$X = Q \begin{pmatrix} & n-k-\ell & k+\ell \\ I & & 0 \\ 0 & & R_0^{-1} \end{pmatrix},$$

then  $A^T A$  and  $B^T B$  are simultaenously diagonalized:

$$X^T A^T A X = \begin{pmatrix} & n-k-\ell & k+\ell \\ n-k-\ell & 0 & 0 \\ k+\ell & 0 & C^T C \end{pmatrix}, \quad (1.4a)$$

$$X^T B^T B X = \begin{pmatrix} & n-k-\ell & k+\ell \\ n-k-\ell & 0 & 0 \\ k+\ell & 0 & S^T S \end{pmatrix}. \quad (1.4b)$$

Thus, we know the “non-trivial” eigenpairs of the generalized eigenvalue problem:

$$A^T A X_{i+n-k-\ell} = \lambda_i B^T B X_{i+n-k-\ell}$$

for  $i = 1, \dots, k+\ell$ , where  $\lambda_i = (\alpha_i/\beta_i)^2$  are “non-trivial” eigenvalues of  $(A^T A, B^T B)$ .  $X_{i+n-k-\ell}$  denotes the  $(i+n-k-\ell)$ th column of  $X$  and are the corresponding eigenvectors.

*Property 5.* Two special cases of the GSVD:

- (a) When  $B$  is square and nonsingular, the GSVD of  $A$  and  $B$  is equivalent to the SVD of  $AB^{-1}$ :

$$AB^{-1} = U(CS^{-1})V^T$$

- (b) If the columns of  $\begin{bmatrix} A^T & B^T \end{bmatrix}^T$  are orthonormal, then the GSVD of  $A$  and  $B$  is equivalent to the Cosine-Sine decomposition (CSD) of  $(A^T, B^T)^T$ :

$$A = UCQ^T, \quad B = VSQ^T \quad (1.5)$$

where  $U$  is  $m$ -by- $m$ ,  $V$  is  $p$ -by- $p$  and  $Q$  is  $n$ -by- $n$  and all of them are orthogonal matrices.

## 1.2 GSVD in Edelman (2019)

In [2], the GSVD of an  $m$ -by- $n$  matrix  $A$  and a  $p$ -by- $n$  matrix  $B$  is defined as follows:

$$A = UCH, \quad B = VSH \quad (1.6)$$

where

- $U$  is  $m$ -by- $m$ , and  $V$  is a  $p$ -by- $p$ , and both are orthogonal matrices.
- $C$  is an  $m$ -by- $(k + \ell)$  matrix and  $S$  is an  $p$ -by- $(k + \ell)$  matrix, and  $C^T C + S^T S = I$ .  $C$  and  $S$  are of the following detailed structures:

$$C = \begin{matrix} & \begin{matrix} k & s & \ell - s \end{matrix} \\ \begin{matrix} k \\ s \\ m - k - s \end{matrix} & \begin{pmatrix} I & 0 & 0 \\ 0 & \Sigma_1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} & \begin{matrix} k & s & \ell - s \end{matrix} \\ \begin{matrix} p - \ell \\ s \\ \ell - s \end{matrix} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & \Sigma_2 & 0 \\ 0 & 0 & I \end{pmatrix} \end{matrix},$$

where  $k + \ell = \text{rank}([A; B])$ ,  $\ell = \text{rank}(B)$ ,  $s = \text{rank}(A) + \text{rank}(B) - \text{rank}([A; B])$ . Furthermore,  $C$  and  $S$  are stored in the arrays  $\alpha$  and  $\beta$  of length  $k + \ell$  such that

$$\begin{aligned} \alpha_1 = \dots = \alpha_k = 1, \quad \Sigma_1 = \text{diag}(\alpha_{k+1}, \dots, \alpha_{k+s}), \quad \alpha_{k+s+1} = \dots = \alpha_{k+\ell} = 0, \\ \beta_1 = \dots = \beta_k = 0, \quad \Sigma_2 = \text{diag}(\beta_{k+1}, \dots, \beta_{k+s}), \quad \beta_{k+s+1} = \dots = \beta_{k+\ell} = 1. \end{aligned}$$

- $H$  is an  $(k + \ell)$ -by- $n$  matrix and has full row rank.

A few remarks are on order:

1. All properties in Section 1.1 hold true by the definition (1.6). In particular, by the RQ factorization of  $H$ :  $H = \begin{bmatrix} 0 & R_0 \end{bmatrix} Q^T$ , where  $R_0$  is an  $(k + \ell)$ -by- $(k + \ell)$  upper triangular matrix and  $Q$  is an  $n$ -by- $n$  orthogonal matrix, then

$$\text{null}(A) \cap \text{null}(B) = \text{span}\{Q(:, 1 : n - k - \ell)\}.$$

In addition, let  $X = Q \begin{pmatrix} I & 0 \\ 0 & R_0^{-1} \end{pmatrix}$ , then the “non-trivial” eigenvalues of the generalized eigenvalue problem  $A^T A x = \lambda B^T B x$  are the square of the generalized singular values of  $A$  and  $B$ , and the last  $(k + \ell)$  columns of  $X$  are the corresponding eigenvectors.

2. From the LAPACK GSVD (1.1) in Section 1.1, there is no value  $s$  to determine the  $s$ -by- $s$  blocks in (1.6). ... How to resolve this issue?

It seems that in the work by Paige and Saunders [3] and Bai and Demmel [4], there is a description of the  $s$ -blocks. ... need to double check.

Q: should we use the GSVD definitions (1.1) or (1.6) in “JuliaX.X”, or leave as options?

### 1.3 GSVD in MATLAB

In MATLAB 2019b [5], the GSVD of an  $m$ -by- $n$  matrix  $A$  and a  $p$ -by- $n$  matrix  $B$  is the following:

$$A = UCX^T, \quad B = V SX^T \quad (1.7)$$

where

- $U$  is  $m$ -by- $m$ ,  $V$  is  $p$ -by- $p$  and both matrices are orthogonal.
- $X$  is an  $n$ -by- $q$  matrix, where  $q = \min\{m + p, n\}$ .
- $C$  is  $m$ -by- $q$ ,  $S$  is  $p$ -by- $q$  and both matrices are nonnegative diagonal.

The nonzero elements of  $S$  are always on its main diagonal. The nonzero elements of  $C$  are on the diagonal  $\text{diag}(C, \max(0, q - m))$ . If  $m \geq q$ , this is the main diagonal of  $C$ .

Both  $C$  and  $S$  are nonnegative and  $C^T C + S^T S = I$ . If  $q > m$ , the rightmost  $m$ -by- $m$  block of  $C$  is diagonal. Otherwise, nonzero elements are on the main diagonal of  $C$ .

Furthermore,  $C^T C = \text{diag}(\alpha_1^2, \dots, \alpha_q^2)$ ,  $S^T S = \text{diag}(\beta_1^2, \dots, \beta_q^2)$ , where  $\alpha_i, \beta_i \in [0, 1]$  for  $i = 1, \dots, q$ . The ratios  $\alpha_i/\beta_i$  are called the *generalized singular values* of the pair  $(A, B)$  and are in non-decreasing order.

The following structures of  $C$  and  $S$  are not explicitly documented in MATLAB, but observed by the author.

1.  $m + p \geq n$ , thus  $q = n$ :

- (a)  $n > m, n \leq p$ :

$$C = \begin{matrix} n-m & m \\ m & \begin{pmatrix} 0 & \Sigma_1 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} n \\ p-n & \begin{pmatrix} \Sigma_2 \\ 0 \end{pmatrix} \end{matrix}$$

where  $\Sigma_1 = \text{diag}(\alpha_{n-m+1}, \dots, \alpha_n)$  and  $\Sigma_2 = \text{diag}(\beta_1, \dots, \beta_n)$ .

- (b)  $n \leq m, n > p$ :

$$C = \begin{matrix} n \\ m-n & \begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} p & n-p \\ p & \begin{pmatrix} \Sigma_2 & 0 \end{pmatrix} \end{matrix}$$

where  $\Sigma_1 = \text{diag}(\alpha_1, \dots, \alpha_n)$  and  $\Sigma_2 = \text{diag}(\beta_1, \dots, \beta_p)$ .

- (c)  $n \leq m, n \leq p$ :

$$C = \begin{matrix} n \\ m-n & \begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} n \\ p-n & \begin{pmatrix} \Sigma_2 \\ 0 \end{pmatrix} \end{matrix}$$

where  $\Sigma_1 = \text{diag}(\alpha_1, \dots, \alpha_n)$  and  $\Sigma_2 = \text{diag}(\beta_1, \dots, \beta_n)$ .

- (d)  $n > m, n > p$ :

$$C = \begin{matrix} n-m & m \\ m & \begin{pmatrix} 0 & \Sigma_1 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} p & n-p \\ p & \begin{pmatrix} \Sigma_2 & 0 \end{pmatrix} \end{matrix}$$

where  $\Sigma_1 = \text{diag}(\alpha_{n-m+1}, \dots, \alpha_n)$  and  $\Sigma_2 = \text{diag}(\beta_1, \dots, \beta_p)$ .

2.  $m + p < n$ , thus  $q = m + p$ :

$$C = \begin{matrix} p & m \\ m & \begin{pmatrix} 0 & \Sigma_1 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} p & m \\ p & \begin{pmatrix} \Sigma_2 & 0 \end{pmatrix} \end{matrix}$$

where  $\Sigma_1 = \text{diag}(\alpha_{p+1}, \dots, \alpha_{p+m})$  and  $\Sigma_2 = \text{diag}(\beta_1, \dots, \beta_p)$ .

A few remarks are in order:

1. The  $n \times q$  matrix  $X$  cannot be guaranteed to be of full rank  $q$ .
2. “The matrix  $X$  has full rank if and only if the matrix  $[A; B]$  has full rank. In fact, the SVD of  $X$  and the condition number of  $X$  are equal to the SVD of  $[A; B]$  and the condition number of  $[A; B]$ , respectively.”
3. The generalized singular values (gsvs) defined in (1.7) could be different from the ones defined in (1.2), see Examples 1.2 and 1.4.
4. By the definition (1.7), we have the factorizations of  $A^T A$  and  $B^T B$ :

$$A^T A = X C^T C X^T, \quad B^T B = X S^T S X^T. \quad (1.8)$$

However, since  $X$  is not guaranteed to be nonsingular, The factorization (1.8) is **not** the simultaneous diagonalization of  $(A^T A, B^T B)$  unless  $X$  is nonsingular. This implies that in general, there is **no connection** between MATLAB’s generalzied singular values (and singular vectors) and the “non-trivial” eigenpairs of  $(A^T A, B^T B)$ . See Examples 1.2 and 1.4.

Meanwhile, *Property 5* is true given this definition,... (a) holds but (b) needs to be verified.

5. MATLAB’s GSVD (1.7) is also different from the one defined in Golub and Van Loan [6, pp. 309], see (1.9) below.

MATLAB manual cites Golub and Van Loand, third edition, 1996... check the definition in the third edition

6. There are two examples on the MATLAB GSVD on MATLAB’s website. are we getting the same results? (looks like all full column rank.

Q: should we communicate with MATLAB about improperly defined GSVD (1.7)? how?

## 1.4 GSVD in Golub and Van Loan

In Golub and Van Loan (4th edition) [6, pp. 309], given an  $m$ -by- $n$  matrix  $A$  and a  $p$ -by- $n$  matrix  $B$  with  $m \geq n$  and  $r = \text{rank}([A; B])$ , the GSVD of  $A$  and  $B$  is:

$$A = UCX^{-1}, \quad B = V SX^{-1} \quad (1.9)$$

where

- $U$  is an  $m$ -by- $m$  orthogonal matrix.
- $V$  is a  $p$ -by- $p$  orthogonal matrix.
- $C$  and  $S$  are  $m$ -by- $n$  and  $p$ -by- $n$ :

$$C = \begin{matrix} & \begin{matrix} q & r-q & n-r \end{matrix} \\ \begin{matrix} q \\ r-q \\ m-r \end{matrix} & \begin{pmatrix} I & 0 & 0 \\ 0 & \Sigma_1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} & \begin{matrix} q & r-q & n-r \end{matrix} \\ \begin{matrix} q \\ r-q \\ p-r \end{matrix} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & \Sigma_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{matrix}$$

where  $q = \max\{r - p, 0\}$ . The diagonal elements of  $C$  and  $S$  are stored in the arrays  $\alpha$  and  $\beta$ :

$$\alpha_1 = \dots = \alpha_q = 1, \quad \Sigma_1 = \text{diag}(\alpha_{q+1}, \dots, \alpha_r), \\ \beta_1 = \dots = \beta_q = 0, \quad \Sigma_2 = \text{diag}(\beta_{q+1}, \dots, \beta_r)$$

and  $\Sigma_1^2 + \Sigma_2^2 = I$ .

- $X$  is an  $n$ -by- $n$  nonsingular matrix.

Q: why there is no need to have two different cases for  $C$  and  $S$  as in LAPACK definition (1.1)?

A few remarks are in order:

1. This definition is due to Van Loan [7]. It holds all properties in Section 1.1 Specifically, for *Property 3*, by  $A(X_1, X_2) = AX = UC = U(C_1, 0)$  and  $B(X_1, X_2) = BX = VS = V(S_1, 0)$ , then we have  $\text{null}(A) \cap \text{null}(B) = \text{span}(X_2)$ , although in this case,  $X_2$  is not an orthonormal basis.
2. The generalized singular value are elements of the set  $\mu(A, B) = \{\alpha_i/\beta_i \mid i = 1, \dots, r\}$ .
3.  $\text{rank}([A; B])$  is the number of “non-trivial???” diagonal entries of  $C$  and  $S$ .
4. By the definition (1.9),  $A^T A$  and  $B^T B$  are simultaneously diagonalized:

$$X^T A^T A X = C^T C, \quad X^T B^T B X = S^T S,$$

Therefore, the first  $r$  quotients of the diagonal entries of  $C^T C$  and  $S^T S$  are the “non-trivial” eigenvalues of the matrix pairs  $(A^T A, B^T B)$ , and the first  $r$  columns of  $X$  are the corresponding eigenvectors.

5. **Note:** MATLAB GSVD (1.7) is also not in line with the GSVD (1.9)!

## 1.5 Examples

We now illustrate our definition 1.1 and that of MATLAB's discussed in Section 1.3 with matrices of small size. Depending on the structures of  $C$  and  $S$  documented in Section 1.1, we devise four pairs: Examples 1 and 2 are contained in “case (1) ( $m \geq k + \ell$ )”, while Examples 3 and 4 fall into “case (2) ( $m < k + \ell$ )”.



**Example 1.1.** Consider a 5-by-4 matrix  $A$  and a 3-by-4 matrix  $B$ :

$$A = \begin{bmatrix} 1 & 2 & 3 & 0 \\ 5 & 4 & 2 & 1 \\ 0 & 3 & 5 & 2 \\ 2 & 1 & 3 & 3 \\ 2 & 0 & 5 & 3 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 0 & 3 & -1 \\ -2 & 5 & 0 & 1 \\ 4 & 2 & -1 & 2 \end{bmatrix}$$

where  $\text{rank}([A; B]) = 4$  and  $\text{rank}(B) = 3$ .

(1). The LAPACK GSVD (1.1) computed by “JuliaGSVD”:

$k = 1$  and  $\ell = 3$ . Since  $m = 5 \geq k + \ell = 1 + 3$ ,  $C$  and  $S$  are of the form in “case (1)”:

$$C = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.894685 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.600408 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.27751 \\ 0.0 & 0.0 & 0.0 & 0.0 \end{bmatrix}, \quad S = \begin{bmatrix} 0.0 & 0.446698 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.799694 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.960723 \end{bmatrix}$$

The generalized singular values computed are

$$\text{Inf}, \quad 2.0028872436786482, \quad 0.7507971450334572, \quad 0.2888559753309598.$$

The computed orthogonal matrices  $U$ ,  $V$ ,  $Q$ , and the  $R$  matrix are:

$$U = \begin{bmatrix} -0.060976 & -0.446679 & -0.448921 & -0.482187 & -0.602266 \\ 0.0904806 & -0.867093 & 0.416172 & 0.115882 & 0.230944 \\ -0.481907 & -0.212508 & -0.636747 & 0.477322 & 0.298869 \\ -0.523214 & 0.0347528 & 0.410748 & 0.420777 & -0.615851 \\ -0.69434 & 0.0475385 & 0.226075 & -0.590913 & 0.339624 \end{bmatrix}$$

$$V = \begin{bmatrix} -0.804633 & -0.328486 & -0.494634 \\ -0.288044 & -0.512512 & 0.808927 \\ -0.519227 & 0.793365 & 0.317765 \end{bmatrix}$$

$$Q = \begin{bmatrix} 0.214542 & 0.484366 & 0.833941 & -0.15461 \\ 0.259709 & 0.413752 & -0.147691 & 0.85997 \\ -0.361334 & 0.767117 & -0.413972 & -0.331052 \\ -0.86946 & -0.0756949 & 0.333702 & 0.356304 \end{bmatrix}$$

$$R = \begin{bmatrix} 5.74065 & -7.07986 & 0.125979 & -0.316232 \\ 0.0 & -7.96103 & -2.11852 & -2.98601 \\ 0.0 & -4.44089e-16 & 5.72211 & -0.43623 \\ 0.0 & 1.33227e-15 & -8.88178e-16 & 5.66474 \end{bmatrix}$$

The residual norms are

$res_A = \frac{\ \tilde{U}^T A \tilde{Q} - \tilde{C} \tilde{R}\ _1}{\max(m,n)\ A\ _1 \epsilon}$	0.35988438508439907
$res_B = \frac{\ \tilde{V}^T B \tilde{Q} - \tilde{S} \tilde{R}\ _1}{\max(p,n)\ B\ _1 \epsilon}$	0.45714285714285713

(2). By GSVD in Julia 1.3 (“svd(A, B)”), we have  $k = 1$  and  $\ell = 3$ .  $D1$  and  $D2$  (equivalent to  $C$  and  $S$  in LAPACK GSVD (1.1)) are:

$$D1 = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.894685 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.600408 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.27751 \\ 0.0 & 0.0 & 0.0 & 0.0 \end{bmatrix}, \quad D2 = \begin{bmatrix} 0.0 & 0.446698 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.799694 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.960723 \end{bmatrix}$$

The computed orthogonal matrices  $U$ ,  $V$ ,  $Q$ , the  $R$  are

$$\begin{aligned}
U &= \begin{bmatrix} -0.060976 & -0.446679 & -0.448921 & 0.482187 & -0.602266 \\ 0.0904806 & -0.867093 & 0.416172 & -0.115882 & 0.230944 \\ -0.481907 & -0.212508 & -0.636747 & -0.477322 & 0.298869 \\ -0.523214 & 0.0347528 & 0.410748 & -0.420777 & -0.615851 \\ -0.69434 & 0.0475385 & 0.226075 & 0.590913 & 0.339624 \end{bmatrix} \\
V &= \begin{bmatrix} -0.804633 & -0.328486 & 0.494634 \\ -0.288044 & -0.512512 & -0.808927 \\ -0.519227 & 0.793365 & -0.317765 \end{bmatrix} \\
Q &= \begin{bmatrix} 0.214542 & 0.484366 & -0.833941 & 0.15461 \\ 0.259709 & 0.413752 & 0.147691 & -0.85997 \\ -0.361334 & 0.767117 & 0.413972 & 0.331052 \\ -0.86946 & -0.0756949 & -0.333702 & -0.356304 \end{bmatrix} \\
R0 &= \begin{bmatrix} 5.74065 & -7.07986 & -0.125979 & 0.316232 \\ 0.0 & -7.96103 & 2.11852 & 2.98601 \\ 0.0 & 0.0 & -5.72211 & 0.43623 \\ 0.0 & 0.0 & 0.0 & 5.66474 \end{bmatrix}
\end{aligned}$$

The residual norms

$res_A = \frac{\ \tilde{U}^T A \tilde{Q} - \tilde{D} \tilde{1} \tilde{R} 0\ _1}{\max(m,n)\ A\ _1 \varepsilon}$	0.35988438508439907
$res_B = \frac{\ \tilde{V}^T B \tilde{Q} - \tilde{D} \tilde{2} \tilde{R} 0\ _1}{\max(p,n)\ B\ _1 \varepsilon}$	0.45714285714285713

(3). The MATLAB GSVD (1.7) computed by “`gsvd(A, B)`”:

Since  $m + p = 5 + 3 > n = 4$ ,  $m = 5 > n = 4$  and  $p = 3 < n = 4$ , the structures of  $C$  and  $S$  are of is the “case 1.(b)” in Section 1.3:

$$C = \begin{bmatrix} 0.2775 & 0 & 0 & 0 \\ 0 & 0.6004 & 0 & 0 \\ 0 & 0 & 0.8947 & 0 \\ 0 & 0 & 0 & 1.0000 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad S = \begin{bmatrix} 0.9607 & 0 & 0 & 0 \\ 0 & 0.7997 & 0 & 0 \\ 0 & 0 & 0.4467 & 0 \end{bmatrix}$$

Consequently, the generalized singular values computed are:

$$0.2889, \quad 0.7508, \quad 2.0029, \quad \text{Inf.}$$

The computed  $U$ ,  $V$  and  $X$  matrix are

$$\begin{aligned}
U &= \begin{bmatrix} 0.4822 & -0.4489 & -0.4467 & -0.0610 & -0.6023 \\ -0.1159 & 0.4162 & -0.8671 & 0.0905 & 0.2309 \\ -0.4773 & -0.6367 & -0.2125 & -0.4819 & 0.2989 \\ -0.4208 & 0.4107 & 0.0348 & -0.5232 & -0.6159 \\ 0.5909 & 0.2261 & 0.0475 & -0.6943 & 0.3396 \end{bmatrix} \\
V &= \begin{bmatrix} 0.4946 & -0.3285 & -0.8046 \\ -0.8089 & -0.5125 & -0.2880 \\ -0.3178 & 0.7934 & -0.5192 \end{bmatrix} \\
X &= \begin{bmatrix} 0.8758 & 4.8394 & -5.1611 & -2.0437 \\ -4.8715 & -1.2203 & -5.5489 & -1.7290 \\ 1.8753 & -2.2244 & -4.2415 & -7.4528 \\ -2.0184 & 1.7541 & -1.1683 & -4.5260 \end{bmatrix}
\end{aligned}$$

The residual norms are

$res_A = \frac{\ A - \tilde{U}\tilde{C}\tilde{X}^T\ _1}{\max(m,n)\ A\ _1\varepsilon}$	0.5222
$res_B = \frac{\ B - \tilde{V}\tilde{S}\tilde{X}^T\ _1}{\max(p,n)\ B\ _1\varepsilon}$	1.3036

#### (4). Findings

- (a) The generalized singular values returned by “LAPACK-GSVD”, “GSVD-Julia1.3” and “MATLAB-GSVD” are the same, but are in different order.
- (b) All quantities computed by “LAPACK-GSVD” and “GSVD-Julia1.3” are the same, up to a sign difference.
- (c) The matrix  $X$  produced by MATLAB-GSVD is non-singular.
- (d) The eigenvalues of  $(A^T A, B^T B)$  computed by MATLAB’s function `eig(A' * A, B' * B)` are

0.08343777448439993, 0.5636963529903901, 4.011557310890648, Inf.

The square roots are

0.2888559753309596, 0.7507971450334572, 2.002887243678647, Inf.

These values are equal to the gsvs computed by LAPACK-GSVD and MATLAB-GSVD.

Note: the “inf” eigenvalue is due to the fact  $B^T B$  is rank deficient.

- (e) The eigenvalues of  $(A^T A, B^T B)$  computed by MATLAB function `dsygvic(n, A' * A, B' * B, tol)`<sup>1</sup> are

4.0116, 0.0834, 0.5637.

The square roots are

2.0029, 0.2889, 0.7508.

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<sup>1</sup><http://cmjiang.cs.ucdavis.edu/xsygvic.html>

**Example 1.2.** Consider a 3-by-4 matrix  $A$  and a 4-by-4 matrix  $B$  but with rank deficiency:

$$A = \begin{bmatrix} 1 & 2 & 1 & 0 \\ 2 & 3 & 1 & 1 \\ 3 & 4 & 1 & 2 \end{bmatrix}, \quad B = \begin{bmatrix} 4 & 5 & 1 & 3 \\ 5 & 6 & 1 & 4 \\ 6 & 7 & 1 & 5 \\ 7 & 1 & -6 & 13 \end{bmatrix}$$

where  $\text{rank}([A; B]) = 2$  and  $\text{rank}(B) = 2$ .

(1). The LAPACK-GSVD (1.1) computed by “JuliaGSVD”:

$k = 0$  and  $\ell = 2$ . Since  $m = 3 > k + \ell = 0 + 2$ , the structure of  $C$  and  $S$  is “case 1”:

$$C = \begin{bmatrix} 0.476231 & 0.0 \\ 0.0 & 0.0697426 \\ 0.0 & 0.0 \end{bmatrix}, \quad S = \begin{bmatrix} 0.87932 & 0.0 \\ 0.0 & 0.997565 \\ 0.0 & 0.0 \\ 0.0 & 0.0 \end{bmatrix}$$

Consequently, the computed gsvs are

$$0.5415903238738987, \quad 0.06991284853891487.$$

The computed matrices  $U$ ,  $V$ ,  $Q$  and  $R$  are:

$$U = \begin{bmatrix} -0.409031 & 0.816105 & -0.408248 \\ -0.56342 & 0.126058 & 0.816497 \\ -0.71781 & -0.563988 & -0.408248 \end{bmatrix}$$

$$V = \begin{bmatrix} -0.472375 & -0.0876731 & -0.390874 & -0.785107 \\ -0.55599 & -0.135916 & -0.53894 & 0.618017 \\ -0.639606 & -0.184159 & 0.745532 & 0.0342253 \\ 0.242159 & -0.969498 & -0.0307137 & -0.0221441 \end{bmatrix}$$

$$Q = \begin{bmatrix} -0.436701 & -0.689898 & 0.299328 & 0.493696 \\ 0.563299 & 0.126599 & 0.793024 & 0.194368 \\ -0.689898 & 0.436701 & 0.493696 & -0.299328 \\ -0.126599 & 0.563299 & -0.194368 & 0.793024 \end{bmatrix}$$

$$R = \begin{bmatrix} 0.0 & 0.0 & -12.2133 & -8.28663 \\ 0.0 & 0.0 & 3.55271e-15 & -18.1154 \end{bmatrix}$$

We tested residues of  $A$  and  $B$  with the computed products  $\tilde{U}$ ,  $\tilde{V}$ ,  $\tilde{Q}$ ,  $\tilde{C}$ ,  $\tilde{S}$  and  $\tilde{R}$ .

$res_A = \frac{\ \tilde{U}^T A \tilde{Q} - \tilde{C} \tilde{R}\ _1}{\max(m, n) \ A\ _1 \epsilon}$	0.6172649988387877
$res_B = \frac{\ \tilde{V}^T B \tilde{Q} - \tilde{S} \tilde{R}\ _1}{\max(p, n) \ B\ _1 \epsilon}$	0.40979208210904405

(2). MATLAB GSVD (1.7) computed by “gsvd(A, B)”:

Since  $m + p = 3 + 4 > n = 4$ ,  $m = 3 < n = 4$  and  $p = 4 = n = 4$ , the structures of  $C$  and  $S$  should be the same as case 1(a) of MATLAB GSVD (1.7) as follows:

$$C = \begin{bmatrix} 0 & 0.0460 & 0 & 0 \\ 0 & 0 & 0.6490 & 0 \\ 0 & 0 & 0 & 0.9946 \end{bmatrix}, \quad S = \begin{bmatrix} 1.0000 & 0 & 0 & 0 \\ 0 & 0.9989 & 0 & 0 \\ 0 & 0 & 0.7608 & 0 \\ 0 & 0 & 0 & 0.1039 \end{bmatrix}$$

Four computed generalized singular values are

$$0, \quad 0.0460, \quad 0.8531, \quad 9.5769.$$

The computed orthogonal matrices  $U$ ,  $V$  and the  $X$  matrix are:

$$U = \begin{bmatrix} 0.0438 & 0.0710 & 0.9965 \\ -0.7618 & -0.6430 & 0.0793 \\ 0.6464 & -0.7626 & 0.0259 \end{bmatrix}$$

$$V = \begin{bmatrix} 0.0621 & 0.0228 & -0.8563 & 0.5121 \\ -0.1574 & 0.3650 & -0.4722 & -0.7868 \\ -0.4326 & 0.8097 & 0.1962 & 0.3445 \\ 0.8855 & 0.4589 & 0.0720 & -0.0075 \end{bmatrix}$$

$$X = \begin{bmatrix} 3.0643 & 9.9974 & -5.3968 & 1.2397 \\ -2.7768 & 8.4399 & -7.4530 & 2.3475 \\ -5.8412 & -1.5575 & -2.0562 & 1.1078 \\ 8.9055 & 11.5549 & -3.3406 & 0.1319 \end{bmatrix}$$

We checked the residues of  $A$  and  $B$  with the computed  $\tilde{U}$ ,  $\tilde{V}$ ,  $\tilde{X}$ ,  $\tilde{C}$  and  $\tilde{S}$ .

$res_A = \frac{\ A - \tilde{U}\tilde{C}\tilde{X}^T\ _1}{\max(m,n)\ A\ _1\varepsilon}$	5.5139
$res_B = \frac{\ B - \tilde{V}\tilde{S}\tilde{X}^T\ _1}{\max(p,n)\ B\ _1\varepsilon}$	1.0600

### (3). Findings

- (a) The matrix  $X$  in MATLAB GSVD (1.7) is singular, with rank 2.
- (b) Neither do the diagonal entries of  $C$  and  $S$  nor the generalize singular values produced in LAPACK GSVD (1.1) and MATLAB GSVD (1.7) bear any resemblance in terms of the number of gsvs and their numerical values.
- (c) The eigenvalues of  $(A^T A, B^T B)$  computed by MATLAB's function `eig(A' * A, B' * B)` are  
 $-0.035807289211371204$ , **0.004887806390825194**,  $0.12085659170178971$ , **0.29332007891383427**.

The square roots are

$$0.0+0.1892281406434339im, \quad \mathbf{0.06991284853891447}, \quad 0.3476443465695792, \quad \mathbf{0.5415903238738985}.$$

Among these values, eigenvalues **0.06991284853891447** and **0.5415903238738985** are found in the computed gsvs of LAPACK GSVD.

- (d) **Note: In this case, two of four eigenvalues computed by MATLAB “eig” are spurious ones. This is caused by the fact that the pencil  $A^T A - \lambda B^T B$  is singular, i.e.,  $A^T A$  and  $B^T B$  have a non-trivial common null space. The function “dsygvic.m” should return only two “corrected” eigenvalues.**  
The computation of the eigenvalues of  $(A^T A, B^T B)$  by MATLAB's function `dsygvic(n, A' * A, B' * B, tol)` caused an exception, the error message is **Singular pencil, exit**.

- (4). By GSVD in Julia 1.3 (`svd(A, B)`), we have  $k = 0$  and  $\ell = 2$ .  $D1$  and  $D2$  (equivalent to  $C$  and  $S$  in the proposed version) are:

$$D1 = \begin{bmatrix} 0.476231 & 0.0 \\ 0.0 & 0.0697426 \\ 0.0 & 0.0 \end{bmatrix}, \quad D2 = \begin{bmatrix} 0.87932 & 0.0 \\ 0.0 & 0.997565 \\ 0.0 & 0.0 \end{bmatrix}$$

The computed orthogonal matrices  $U$ ,  $V$ ,  $Q$ , the  $R0$  matrix (equivalent to  $R$  in the proposed version) are:

$$\begin{aligned}
U &= \begin{bmatrix} 0.409031 & 0.816105 & -0.408248 \\ 0.56342 & 0.126058 & 0.816497 \\ 0.71781 & -0.563988 & -0.408248 \end{bmatrix} \\
V &= \begin{bmatrix} 0.472375 & -0.0876731 & -0.390874 & -0.785107 \\ 0.55599 & -0.135916 & -0.53894 & 0.618017 \\ 0.639606 & -0.184159 & 0.745532 & 0.0342253 \\ -0.242159 & -0.969498 & -0.0307137 & -0.0221441 \end{bmatrix} \\
Q &= \begin{bmatrix} -0.436701 & -0.689898 & -0.299328 & 0.493696 \\ 0.563299 & 0.126599 & -0.793024 & 0.194368 \\ -0.689898 & 0.436701 & -0.493696 & -0.299328 \\ -0.126599 & 0.563299 & 0.194368 & 0.793024 \end{bmatrix} \\
R0 &= \begin{bmatrix} 0.0 & 0.0 & -12.2133 & 8.28663 \\ 0.0 & 0.0 & 0.0 & -18.1154 \end{bmatrix}
\end{aligned}$$

All these quantities are essentially (up to a sign) the same with JuliaGSVD.

Still, we tested residuals of  $A$  and  $B$  with the computed products  $\tilde{U}$ ,  $\tilde{V}$ ,  $\tilde{Q}$ ,  $\tilde{D}1$ ,  $\tilde{D}2$  and  $\tilde{R}0$ .

$res_A = \frac{\ \tilde{U}^T A \tilde{Q} - \tilde{D}1 \tilde{R}0\ _1}{\max(m,n)\ A\ _1 \varepsilon}$	0.5068000688771875
$res_B = \frac{\ \tilde{V}^T B \tilde{Q} - \tilde{D}2 \tilde{R}0\ _1}{\max(p,n)\ B\ _1 \varepsilon}$	0.5689371432283518

**Example 1.3.** Let  $A$  be a 3-by-4 matrix and  $B$  be a 4-by-4 matrix:

$$A = \begin{bmatrix} 1 & 4 & 1 & 0 \\ 5 & 3 & 1 & 1 \\ 3 & 0 & 1 & 2 \end{bmatrix}, \quad B = \begin{bmatrix} 4 & 5 & 1 & 3 \\ -2 & 0 & 1 & 4 \\ 3 & 2 & 1 & -5 \\ 1 & 1 & -6 & 3 \end{bmatrix}$$

(1). The LAPACK GSVD (1.1) computed by “JuliaGSVD”:

$k = 0$  and  $\ell = 4$ . Since  $m = 3$  and  $m < k + \ell$ ,  $C$  and  $S$  should be contained in case (2) in Section 1.1:

$$C = \begin{bmatrix} 0.99144 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.681061 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.167854 & 0.0 \end{bmatrix}, \quad S = \begin{bmatrix} 0.130566 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.732227 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.985812 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 \end{bmatrix}$$

The generalized singular values computed are

$$7.593384394490093, 0.930122554989402, 0.17026951585960612, 0.0.$$

The computed orthogonal matrices  $U$ ,  $V$ ,  $Q$ , and the  $R$  matrix are:

$$U = \begin{bmatrix} -0.519777 & 0.747619 & 0.413398 \\ 0.470025 & 0.654341 & -0.592381 \\ 0.713378 & 0.113599 & 0.691511 \end{bmatrix}$$

$$V = \begin{bmatrix} 0.259832 & 0.927018 & 0.177229 & -0.20424 \\ -0.733955 & 0.0402919 & 0.652334 & -0.184789 \\ -0.597084 & 0.369645 & -0.576157 & 0.418206 \\ -0.1931. & -0.0487437 & -0.459449 & -0.865588 \end{bmatrix}$$

$$Q = \begin{bmatrix} -0.685431 & -0.564405 & -0.459976 & -0.00724571 \\ 0.681731 & -0.704114 & -0.149854 & -0.130423 \\ -0.127188 & -0.380896 & 0.646684 & 0.648491 \\ -0.221923 & -0.201466 & 0.589716 & -0.749931 \end{bmatrix}$$

$$R = \begin{bmatrix} -3.71474 & -2.42556 & -0.179891 & -0.941672 \\ -7.20246e-16 & -9.84284 & -1.8323 & -0.522579 \\ -8.91076e-17 & 2.04711e-15 & 6.16149 & -1.43582 \\ 1.84152e-15 & 1.41087e-15 & 1.2978e-15 & 8.05363 \end{bmatrix}$$

We tested residues of  $A$  and  $B$  with the computed products  $\tilde{U}, \tilde{V}, \tilde{Q}, \tilde{C}, \tilde{S}$  and  $\tilde{R}$ .

$res_A = \frac{\ \tilde{U}^T A \tilde{Q} - \tilde{C} \tilde{R}\ _1}{\max(m, n) \ A\ _1 \varepsilon}$	0.41810247019514407
$res_B = \frac{\ \tilde{V}^T B \tilde{Q} - \tilde{S} \tilde{R}\ _1}{\max(p, n) \ B\ _1 \varepsilon}$	0.8941315014073346

(2). MATLAB GSVD (1.7) computed by “`gsvd(A, B)`”:

$m + p = 3 + 4 \geq n = 4$ ,  $m = 3 < n = 4$  and  $p = 4 \leq n = 4$ , the structures of  $C$  and  $S$  are the same as case 1.(a) in Section 1.3.

$$C = \begin{bmatrix} 0 & 0.1679 & 0 & 0 \\ 0 & 0 & 0.6811 & 0 \\ 0 & 0 & 0 & 0.9914 \end{bmatrix}, \quad S = \begin{bmatrix} 1.0000 & 0 & 0 & 0 \\ 0 & 0.9858 & 0 & 0 \\ 0 & 0 & 0.7322 & 0 \\ 0 & 0 & 0 & 0.1306 \end{bmatrix}$$

The generalized singular values computed are:

$$0, 0.1703, 0.9301, 7.5934.$$

The computed orthogonal matrices  $U$ ,  $V$  and the  $X$  matrix are given below.

$$U = \begin{bmatrix} 0.4134 & -0.7476 & 0.5198 \\ -0.5924 & -0.6543 & -0.4700 \\ 0.6915 & -0.1136 & -0.7134 \end{bmatrix}$$

$$V = \begin{bmatrix} 0.2042 & 0.1772 & -0.9270 & -0.2598 \\ 0.1848 & 0.6523 & -0.0403 & 0.7340 \\ -0.4182 & -0.5762 & -0.3696 & 0.5971 \\ 0.8656 & -0.4594 & 0.0487 & 0.1931 \end{bmatrix}$$

$$X = \begin{bmatrix} 0.0584 & -2.8237 & -6.4020 & -4.0048 \\ 1.0504 & -0.7361 & -7.2732 & 0.6748 \\ -5.2227 & 3.0534 & -2.2253 & -0.6694 \\ 6.0397 & 4.7103 & -1.2944 & -1.9132 \end{bmatrix}$$

We checked the residues of  $A$  and  $B$  with the computed  $\tilde{U}$ ,  $\tilde{V}$ ,  $\tilde{X}$ ,  $\tilde{C}$  and  $\tilde{S}$ .

$res_A = \frac{\ A - \tilde{U}\tilde{C}\tilde{X}^T\ _1}{\max(m,n)\ A\ _1\varepsilon}$	3.5278
$res_B = \frac{\ B - \tilde{V}\tilde{S}\tilde{X}^T\ _1}{\max(p,n)\ B\ _1\varepsilon}$	0.5000

### (3). Findings

- (a) The generalized singular values computed by “JuliaGSVD” and “MATLAB-SVD” are the same. However, the order are opposite.
- (b) The  $X$  matrix produced by MATLAB is non-singular.
- (c) The eigenvalues of  $(A^T A, B^T B)$  computed by MATLAB’s function `eig(A' * A, B' * B)` are

$$-1.8035125057805033e^{-15}, \quad \mathbf{0.028991708031064364}, \quad \mathbf{0.8651279673000131}, \quad \mathbf{57.659486562484965}.$$

The square roots are

$$0.0 + 4.2467781973874066e^{-8} \text{im}, \quad \mathbf{0.17026951585960526}, \quad \mathbf{0.930122554989402}, \quad \mathbf{7.593384394490046}.$$

Among these values, eigenvalues **0.17026951585960526**, **0.930122554989402** and **7.593384394490046** are found in the computed gsvs of LAPACK GSVD and MATLAB GSVD.

- (d) One of the eigenvalues computed by MATLAB’s `eig` is spurious. The eigenvalues of  $(A^T A, B^T B)$  computed by MATLAB’s function `dsygvic(n, A' * A, B' * B, tol)` are

$$57.6595, \quad 0.8651, \quad 0.0000, \quad 0.0290.$$

The square roots are

$$7.5934, \quad 0.9301, \quad 0.0000, \quad 0.1703.$$

all of which are identical to the computed gsvs of LAPACK-GSVD and MATLAB-GSVD.



- (4). Similarly, we test GSVD in Julia 1.3 with the same inputs. For the numerical rank,  $k = 0$  and  $\ell = 4$ .  $D1$  and  $D2$  (equivalent to  $C$  and  $S$  in the proposed version) are:

$$D1 = \begin{bmatrix} 0.99144 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.681061 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.167854 & 0.0 \end{bmatrix}, \quad D2 = \begin{bmatrix} 0.130566 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.732227 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.985812 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 \end{bmatrix}$$

The computed orthogonal matrices  $U$ ,  $V$ ,  $Q$ , the  $R0$  matrix (equivalent to  $R$  in the proposed version) are:

$$U = \begin{bmatrix} 0.519777 & 0.747619 & 0.413398 \\ -0.470025 & 0.654341 & -0.592381 \\ -0.713378 & 0.113599 & 0.691511 \end{bmatrix}$$

$$V = \begin{bmatrix} -0.259832 & 0.927018 & 0.177229 & 0.20424 \\ 0.733955 & 0.0402919 & 0.652334 & 0.184789 \\ 0.597084 & 0.369645 & -0.576157 & -0.418206 \\ 0.1931 & -0.0487437 & -0.459449 & 0.865588 \end{bmatrix}$$

$$Q = \begin{bmatrix} -0.685431 & 0.564405 & 0.459976 & 0.00724571 \\ 0.681731 & 0.704114 & 0.149854 & 0.130423 \\ -0.127188 & 0.380896 & -0.646684 & -0.648491 \\ -0.221923 & 0.201466 & -0.589716 & 0.749931 \end{bmatrix}$$

$$R0 = \begin{bmatrix} 3.71474 & -2.42556 & -0.179891 & -0.941672 \\ 0.0 & 9.84284 & 1.8323 & 0.522579 \\ 0.0 & 0.0 & -6.16149 & 1.43582 \\ 0.0 & 0.0 & 0.0 & 8.05363 \end{bmatrix}$$

All these quantities are essentially (up to a sign) the same with JuliaGSVD.

Still, we tested residuals of  $A$  and  $B$  with the computed products  $\tilde{U}$ ,  $\tilde{V}$ ,  $\tilde{Q}$ ,  $\tilde{D}1$ ,  $\tilde{D}2$  and  $\tilde{R}0$ .

$res_A = \frac{\ \tilde{U}^T A \tilde{Q} - \tilde{D}1 \tilde{R}0\ _1}{\max(m,n)\ A\ _1 \varepsilon}$	0.3536371804643456
$res_B = \frac{\ \tilde{V}^T B \tilde{Q} - \tilde{D}2 \tilde{R}0\ _1}{\max(p,n)\ B\ _1 \varepsilon}$	0.59375

**Example 1.4.** Given a 3-by-5 matrix  $A$  and a 4-by-5 matrix  $B$  which are rank deficient:

$$A = \begin{bmatrix} 1 & 4 & 2 & 3 & 0 \\ 3 & 4 & 0 & -2 & 1 \\ 4 & 7 & 5 & 6 & 3 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 4 & 2 & 3 & 0 \\ 2 & 5 & 3 & 4 & 1 \\ 3 & 6 & 4 & 5 & 2 \\ 0 & 1 & -1 & 3 & 1 \end{bmatrix}$$

(1). The LAPACK GSVD (1.1) computed by “JuliaGSVD”:

$k = 1, \ell = 3$  and  $m = 3 < k + \ell = 4$ . Both  $B$  and  $[A; B]$  are not in full rank, the structures of  $C$  and  $S$  comply with those of case (2) in Section 1.1.

$$C = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.849235 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.605834 & 0.0 \end{bmatrix}, \quad S = \begin{bmatrix} 0.0 & 0.528015 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.795591 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 \end{bmatrix}$$

The generalized singular values computed are

$$\text{Inf}, 1.6083530545973714, 0.7614900645668164, 0.0.$$

The computed orthogonal matrices  $U$ ,  $V$ ,  $Q$ , and the  $R$  matrix are:

$$U = \begin{bmatrix} -2.22045e-16 & 0.355381 & -0.934722 \\ 1.0 & -1.74736e-16 & -1.8521e-16 \\ -2.2915e-16 & -0.934722 & -0.355381 \end{bmatrix}$$

$$V = \begin{bmatrix} 0.571577 & -0.711781 & 1.07608e-17 & -0.408248 \\ -0.120069 & -0.564727 & -2.13123e-16 & 0.816497 \\ -0.811716 & -0.417673 & -1.59451e-16 & -0.408248 \\ 1.38917e-16 & 1.22399e-16 & -1.0 & 3.46945e-17 \end{bmatrix}$$

$$Q = \begin{bmatrix} -0.735494 & -0.356936 & -0.479812 & 0.318474 & 3.59984e-16 \\ 0.29657 & -0.540179 & 0.367864 & 0.633716 & 0.288675 \\ 0.130491 & 0.610611 & -0.189162 & 0.700722 & -0.288675 \\ -0.237256 & 0.432143 & 0.0711454 & 0.0435931 & 0.866025 \\ 0.545689 & -0.145639 & -0.770462 & -0.0637737 & 0.288675 \end{bmatrix}$$

$$R = \begin{bmatrix} 0.0 & -4.24145 & -0.880735 & 3.33933 & -0.288675 \\ 0.0 & 0.0 & 2.7394 & -8.38306 & -5.97906 \\ 0.0 & 0.0 & -1.77636e-15 & -12.2122 & -8.79399 \\ 0.0 & 0.0 & -4.996e-16 & 2.22045e-16 & -3.4641 \end{bmatrix}$$

We can verify that  $R$  has a zero column in the leftmost since  $k + l < n$ .

We tested residues of  $A$  and  $B$  with the computed products  $\tilde{U}, \tilde{V}, \tilde{Q}, \tilde{C}, \tilde{S}$  and  $\tilde{R}$ .

$res_A = \frac{\ \tilde{U}^T A \tilde{Q} - \tilde{C} \tilde{R}\ _1}{\max(m, n) \ A\ _1 \epsilon}$	0.36
$res_B = \frac{\ \tilde{V}^T B \tilde{Q} - \tilde{S} \tilde{R}\ _1}{\max(p, n) \ B\ _1 \epsilon}$	0.589976856064605

(2). MATLAB GSVD (1.7) computed by “`gsvd(A, B)`”:

$m + p = 3 + 4 \geq n = 5$  and  $m = 3 < n = 5$ ,  $p = 4 < n = 5$ , the structures of  $C$  and  $S$  are the form of case 1.(d) in Section 1.3.

$$C = \begin{bmatrix} 0 & 0 & 0.8178 & 0 & 0 \\ 0 & 0 & 0 & 0.9995 & 0 \\ 0 & 0 & 0 & 0 & 1.0000 \end{bmatrix}, \quad S = \begin{bmatrix} 1.0000 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 \\ 0 & 0 & 0.5755 & 0 & 0 \\ 0 & 0 & 0 & 0.0312 & 0 \end{bmatrix}$$

The generalized singular values computed are

$$0, 0, 1.4209, 32.0780, \text{Inf.}$$

The computed orthogonal matrices  $U$ ,  $V$  and the  $X$  matrix are:

$$U = \begin{bmatrix} -0.1968 & 0.9805 & 0.0000 \\ 0.0000 & -0.0000 & 1.0000 \\ -0.9805 & -0.1968 & -0.0000 \end{bmatrix}$$

$$V = \begin{bmatrix} -0.8338 & 0 & 0.3365 & 0.4376 \\ -0.5289 & 0.0000 & -0.2600 & -0.8079 \\ -0.1581 & 0.0000 & -0.9051 & 0.3947 \\ -0.0000 & -1.0000 & -0.0000 & -0.0000 \end{bmatrix}$$

$$X = \begin{bmatrix} -2.3660 & 0.0000 & -5.0363 & 0.1935 & 3.0000 \\ -6.9285 & -1.0000 & -9.3550 & 2.5457 & 4.0000 \\ -3.8868 & 1.0000 & -6.4759 & 0.9776 & 0.0000 \\ -5.4077 & -3.0000 & -7.9154 & 1.7617 & -2.0000 \\ -0.8451 & -1.0000 & -3.5968 & -0.5906 & 1.0000 \end{bmatrix}$$

We checked the residues of  $A$  and  $B$  with the computed  $\tilde{U}$ ,  $\tilde{V}$ ,  $\tilde{X}$ ,  $\tilde{C}$  and  $\tilde{S}$ .

$res_A = \frac{\ A - \tilde{U}\tilde{C}\tilde{X}^T\ _1}{\max(m,n)\ A\ _1\varepsilon}$	0.4800
$res_B = \frac{\ B - \tilde{V}\tilde{S}\tilde{X}^T\ _1}{\max(p,n)\ B\ _1\varepsilon}$	0.4000

### (3). Findings

- (a) The matrix  $X$  in MATLAB GSVD (1.7) is singular, whose rank is 4.
- (b) Neither do the diagonal entries of  $C$  and  $S$  nor the generalize singular values produced in LAPACK GSVD (1.1) and MATLAB GSVD (1.7) share any in common in terms of the number of gsvs and their numerical values.
- (c) The eigenvalues of  $(A^T A, B^T B)$  computed by MATLAB's function `eig(A'*A, B'*B)` are  $-0.34554912453318243, 1.3025318975863486e^{-16}, \mathbf{0.5798671184339763}, \mathbf{2.586799548232693}, \text{Inf.}$

The square roots are

$$0.0+0.5878342662121547\text{im}, 1.1412851955520796e^{-8}, \mathbf{0.7614900645668178}, \mathbf{1.6083530545973708}, \text{Inf.}$$

Among these values, eigenvalues **0.7614900645668178** and **1.6083530545973708** are found in the computed gsvs of LAPACK GSVD.

- (d) The computation of the eigenvalues of  $(A^T A, B^T B)$  by MATLAB's function `dsygvic(n, A'*A, B'*B, tol)` threw an error at line 328. I tried to change  $k$  to  $k(1)$ , thus the square roots of the eigenvalues are

$$0.0046, \quad 0.7710.$$

which makes no sense.

- (4). Again, same inputs are tested in Julia 1.3. For the numerical rank determination,  $k = 1$  and  $\ell = 3$ .  $D1$  and  $D2$  (equivalent to  $C$  and  $S$  in the proposed version) are:

$$D1 = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.849235 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.605834 & 0.0 \end{bmatrix}, \quad D2 = \begin{bmatrix} 0.0 & 0.528015 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.795591 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 \end{bmatrix}$$

The computed orthogonal matrices  $U$ ,  $V$ ,  $Q$ , the  $R0$  matrix (equivalent to  $R$  in the proposed version) are:

$$U = \begin{bmatrix} -2.22045e-16 & -0.355381 & -0.934722 \\ 1.0 & 1.74736e-16 & -1.8521e-16 \\ -2.2915e-16 & 0.934722 & -0.355381 \end{bmatrix}$$

$$V = \begin{bmatrix} -0.571577 & -0.711781 & 1.94289e-16 & -0.408248 \\ 0.120069 & -0.564727 & 2.35922e-16 & 0.816497 \\ 0.811716 & -0.417673 & -1.82146e-17 & -0.408248 \\ 7.69338e-17 & 2.44055e-16 & 1.0 & 3.46945e-17 \end{bmatrix}$$

$$Q = \begin{bmatrix} -0.735494 & -0.356936 & -0.479812 & -0.318474 & -1.66533e-16 \\ 0.29657 & -0.540179 & 0.367864 & -0.633716 & -0.288675 \\ 0.130491 & 0.610611 & -0.189162 & -0.700722 & 0.288675 \\ -0.237256 & 0.432143 & 0.0711454 & -0.0435931 & -0.866025 \\ 0.545689 & -0.145639 & -0.770462 & 0.0637737 & -0.288675 \end{bmatrix}$$

$$R0 = \begin{bmatrix} 0.0 & -4.24145 & -0.880735 & -3.33933 & 0.288675 \\ 0.0 & 0.0 & -2.7394 & -8.38306 & -5.97906 \\ 0.0 & 0.0 & 0.0 & 12.2122 & 8.79399 \\ 0.0 & 0.0 & 0.0 & 0.0 & -3.4641 \end{bmatrix}$$

It is clear that the leftmost column of  $R0$  is all zeros.

All these quantities are essentially (up to a sign) the same with JuliaGSVD.

Still, we tested residuals of  $A$  and  $B$  with the computed products  $\tilde{U}$ ,  $\tilde{V}$ ,  $\tilde{Q}$ ,  $\tilde{D}1$ ,  $\tilde{D}2$  and  $\tilde{R}0$ .

$res_A = \frac{\ \tilde{U}^T A \tilde{Q} - \tilde{D}1 \tilde{R}0\ _1}{\max(m,n)\ A\ _{1\varepsilon}}$	0.4449492156962062
$res_B = \frac{\ \tilde{V}^T B \tilde{Q} - \tilde{D}2 \tilde{R}0\ _1}{\max(p,n)\ B\ _{1\varepsilon}}$	0.305570013362164

## 2 Algorithms

### 2.1 GSVD algorithm

The algorithm consists of four steps. First step is a pre-processing step where the input matrix pair is reduced to a triangular pair while revealing their ranks [8]. We further reduce two upper triangular matrices to one upper triangular matrix in the QR decomposition step. Next is the CS decomposition of a matrix with orthonormal columns that is partitioned into two blocks. [7] The last step is post-processing to get the final product of the decomposition.

**Step 1. Pre-processing:** To reduce “regular matrices to their triangular form and reveal rank”, we employ the QR decomposition with column pivoting followed by RQ decomposition [6] as well as QR decomposition. We detail this in nine substeps below.

(1) QR decomposition with column pivoting of  $B$ :

$$BP = V \begin{matrix} & \ell & n-\ell \\ \ell & & \\ p-\ell & & \end{matrix} \begin{pmatrix} B_{11} & B_{12} \\ 0 & 0 \end{pmatrix}$$

(2) Update  $A := AP$

(3) Set  $Q := I_n$  and update  $Q := QP$

(4) If  $n > \ell$ :

- RQ decomposition of  $(B_{11} \ B_{12})$ :

$$\begin{matrix} \ell & n-\ell & & n-\ell & \ell \\ \ell & (B_{11} & B_{12}) = \ell & (0 & B_{13})Z \end{matrix}$$

- Update  $A := AZ^T$
- Update  $Q := QZ^T$

(5) Partition

$$A = m \begin{matrix} & n-\ell & \ell \\ (A_1 & A_2), \end{matrix}$$

the QR decomposition with column pivoting of  $A_1$  is:

$$A_1 P_1 = U \begin{matrix} & k & n-\ell-k \\ k & & \\ m-k & & \end{matrix} \begin{pmatrix} A_{11} & A_{12} \\ 0 & 0 \end{pmatrix}$$

(6) Update  $A_2 := U^T A_2$

$$(7) \text{ Partition } A = \begin{matrix} & k & n-\ell-k & \ell \\ m-k & \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ 0 & 0 & A_{23} \end{pmatrix} \end{matrix}$$

(8) Update  $Q(:, 1 : n - \ell) := Q(:, 1 : n - \ell)P_1$

(9) If  $n - \ell > k$ :

- RQ decomposition of  $(A_{11} \ A_{12})$ :

$$\begin{matrix} & k & n-\ell-k & & n-\ell-k & k \\ k & (A_{11} & A_{12}) & = k & \begin{pmatrix} 0 & A_{12} \end{pmatrix} & Z_1 \end{matrix}$$

$$\text{and it results } A = \begin{matrix} & n-\ell-k & k & \ell \\ k & \begin{pmatrix} 0 & A_{12} & A_{13} \\ 0 & 0 & A_{23} \end{pmatrix} \\ m-k & \end{matrix}$$

- Update  $Q(:, 1 : n - \ell) = Q(:, 1 : n - \ell)Z_1^T$

(10) If  $m > k$ :

Let

$$A_2 = \begin{matrix} & \ell \\ k & \begin{pmatrix} A_{13} \\ A_{23} \end{pmatrix} \\ m-k & \end{matrix}$$

- QR decomposition of  $A_{23}$ :

$$A_{23} = U_1 \begin{matrix} & \ell \\ \ell & \begin{pmatrix} A_{23} \\ 0 \end{pmatrix} \\ m-k-\ell & \end{matrix}$$

- Update  $U(:, k + 1 : m) = U(:, k + 1 : m)U_1$

In summary, we have the following decomposition at the end of the pre-processing:

$$A = UR_AQ^T, \quad B = VR_BQ^T \quad (2.1)$$

where

- If  $m - k - \ell \geq 0$ :

$$R_A = \begin{matrix} & n-k-\ell & k & \ell \\ k & \begin{pmatrix} 0 & A_{12} & A_{13} \\ \ell & 0 & A_{23} \\ m-k-\ell & 0 & 0 \end{pmatrix} \\ \ell & \end{matrix}, \quad R_B = \begin{matrix} & n-k-\ell & k & \ell \\ \ell & \begin{pmatrix} 0 & 0 & B_{13} \\ 0 & 0 & 0 \end{pmatrix} \\ p-\ell & \end{matrix}$$

where  $R_A$  and  $R_B$  overwrite  $A$  and  $B$ , respectively, and  $A_{12}$  and  $B_{13}$  are non-singular upper triangular matrix.  $\ell$  is the rank of  $B$ ,  $k + \ell$  is the rank of  $[A^T \ B^T]^T$ .  $A_{23}$  is  $\ell$ -by- $\ell$  upper triangular,

- If  $m - k - \ell < 0$ :

$$R_A = \begin{matrix} & n-k-\ell & k & \ell \\ k & \begin{pmatrix} 0 & A_{12} & A_{13} \\ 0 & 0 & A_{23} \end{pmatrix} \\ m-k & \end{matrix}, \quad R_B = \begin{matrix} & n-k-\ell & k & \ell \\ \ell & \begin{pmatrix} 0 & 0 & B_{13} \\ 0 & 0 & 0 \end{pmatrix} \\ p-\ell & \end{matrix},$$

where  $R_A$  and  $R_B$  overwrite  $A$  and  $B$ , respectively, and  $A_{12}$  and  $B_{13}$  are non-singular upper triangular matrix.  $\ell$  is the rank of  $B$ ,  $k + \ell$  is the rank of  $[A^T \ B^T]^T$ .  $A_{23}$  is  $(m - k)$ -by- $\ell$  upper trapezoidal.

**Step 2. QR decomposition of  $[A_{23}^T \ B_{13}^T]^T$ :**

- If  $m - k - \ell \geq 0$ :

$$\begin{matrix} & \ell \\ \ell & \begin{pmatrix} A_{23} \\ B_{23} \end{pmatrix} \\ \ell & \end{matrix} = \begin{matrix} & \ell \\ \ell & \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} \\ \ell & \end{matrix} R_{23}$$

- If  $m - k - \ell < 0$ :

$$\begin{matrix} & \ell \\ m-k & \left( \begin{matrix} A_{23} \\ B_{23} \end{matrix} \right) \\ \ell & \end{matrix} = \begin{matrix} & \ell \\ m-k & \left( \begin{matrix} Q_1 \\ Q_2 \end{matrix} \right) \\ \ell & \end{matrix} R_{23}$$

Thus, (2.1) can be rewritten as:

$$A = U(Q_A \hat{R})Q^T, \quad B = V(Q_B \hat{R})Q^T \quad (2.2)$$

where

- If  $m - k - \ell \geq 0$ :

$$Q_A = \begin{matrix} & k & \ell \\ & \ell & \\ m-k-\ell & \left( \begin{matrix} I & 0 \\ 0 & Q_1 \end{matrix} \right) \\ & 0 & 0 \end{matrix}, \quad Q_B = \begin{matrix} & k & \ell \\ & \ell & \\ p-\ell & \left( \begin{matrix} 0 & Q_2 \\ 0 & 0 \end{matrix} \right) \\ & 0 & 0 \end{matrix}, \quad \hat{R} = \begin{matrix} & n-k-\ell & k & \ell \\ & 0 & A_{12} & B_{13} \\ & 0 & 0 & R_{23} \end{matrix}$$

- If  $m - k - \ell < 0$ :

$$Q_A = \begin{matrix} & k & \ell \\ & \ell & \\ m-k & \left( \begin{matrix} I & 0 \\ 0 & Q_1 \end{matrix} \right) \\ & 0 & 0 \end{matrix}, \quad Q_B = \begin{matrix} & k & \ell \\ & \ell & \\ p-\ell & \left( \begin{matrix} 0 & Q_2 \\ 0 & 0 \end{matrix} \right) \\ & 0 & 0 \end{matrix}, \quad \hat{R} = \begin{matrix} & n-k-\ell & k & \ell \\ & 0 & A_{12} & B_{13} \\ & 0 & 0 & R_{23} \end{matrix}$$

**Step 3. CS decomposition of  $Q_1$  and  $Q_2$ :**

$$Q_1 = U_1 \Sigma_1 Z_1^T, \quad Q_2 = V_1 \Sigma_2 Z_1^T \quad (2.3)$$

where

- If  $m - k - \ell \geq 0$ :

$U_1$ ,  $Z_1$  and  $V_1$  are  $\ell$ -by- $\ell$  orthogonal matrices, and  $\Sigma_1$  and  $\Sigma_2$  are  $\ell$ -by- $\ell$  diagonal matrices, and  $\Sigma_1^T \Sigma_1 + \Sigma_2^T \Sigma_2 = I_\ell$ .

- If  $m - k - \ell < 0$ :

$U_1$  is  $(m-k)$ -by- $(m-k)$  orthogonal and  $Z_1$  and  $V_1$  are  $\ell$ -by- $\ell$  orthogonal.  $\Sigma_1$  is  $(m-k)$ -by- $\ell$  diagonal,  $\Sigma_2$  is  $\ell$ -by- $\ell$  diagonal and  $\Sigma_1^T \Sigma_1 + \Sigma_2^T \Sigma_2 = I_\ell$ .

Combining (2.2) and (2.3), we have

$$A = U(\hat{U}C\hat{Q}^T)\hat{R}Q^T, \quad B = V(\hat{V}S\hat{Q}^T)\hat{R}Q^T \quad (2.4)$$

where

- If  $m - k - \ell \geq 0$ :

$$\hat{U} = \begin{matrix} & k & \ell & m-k-\ell \\ & \ell & & \\ m-k-\ell & \left( \begin{matrix} I & 0 & 0 \\ 0 & U_1 & 0 \\ 0 & 0 & I \end{matrix} \right) \\ & 0 & 0 & 0 \end{matrix}, \quad \hat{V} = \begin{matrix} & \ell & p-\ell \\ & \ell & \\ p-\ell & \left( \begin{matrix} V_1 & 0 \\ 0 & I \end{matrix} \right) \\ & 0 & 0 \end{matrix}, \quad \hat{Q}^T = \begin{matrix} & k & \ell \\ & \ell & \\ p-\ell & \left( \begin{matrix} I & 0 \\ 0 & Z_1^T \end{matrix} \right) \\ & 0 & 0 \end{matrix}$$

and

$$C = \begin{matrix} & k & \ell \\ & \ell & \\ m-k-\ell & \left( \begin{matrix} I & 0 \\ 0 & \Sigma_1 \\ 0 & 0 \end{matrix} \right) \\ & 0 & 0 \end{matrix}, \quad S = \begin{matrix} & k & \ell \\ & \ell & \\ p-\ell & \left( \begin{matrix} 0 & \Sigma_2 \\ 0 & 0 \end{matrix} \right) \\ & 0 & 0 \end{matrix}$$

- If  $m - k - \ell < 0$ :

$$\hat{U} = \begin{matrix} & k & m-k \\ m-k & \begin{pmatrix} I & 0 \\ 0 & U_1 \end{pmatrix} \end{matrix}, \quad \hat{V} = \begin{matrix} & \ell & p-\ell \\ p-\ell & \begin{pmatrix} V_1 & 0 \\ 0 & I \end{pmatrix} \end{matrix}, \quad \hat{Q}^T = \begin{matrix} & k & \ell \\ p-\ell & \begin{pmatrix} I & 0 \\ 0 & Z_1^T \end{pmatrix} \end{matrix}$$

and

$$C = \begin{matrix} & k & \ell \\ m-k & \begin{pmatrix} I & 0 \\ 0 & \Sigma_1 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} & k & \ell \\ p-\ell & \begin{pmatrix} 0 & \Sigma_2 \\ 0 & 0 \end{pmatrix} \end{matrix}$$

The algorithm for computing the CS decomposition is in Section 2.2.

#### Step 4. Post-processing:

- $U := U\hat{U}$ .
- $V := V\hat{V}$ .
- Formulate  $R$  by RQ decomposition:  $\hat{Q}^T \hat{R} = RQ_3$
- $Q := QQ_3^T$

Then we obtain the desired GSVD (1.1), i.e.,

$$A = UCRQ^T, \quad B = VSRQ^T \quad (2.5)$$

where  $C$  and  $S$  have the following structures:

- If  $m - k - \ell \geq 0$ :

$$C = \begin{matrix} & k & \ell \\ \ell & \begin{pmatrix} I & 0 \\ 0 & \Sigma_1 \end{pmatrix} \\ m-k-\ell & \begin{pmatrix} 0 & 0 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} & k & \ell \\ p-\ell & \begin{pmatrix} 0 & \Sigma_2 \\ 0 & 0 \end{pmatrix} \end{matrix}$$

- If  $m - k - \ell < 0$ :

$$C = \begin{matrix} & k & m-k & k+\ell-m \\ m-k & \begin{pmatrix} I & 0 & 0 \\ 0 & \Sigma_1 & 0 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} & k & m-k & k+\ell-m \\ k+\ell-m & \begin{pmatrix} 0 & \Sigma_2 & 0 \\ 0 & 0 & I \\ p-\ell & 0 & 0 \end{pmatrix} \end{matrix}$$

In either case,  $\Sigma_1^2 + \Sigma_2^2 = I$ .

**Remark 2.1.** Michael Stewart [9] describes an alternative rank revealing mechanism of  $[A; B]$  and claims that it can more reliably determine the partitioning of a GSVD and shows improved numerical reliability.

**Remark 2.2.** The algorithm presented here is “similar to” ... Golub and Van Loan [6, pp. 502–503] introduced an algorithm to compute GSVD using CS decomposition for tall, full-rank matrix pairs.

Assume that  $A$  is  $m$ -by- $n$  and  $B$  is  $p$ -by- $n$  with  $m \geq n$  and  $p \geq n$ , computes an  $m$ -by- $m$  orthogonal matrix  $U$ , a  $p$ -by- $p$  orthogonal matrix  $V$ , an  $n$ -by- $n$  nonsingular matrix  $X$  and  $m$ -by- $n$  diagonal matrix  $C$ ,  $p$ -by- $n$  diagonal matrix  $S$  such that  $U^T A X = C$  and  $V^T B X = S$ .

*Step 1* Compute the regular QR decomposition of  $\begin{pmatrix} A \\ B \end{pmatrix}$ :  $\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} R$



*Step 2* Compute the CS decomposition of  $Q_1$  and  $Q_2$ :

$$U^T Q_1 Z = C = \text{diag}(\alpha_1, \dots, \alpha_n), \quad V^T Q_2 Z = S = \text{diag}(\beta_1, \dots, \beta_n).$$

*Step 3* Solve  $RX = Z$  for  $X$ .

**Remark 2.3.** LAPACK GSVD algorithm [1, pp. 51–53] has two phases. First is a pre-processing step as described in Section 2.1. Next is a **Jacobi-style method** [3, 4] to compute the GSVD of two square upper triangular matrices, namely,  $A_{23}$  and  $B_{13}$  in (2.1) such that

$$A_{23} = U_1 C R Q_1^T, \quad B_{13} = V_1 S R Q_1^T. \quad (2.6)$$

Here  $U_1$ ,  $V_1$  and  $Q_1$  are orthogonal matrices,  $C$  and  $S$  are both real nonnegative matrices satisfying  $C^T C + S^T S = I$ ,  $S$  is nonsingular, and  $R$  is upper triangular and nonsingular.

## 2.2 CS Decomposition

### 2.2.1 Definition

Suppose we have an  $(m+p) \times n$  matrix  $Q$  such that  $m+p \geq n$  and has orthonormal columns. If we partition  $Q$  into 2-by-1 form as  $[Q_1; Q_2]$ , then the CS decomposition of  $Q_1$  and  $Q_2$  is the following:

$$Q_1 = UCZ^T, \quad Q_2 = VSZ^T \quad (2.7)$$

where

- $U$  is  $m$ -by- $m$ ,  $V$  is  $p$ -by- $p$ , and  $Z$  is  $n$ -by- $n$ , all are orthogonal.
- $C$  is  $m$ -by- $n$  real non-negative diagonal, and  $S$  is  $p$ -by- $n$  real non-negative with the top right diagonal block, and  $C^T C + S^T S = I$ .

$C$  and  $S$  have the following detailed structures:

1.  $m \geq n$  and  $p \geq n$ :

$$C = \begin{matrix} & n \\ m-n & \begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} & n \\ p-n & \begin{pmatrix} \Sigma_2 \\ 0 \end{pmatrix} \end{matrix}$$

2.  $m \geq n$  and  $p < n$ :

$$C = \begin{matrix} & n-p & p \\ n-p & \begin{pmatrix} I & 0 \\ 0 & \Sigma_1 \end{pmatrix} \\ p & \begin{pmatrix} 0 & \Sigma_1 \\ 0 & 0 \end{pmatrix} \\ m-n & \end{matrix}, \quad S = \begin{matrix} & n-p & p \\ n-p & \begin{pmatrix} 0 & \Sigma_2 \end{pmatrix} \\ p & \end{matrix}$$

3.  $m \leq n$  and  $p \geq n$ :

$$C = \begin{matrix} & m & n-m \\ m & \begin{pmatrix} \Sigma_1 & 0 \end{pmatrix} \\ n-m & \begin{pmatrix} 0 & I \\ 0 & 0 \end{pmatrix} \\ p-n & \end{matrix}, \quad S = \begin{matrix} & m & n-m \\ n-m & \begin{pmatrix} \Sigma_2 & 0 \\ 0 & I \end{pmatrix} \\ p-n & \begin{pmatrix} 0 & 0 \end{pmatrix} \end{matrix}$$

4.  $m \leq n$  and  $p < n$ :

$$C = \begin{matrix} & n-p & t & n-m \\ n-p & \begin{pmatrix} I & 0 & 0 \\ 0 & \Sigma_1 & 0 \end{pmatrix} \\ t & \end{matrix}, \quad S = \begin{matrix} & n-p & t & n-m \\ n-m & \begin{pmatrix} 0 & \Sigma_2 & 0 \\ 0 & 0 & I \end{pmatrix} \\ t & \end{matrix}$$

where  $t = m + p - n$ .

where  $\Sigma_1$  and  $\Sigma_2$  are diagonal matrices and satisfy  $\Sigma_1^2 + \Sigma_2^2 = I$ .

**Why called the CSD?** Write  $C^T C = \text{diag}(\alpha_1^2, \alpha_2^2, \dots, \alpha_n^2)$  and  $S^T S = \text{diag}(\beta_1^2, \beta_2^2, \dots, \beta_n^2)$ , we have

$$\alpha_i^2 + \beta_i^2 = 1 \quad \text{for } i = 1, 2, \dots, n \quad (2.8)$$

CS decomposition is named after cosine and sine due to the resemblance between (2.8) and cosine-sine relation. Thus, we name  $\alpha_i$  and  $\beta_i$  cosine and sine values, respectively. To align with the growth of cosine and sine values between angles of 0 and  $\frac{\pi}{2}$  in Euclidean geometry,  $\alpha_i$  are placed in non-increasing order while  $\beta_i$  are sorted in non-decreasing order.

**Remark 2.4.** LAPACK provides a routine to compute the CSD of a 2-by-1 partitioned matrix, which is developed by Sutton [10].

Given an  $(m+p)$ -by- $n$  matrix  $Q$  with orthonormal columns that has been partitioned into a 2-by-1 block structure:

$$Q = \begin{matrix} & n \\ m & \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} \\ p \end{matrix}$$

There exist an  $m$ -by- $m$  matrix  $U$ , a  $p$ -by- $p$  matrix  $V$ , and an  $n$ -by- $n$  matrix  $Z$  (all are orthogonal) such that:

$$\begin{pmatrix} U & 0 \\ 0 & V \end{pmatrix}^T \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} Z = \begin{pmatrix} C \\ S \end{pmatrix} = \begin{pmatrix} I_1 & 0 & 0 \\ 0 & \Sigma_1 & 0 \\ 0 & 0 & 0 \\ \hline 0 & 0 & 0 \\ 0 & \Sigma_2 & 0 \\ 0 & 0 & I_2 \end{pmatrix}$$

where  $\Sigma_1$  and  $\Sigma_2$  are  $r$ -by- $r$  non-negative diagonal matrices satisfying  $\Sigma_1^2 + \Sigma_2^2 = I$ , where  $r = \min\{m, p, n, m+p-n\}$ .  $I_1$  is a  $k_1$ -by- $k_1$  identity matrix and  $I_2$  is a  $k_2$ -by- $k_2$  identity matrix, where  $k_1 = \max\{n-p, 0\}$ ,  $k_2 = \max\{n-m, 0\}$ .

We observe that the detailed structures of  $C$  and  $S$  match the structures of  $C$  and  $S$  in the definition (2.7).

### 2.2.2 Algorithm

Now, we present an algorithm to compute the CS decomposition. The algorithm extends the one proposed by Van Loan [11].

First, we set  $q_1 = \min\{m, n\}$  and  $q_2 = \min\{p, n\}$ . We split this algorithm into two cases:  $m \leq p$  and  $m > p$ .

1. If  $m \leq p$ :

Step 1. SVD of  $Q_2$  such that:

$$Q_2 = V S Z^T, \tag{2.9}$$

where  $V$  is  $p$ -by- $p$  and  $Z$  is  $n$ -by- $n$ , both are orthogonal matrices.  $S$  has the following structure:

$$S = \begin{matrix} & q_2 & n-q_2 \\ q_2 & \begin{pmatrix} \Sigma & 0 \\ 0 & 0 \end{pmatrix} \\ p-q_2 \end{matrix}$$

where  $q_2 = \min\{p, n\}$ ,  $\Sigma = \text{diag}(\beta_n, \dots, \beta_{n-q_2+1})$  such that  $1 \geq \beta_n \geq \beta_{n-1} \geq \dots \geq \beta_{n-q_2+1} \geq 0$ .

This means we need to reverse the order of  $\beta_i$  to preserve that the sine values are in non-decreasing order. Thus,

- Reorder the diagonal entries of  $S$  in non-decreasing, such that:

$$S = \begin{matrix} & n-q_2 & q_2 \\ q_2 & \begin{pmatrix} 0 & \hat{\Sigma} \\ 0 & 0 \end{pmatrix} \\ p-q_2 \end{matrix}$$

where  $\hat{\Sigma} = \text{diag}(\beta_{n-q_2+1}, \dots, \beta_n)$

- Reverse the first  $q_2$  columns of  $V$ :  $V(:, 1:q_2) = V(:, q_2:-1:1)$ .
- Reverse the columns of  $Z$ :  $Z = Z(:, n:-1:1)$ .

Since  $Q_2$  has  $(n - q_2)$  zero singular values,  $\beta_1 = \beta_2 = \dots = \beta_{n-q_2} = 0$  and correspondingly,  $\alpha_1 = \alpha_2 = \dots = \alpha_{n-q_2} = 1$ .

*Step 2.* Determine  $r$  such that  $0 \leq \beta_{n-q_2+1} \leq \dots \leq \beta_r \leq \frac{1}{\sqrt{2}} < \beta_{r+1} \leq \dots \leq \beta_n \leq 1$ .

*Step 3.*  $T = Q_1 Z$ .

*Step 4.* QR decomposition of  $T$ :

$$T = UR, \quad (2.10)$$

where  $U$  is an  $m$ -by- $m$  orthogonal matrix,

$$R = \begin{matrix} & n - q_2 & r - n + q_2 & q_1 - r & n - q_1 \\ \begin{matrix} n - q_2 \\ r - n + q_2 \\ q_1 - r \\ m - q_1 \end{matrix} & \begin{pmatrix} I & \epsilon & \epsilon & \epsilon \\ 0 & R_{22} & \epsilon & \epsilon \\ 0 & 0 & R_{33} & R_{34} \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{matrix} \quad (2.11)$$

where  $q_1 = \min\{m, n\}$ , and  $R_{22} = \text{diag}(\alpha_{n-q_2+1}, \dots, \alpha_r)$ .

Combining *Step 3* and *Step 4*, we obtain:

$$Q_1 = URZ^T \quad (2.12)$$

The formula above can be treated as the SVD of  $Q_1$ .

Thus, the fact that  $Q_1$  has  $(n - q_1)$  zero singular values implies that  $\alpha_{q_1} = \dots = \alpha_l = 0$ , and  $\beta_{q_1} = \dots = \beta_l = 1$ , respectively.

*Step 5.* SVD of  $(R_{33} \ R_{34})$  such that:

$$(R_{33} \ R_{34}) = U_r C_r Z_r^T \quad (2.13)$$

where  $U_r$  is a  $(q_1 - r)$ -by- $(q_1 - r)$  orthogonal matrix,  $Z_r$  is an  $(n - r)$ -by- $(n - r)$  orthogonal matrix and  $C_r$  is a  $(q_1 - r)$ -by- $(n - r)$  matrix with the main diagonal entries storing non-zero  $\alpha_{r+1}, \dots, \alpha_{q_1}$ .

*Step 6.* Plugging (2.13) into (2.12), and update  $U$ ,  $R$  and  $Z$  accordingly:

- Update the  $(r + 1)$  to  $q_1$  columns of  $U$ :

$$U = U \begin{matrix} & r & q_1 - r & m - q_1 \\ \begin{matrix} r \\ q_1 - r \\ m - q_1 \end{matrix} & \begin{pmatrix} I & 0 & 0 \\ 0 & U_r & 0 \\ 0 & 0 & I \end{pmatrix} \end{matrix}$$

- Update the last  $(n - r)$  columns of  $Z$ :

$$Z = Z \begin{matrix} & r & n - r \\ \begin{matrix} r \\ n - r \end{matrix} & \begin{pmatrix} I & 0 \\ 0 & Z_r \end{pmatrix} \end{matrix}$$

- Rewrite  $R$  to formulate  $C$ :

$$C = \begin{matrix} & n - q_2 & r - n + q_2 & q_1 - r & n - q_1 \\ \begin{matrix} n - q_2 \\ r - n + q_2 \\ q_1 - r \\ m - q_1 \end{matrix} & \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & R_{22} & 0 & 0 \\ 0 & 0 & C_r(:, 1 : q_1 - r) & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{matrix}$$

Now, we have the final decomposition of  $Q_1$ :

$$Q_1 = UCZ^T \quad (2.14)$$

*Step 7.* Since  $Z$  is updated, we need to modify  $V$  as well:

- Set  $W$ :  $W = S_1 Z_r(1 : q_2 - r, 1 : q_2 - r)$ , where  $S_1 = \text{diag}(\beta_{r+1}, \dots, \beta_{q_2})$ ,
- QR decomposition of  $W$ :

$$W = Q_w R_w \quad (2.15)$$

- Update middle  $(q_2 - r)$  columns of  $V$ :  
Let  $\ell = \min\{r, n - q_2\}$ ,

$$V = V \begin{matrix} & r - \ell & q_2 - r & p - q_2 + \ell \\ \begin{matrix} r - \ell \\ q_2 - r \\ p - q_2 + \ell \end{matrix} & \begin{pmatrix} I & 0 & 0 \\ 0 & Q_w & 0 \\ 0 & 0 & I \end{pmatrix} \end{matrix}$$

In summary, we obtain:

$$Q_1 = UCZ^T, \quad Q_2 = VSZ^T \quad (2.16)$$

and

$$C = \begin{matrix} & n - q_2 & t & n - q_1 \\ \begin{matrix} n - q_2 \\ t \\ m - q_1 \end{matrix} & \begin{pmatrix} I & 0 & 0 \\ 0 & \Sigma_1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{matrix}, \quad S = \begin{matrix} & n - q_2 & t & n - q_1 \\ \begin{matrix} t \\ n - m \\ p - q_2 \end{matrix} & \begin{pmatrix} 0 & \Sigma_2 & 0 \\ 0 & 0 & I \\ 0 & 0 & 0 \end{pmatrix} \end{matrix}$$

where  $t = q_1 + q_2 - n$ ,  $\Sigma_1 = \text{diag}(\alpha_{\ell - q_2 + 1}, \dots, \alpha_{q_1})$  and  $\Sigma_2 = \text{diag}(\beta_{\ell - q_2 + 1}, \dots, \beta_{q_1})$ .

2. If  $m > p$ :

*Step 1.* Full SVD of  $Q_1$  such that:

$$Q_1 = UCZ^T \quad (2.17)$$

$U$  is  $m$ -by- $m$ ,  $Z$  is  $n$ -by- $n$ , both are orthogonal matrices.  $C$  is  $m$ -by- $n$  with singular values  $1 \geq \alpha_1 \geq \dots \geq \alpha_{q_1} \geq 0$  placed in the main diagonal. Since  $Q_1$  has  $(n - q_1)$  zero singular values, we obtain  $\alpha_{q_1 + 1} = \dots = \alpha_n = 0$ , and  $\beta_{q_1 + 1} = \dots = \beta_n = 1$ , respectively.

*Step 2.* Determine  $r$  such that  $1 \geq \alpha_1 \geq \dots \geq \alpha_r \geq \frac{1}{\sqrt{2}} > \alpha_{r+1} \geq \dots \geq \alpha_n \geq 0$ .

*Step 3.*  $T = Q_2 Z$ .

*Step 4.* QL decomposition of  $T$ :

$$T = VL, \quad (2.18)$$

where  $V$  is a  $p$ -by- $p$  orthogonal matrix,

$$L = \begin{matrix} & n - q_2 & r & q_1 + q_2 - n - r & n - q_1 \\ \begin{matrix} p - q_2 \\ r \\ q_1 + q_2 - n - r \\ n - q_1 \end{matrix} & \begin{pmatrix} 0 & 0 & 0 & 0 \\ L_{11} & L_{12} & 0 & 0 \\ \epsilon & \epsilon & L_{23} & 0 \\ \epsilon & \epsilon & \epsilon & I \end{pmatrix} \end{matrix} \quad (2.19)$$

and  $L_{23} = \text{diag}(\beta_{n - q_2 + r + 1}, \dots, \beta_{q_1})$ .

To be consistent with the structure of  $S$  given above, we pre-multiply  $T$  with a permutation matrix  $P$  in an effort to move the top  $(n - q_2)$  rows to the bottom.

$$P = \begin{matrix} & p - q_2 & r & q_2 - r \\ \begin{matrix} r \\ q_2 - r \\ p - q_2 \end{matrix} & \begin{pmatrix} 0 & I & 0 \\ 0 & 0 & I \\ I & 0 & 0 \end{pmatrix} \end{matrix}$$

Combining *Step 3* and *Step 4*, we get:

$$Q_2 = V(P^{-1}PL)Z^T \quad (2.20)$$

This formula can be regarded as the SVD of  $Q_2$ . Therefore, the fact that  $Q_2$  has  $(n - q_2)$  zero singular values indicates that  $\alpha_1 = \dots = \alpha_{n-q_2} = 1$ , and  $\beta_1 = \dots = \beta_{n-q_2} = 0$ , respectively.

*Step 5.* SVD of  $(L_{11} \ L_{12})$  such that:

$$(L_{11} \ L_{12}) = V_l S_l Z_l^T \quad (2.21)$$

where  $V_l$  is  $r$ -by- $r$  orthogonal matrix,  $Z_l$  is  $(n - q_2 + r)$ -by- $(n - q_2 + r)$  orthogonal matrix and  $S_l$  is  $r$ -by- $(n - q_2 + r)$  and contains the  $r$  singular values in a non-increasing fashion. However, by the nature of sine, we want to reverse the ordering of  $\beta_i$ . Accordingly, we need to reverse the columns of  $V_l$  and  $Z_l$ .

- Reorder the diagonal entries of  $S_l$  in non-decreasing order, such that:

$$S_l = \begin{matrix} & r & n - q_2 \\ r & \begin{pmatrix} \Sigma & 0 \end{pmatrix} \end{matrix}$$

where  $\Sigma = \text{diag}(\beta_{n-q_2+1}, \dots, \beta_{n-q_2+r})$

- Reverse the columns of  $V_l$ :  $V_l = V_l(:, r : -1 : 1)$ .
- Reverse the columns of  $Z_l$ :  $Z_l = Z_l(:, n - q_2 + r : -1 : 1)$ .

*Step 6.* To plug (2.21) into (2.20), we shall update  $V$ ,  $L$  and  $Z$  accordingly:

- Update  $V$ :

$$V = \begin{matrix} & p - q_2 & r & q_2 - r \\ \begin{matrix} p - q_2 \\ r \\ q_2 - r \end{matrix} & \begin{pmatrix} I & 0 & 0 \\ 0 & U_r & 0 \\ 0 & 0 & I \end{pmatrix} \end{matrix} P^{-1}$$

- Update the first  $(r + n - q_2)$  columns of  $Z$ :

$$Z = \begin{matrix} & r + n - q_2 & q_2 - r \\ \begin{matrix} r + n - q_2 \\ q_2 - r \end{matrix} & \begin{pmatrix} Z_l & 0 \\ 0 & I \end{pmatrix} \end{matrix}$$

- Rewrite  $L$  to formulate  $S$ :

$$S = \begin{matrix} & n - q_2 & r & q_1 + q_2 - n - r & n - q_1 \\ \begin{matrix} r \\ q_1 + q_2 - n - r \\ n - q_1 \\ p - q_2 \end{matrix} & \begin{pmatrix} 0 & S_l(:, 1 : r) & 0 & 0 \\ 0 & 0 & L_{23} & 0 \\ 0 & 0 & 0 & I \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{matrix}$$

*Step 7.* Since  $Z$  is updated, we need to modify  $U$  as well:

- Set  $W$ :  
Let  $C_1 = \text{diag}(\alpha_1, \dots, \beta_{r+n-q_2})$ ,  $W = C_1 Z_l$ .
- QR decomposition of  $W$ :

$$W = Q_w R_w \quad (2.22)$$

- Update  $U$ :

$$U = U \begin{matrix} & r+n-q_2 & m+r-l+q_2 \\ r+n-q_2 & & \\ m+r-l+q_2 & & \end{matrix} \begin{pmatrix} Q_w & 0 \\ I & 0 \end{pmatrix}$$

Putting all the 7 steps together, we have:

$$Q_1 = UCZ^T, \quad Q_2 = VSZ^T \quad (2.23)$$

and

$$C = \begin{matrix} & n-q_2 & t & n-q_1 \\ n-q_2 & & & \\ t & & & \\ m-q_1 & & & \end{matrix} \begin{pmatrix} I & 0 & 0 \\ 0 & \Sigma_1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad S = \begin{matrix} & n-q_2 & t & n-q_1 \\ t & & & \\ n-m & & & \\ p-q_2 & & & \end{matrix} \begin{pmatrix} 0 & \Sigma_2 & 0 \\ 0 & 0 & I \\ 0 & 0 & 0 \end{pmatrix}$$

where  $t = q_1 + q_2 - n$ ,  $\Sigma_1 = \text{diag}(\alpha_{l-q_2+1}, \dots, \alpha_{q_1})$  and  $\Sigma_2 = \text{diag}(\beta_{l-q_2+1}, \dots, \beta_{q_1})$ .

**Remark 2.5.** We justify here why we choose  $\frac{1}{\sqrt{2}}$  as the threshold in *Step 2* of both cases. Since  $Q_1^T Q_1 + Q_2^T Q_2 = I$  and  $\|Q_1^T Q_1 + Q_2^T Q_2\|_1 = 1$ , the singular values of  $Q_1$  and  $Q_2$  lie between 0 and 1.  $\frac{1}{\sqrt{2}}$  is the exact midpoint in between so that it nicely separates large singular values from tiny singular values. This theoretical yet empirical choice is first suggested by Van Loan in [11] because the midpoint balances the backward error defined in (4.2) - (4.5) and performance.

**Remark 2.6.** In *Step 4* of case 1,  $R$  is upper triangular in exact arithmetics, but the upper-right 5 block matrices are effectively zero matrices. Here, we rationalize this assertion.

If we analyse the  $T$  matrix we computed in *Step 3*, we have:

$$\begin{aligned} T^T T &= (Q_1 Z)^T (Q_1 Z) \\ &= Z^T Q_1^T Q_1 Z \\ &= Z^T (I - Q_2^T Q_2) Z \\ &= Z^T (I - Z S^T V^T V S Z^T) Z \\ &= Z^T (I - Z S^T S Z^T) Z \\ &= I - S^T S \\ &= \text{diag}(1 - \beta_1^2, 1 - \beta_2^2, \dots, 1 - \beta_n^2), \end{aligned}$$

which indicates that the norms of each column of  $T$  are in non-increasing order. Further, it implies that  $\sigma_{\min}(T_1) \geq \sigma_{\min}(T_2) \geq \dots \geq \sigma_{\min}(T_r)$  where  $T_i$  is the first  $i$  columns of  $T$  and  $r = \text{rank}(T)$ . This can be proven by **Corollary 2.4.4** in [6, pp. 78–78] by Golub and Van Loan.

Before we proceed, we present the following theorem and its proof.

**Theorem 2.7.** Let  $X$  be an  $m$ -by- $n$  matrix whose rank  $= \min(m, n)$  and

$$X^T X = D^T D + E,$$

where  $\|E\| = O(\epsilon)$  and  $D = \text{diag}(\|x_1\|, \|x_2\|, \dots, \|x_n\|)$  and  $x_i$  denotes the  $i$ -th column of  $X$ .

Applying the full QR decomposition of  $X$ , one obtains:

$$X = QR, \quad (2.24)$$

where  $Q$  is an  $m$ -by- $m$  orthogonal matrix.  $R$  is an  $m$ -by- $n$  upper triangular matrix if  $m \geq n$ . Otherwise,  $R$  is upper trapezoidal.

Let  $X_i$  be the first  $i$  columns of  $X$ , then for  $i, j$  where  $i < j \leq \min(m, n)$ , we have

$$|R(i, j)| \leq \min\{\|x_j\|, \frac{\|E\|}{\sigma_{\min}(X_i)}\}. \quad (2.25)$$

*Proof.* This theorem is proved by Van Loan in **Theorem 3.2** [11, pp. 484–485].  $\square$

From this theorem along with the  $\frac{1}{\sqrt{2}}$  threshold we justified above, it follows that, for  $i = 1, 2, \dots, r$ ,

$$|R(i, j)| \leq \frac{\epsilon}{\sigma_{\min}(T_i)} \leq \frac{\epsilon}{\sqrt{1 - \beta_r^2}} \leq \sqrt{2}\epsilon.$$

By that, we know that  $R(1 : n - q_2, n - q_2 + 1 : r)$ ,  $R(1 : n - q_2, r + 1 : q_1)$ ,  $R(1 : n - q_2, q_1 + 1 : n)$ ,  $R(n - q_2 + 1 : r, r + 1 : q_1)$  and  $R(n - q_2 + 1 : r, q_1 + 1 : n)$ , namely the 5 upper right block matrices of  $R$  in (2.11) are effectively zero matrices.

The justification why the 5 lower left block matrices are effective zero matrices in (2.19) in *Step 4* of case 2 is similar.

*This remark of justification is pretty long, but I think it makes more sense to put it here rather than an independent subsection since all three remarks in this section are justifications. Is it a good practice to include a theorem inside a remark? I skip the proof part because it's too long. What's your consideration?*

**Remark 2.8.** Justifications why we're using our own CS decomposition, not LAPACK's CSD Algorithm – two-phases:

1. The matrix is reduced to a bidiagonal block form.
2. The blocks are simultaneously diagonalized using techniques from the bidiagonal SVD algorithms.
3. Reference: Brian D. Sutton. Computing the complete CS decomposition. Numer. Algorithms, 50(1):33-65, 2009.



## 3 Software

### 3.1 Interface design

The products of the GSVD are six matrices and two integers indicating the rank. To follow Julia's convention, we encapsulate all the products into a composite type named `GeneralizedSVD`. In this way, users do not need to explicitly enumerate every matrix or integer in the return statement. In addition, doing so will facilitate those who only want to access part of the products. Hence, we define the composite type as a struct.

```
struct GeneralizedSVD{T} <: Factorization{T}
    U::AbstractMatrix{T}
    V::AbstractMatrix{T}
    Q::AbstractMatrix{T}
    C::AbstractMatrix{T}
    S::AbstractMatrix{T}
    k::Int
    l::Int
    R::AbstractMatrix{T}
end
```

**Interface 1** We adopt the practice of polymorphism when designing the interface of the GSVD. This enables SVD of one matrix and GSVD of a matrix pair to share a single interface with entities of different input parameters. Such polymorphism allows a function to be written generically and thus maintain the language's expressiveness. We now present the interface below.

```
svd(A, B) -> GeneralizedSVD
```

Compute the generalized SVD of A and B, returning a `GeneralizedSVD` factorization object F, such that  $A = F \cdot U \cdot F^T \cdot C \cdot F^T \cdot R \cdot F^T \cdot Q^T$  and  $B = F \cdot V \cdot F^T \cdot S \cdot F^T \cdot R \cdot F^T \cdot Q^T$ .

For an m-by-n matrix A and p-by-n matrix B,

- U is an m-by-m orthogonal matrix,
- V is a p-by-p orthogonal matrix,
- Q is an n-by-n orthogonal matrix,
- C is an m-by-(k+1) diagonal matrix with 1s in the first K entries,
- S is a p-by-(k+1) matrix whose top right L-by-L block is diagonal,
- R is a (k+1)-by-n matrix whose rightmost (k+1)-by-(k+1) block is nonsingular upper block triangular,
- k+1 is the effective numerical rank of the matrix  $[A; B]$ .

Iterating the decomposition produces the components U, V, Q, C, S, and R.

**Interface 2** As used elsewhere in Julia, we provide another interface that overrides input matrices.

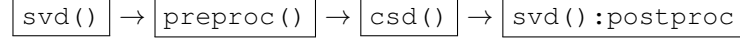
```
svd!(A, B) -> GeneralizedSVD
```

`svd!` is the same as `svd`, but modifies the arguments A and B in-place, instead of making copies.

### 3.2 Architecture

We implement the GSVD algorithm described in the previous section in Julia 1.3 using `Float64` data. The structural unit called `Module` is native to Julia to group relevant functions and definitions. Considering that the CS decomposition not only serves as a building block for our GSVD algorithm, but is also a powerful tool in other applications, it is wise to separate CS decomposition as a standalone module called `CSD`. The main module is `GSVD`.

The algorithm starts from the main function `svd()` under module `GSVD`. It then calls `preproc()`. Once return, it calls `csd` intermodularly. Finally, the main function post processes to formulate the outputs.



### 3.3 Implementation details

*Step 1* Pre-processing:

This step is to reduce two input matrices  $A$  and  $B$  into two upper triangular forms. This is done via a call to `preproc()`. This function makes use of three fundamental orthogonal decompositions. First is QR decomposition with column pivoting to reveal the numerical rank of  $B$  and  $[A; B]$  without forming the matrix explicitly. This is done by a call to `qr(A, pivot=Val(true))`. Second is RQ decomposition via a call to `LAPACK.gerqf!()`. Last is QR decomposition by calling `qr()`. Upon return to `svd()`, two of the upper triangular matrices overwrites  $A$  and  $B$ , the orthogonal matrices are placed in  $U$ ,  $V$ , and  $Q$  and rank information is stored in  $K$  and  $L$ .

*Step 2* QR decomposition:

This step is to reduce two upper triangular matrices to one and is done by directly calling `qr()`. On exit,  $Q_1$  and  $Q_2$  overwrites  $A$  and  $B$ .

*Step 3* CS decomposition:

This step calls `csd()` from module `CSD`. This function requires SVD, QR decomposition and QL decomposition and is done by calls to `svd()`, `qr()` and `LAPACK.geqlf!()` respectively. it return  $U_1, V_1, Z_1, C, S$  on exit.

*Step 4* Post-processing: In this step, we update matrix  $U$ ,  $V$  and  $Q$  by matrix-matrix multiply. To formulate  $R$ , we utilize RQ decomposition via a call to `LAPACK.gerqf!()`. Finally, we put matrices  $U, V, C, S, Q$  and  $K, L$  into the constructor of `GeneralizedSVD` as return.

### 3.4 GSVD in other languages: a comparison

We list several major languages that feature GSVD, shown in Table 1.

Language	GSVD Documentation
Native Julia (proposed)	<code>svd(A, B) -&gt; GeneralizedSVD</code> Computes the generalized SVD of A and B, returning a GSVD factorization object F, such that $A = F.U*F.C*F.R*F.Q'$ and $B = F.V*F.S*F.R*F.Q'$ .
Julia 1.3 (LAPACK wrapper)	<code>svd(A, B) -&gt; GeneralizedSVD</code> Computes the generalized SVD of A and B, returning a GeneralizedSVD factorization object F, such that $A = F.U*F.D1*F.R0*F.Q'$ and $B = F.V*F.D2*F.R0*F.Q'$ .
MATLAB (2019b)	<code>[U,V,X,C,S] = gsvd(A,B)</code> Returns unitary matrices U and V, a (usually) square matrix X, and nonnegative diagonal matrices C and S so that $A = U*C*X'$ , $B = V*S*X'$ , $C'*C + S'*S = I$ .
Mathematica	<code>SingularValueDecomposition[m,a]</code> Gives a list of matrices $\{u, ua, w, wa, v\}$ such that m can be written as $u.w.Conjugate[Transpose[v]]$ and a can be written as $ua.wa.Conjugate[Transpose[v]]$ .
R (geigen v2.3, LAPACK wrapper)	<code>z &lt;- gsvd(A, B)</code> Computes The Generalized Singular Value Decomposition of matrices A and B such that $A = U D_1 [0 \ R] Q^T$ and $B = V D_2 [0 \ R] Q^T$ . Note that the return value is the same as the output of LAPACK 3.6 and above.
Python (R. Luo's thesis)	Didn't disclose API design. The author defined GSVD as follows: Given two $M_i$ -by- $N$ column-matched but row-independent matrices $D_i$ , each with full column rank and $N \leq M_i$ , the GSVD is an exact simultaneous factorization $D_i = U_i \Sigma_i V^T, i = 1, 2$ . $U_i$ is $M_i$ -by- $N$ and are column-wise orthonormal and $V$ is $N$ -by- $N$ nonsingular matrix with normalized rows. $diag(\Sigma_i)$ returns two lists of $N$ positive values and the ratios are called the generalized singular values.

Table 1: GSVD in different languages

## 4 Testing and Performance

### 4.1 Accuracy (backward stability)

**Metric.** We define the following metrics in order to test backward stability:

$$res_A = \frac{\|U^T A Q - C R\|_1}{\max(m, n) \|A\|_1 \epsilon} \quad (4.1)$$

$$res_b = \frac{\|V^T B Q - S R\|_1}{\max(p, n) \|B\|_1 \epsilon} \quad (4.2)$$

$$orth_U = \frac{\|I - U^T U\|_1}{m \epsilon} \quad (4.3)$$

$$orth_V = \frac{\|I - V^T V\|_1}{p \epsilon} \quad (4.4)$$

$$orth_Q = \frac{\|I - Q^T Q\|_1}{n \epsilon} \quad (4.5)$$

where  $\epsilon$  is machine precision of input data type.

#### 4.1.1 Numerical examples of small matrices

We also record the stability metrics computed by both versions in Julia in Table 2.

	Version	$res_A$	$res_B$	$orth_U$	$orth_V$	$orth_Q$
Example 1	proposed	0.2956	0.5646	0.5308	1.0417	1.1790
	Julia 1.3	0.3599	0.4571	0.9117	1.7083	1.3250
Example 2	proposed	0.6173	0.4098	1.5000	0.5613	1.3998
	Julia 1.3	0.5068	0.5689	1.4583	0.9245	1.2483
Example 3	proposed	0.4181	0.8941	0.7500	1.3940	1.3277
	Julia 1.3	0.3536	0.5938	1.4791	1.9540	1.1062
Example 4	proposed	0.3600	0.5900	0.6558	0.5385	1.4362
	Julia 1.3	0.4449	0.3056	1.3225	0.7205	1.1814

Table 2: Stability profiling for small matrices

#### 4.1.2 Random dense matrices

**Test matrix generation.** As discussed in Section 1.1, we test stability on four cases depending on the row and column size of the input matrix pair. In this section, we test random dense matrices of `Float64`. For each case, we choose four subcases from low to high matrix size. We generate a total of 320 random matrix pairs, 20 for each subcase.

**Results.** As a demonstration, we list the results of five stability metrics for each subcase of a single test run in Table 3. All 320 test runs yield results no greater than two.

	$m$	$p$	$n$	$k+l$	$res_A$	$res_B$	$orth_U$	$orth_V$	$orth_Q$
$m \geq n$ $p \geq n$	60	50	40	40	0.1607	0.2710	0.7924	1.0079	0.4609
	300	250	200	200	0.0369	0.0484	0.5041	0.6408	0.3202
	900	750	600	600	0.0181	0.0193	0.3952	0.5157	0.2307
	1500	1250	1000	1000	0.0120	0.0142	0.3702	0.4129	0.1847
$m \geq n > p$	60	40	50	50	0.1529	0.2261	0.7653	1.1960	0.6074
	300	200	250	250	0.0412	0.0620	0.5559	0.7492	0.3150
	900	600	750	750	0.0169	0.0232	0.4174	0.5250	0.2411
	1500	1000	1250	1250	0.0122	0.0160	0.3726	0.4723	0.2080
$p \geq n > m$	40	60	50	50	0.1672	0.2028	1.1293	0.9373	0.4217
	200	300	250	250	0.0595	0.0530	0.7064	0.5855	0.3065
	600	900	750	750	0.0231	0.0231	0.5178	0.4186	0.2112
	1000	1500	1250	1250	0.0164	0.0153	0.4543	0.3673	0.1778
$n > m$ $n > p$	20	30	60	50	0.0483	0.0464	0.5472	0.5358	0.4547
	200	300	600	500	0.0120	0.0105	0.3036	0.3030	0.2374
	400	600	1200	1000	0.0081	0.0072	0.2888	0.2813	0.2315
	1000	1500	3000	2500	0.0053	0.0047	0.2700	0.2605	0.2410

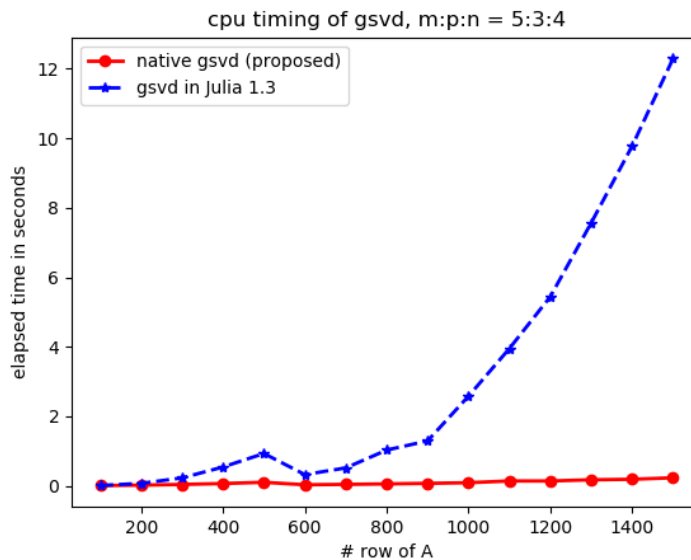
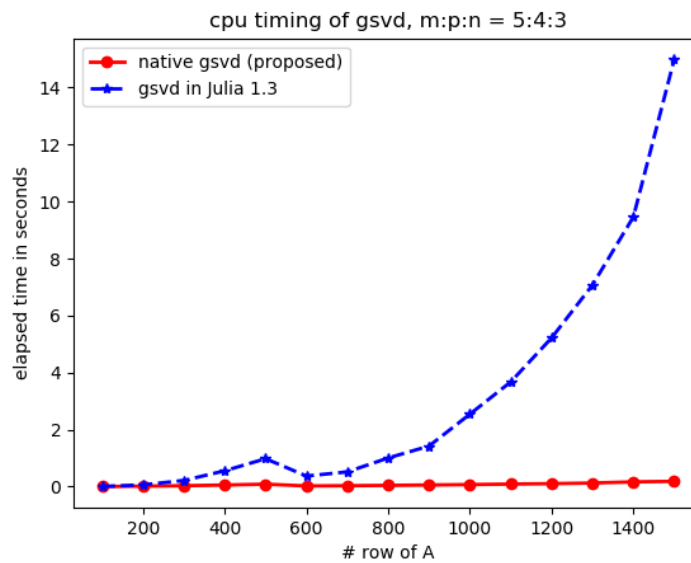
Table 3: Stability profiling for random dense matrices

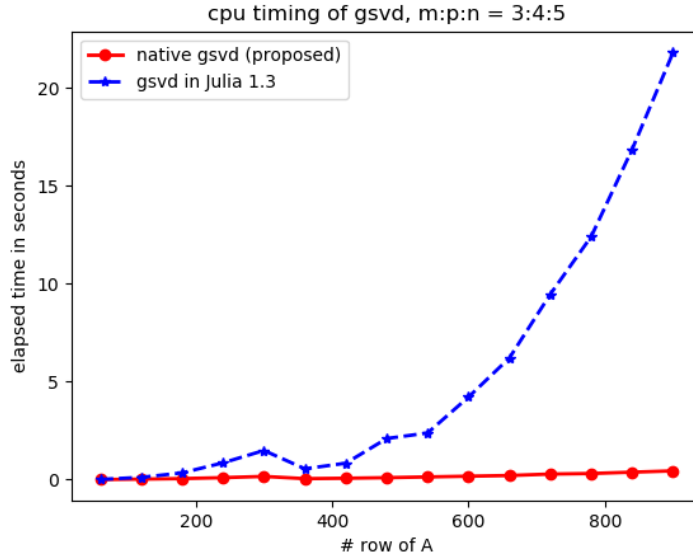
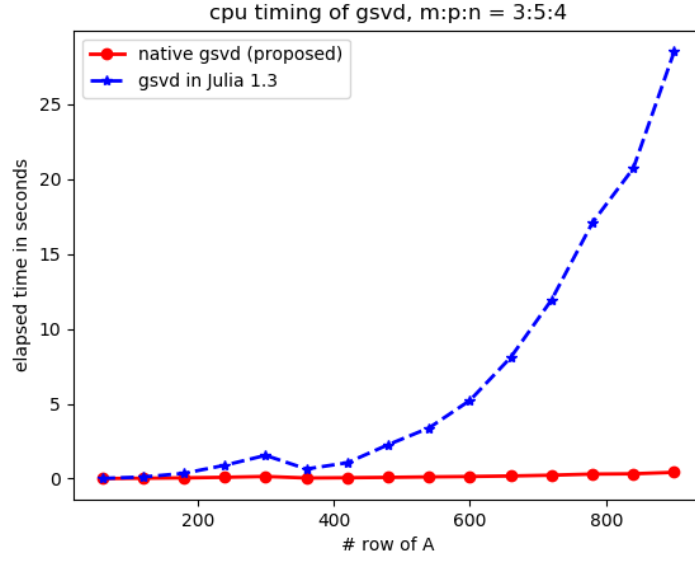
#### 4.1.3 Special types of matrices

## 4.2 Timing

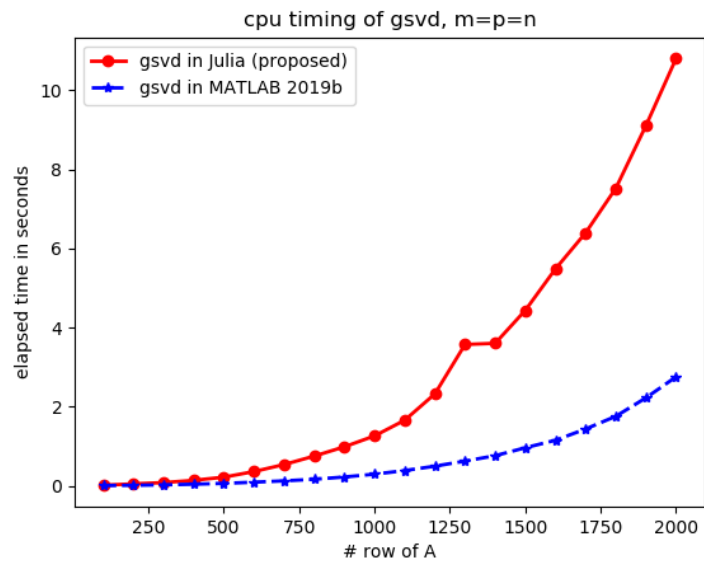
We want to evaluate the timing performance of our implementation between current version in Julia and MATLAB.

**vs. Julia 1.3** For the comparison with Julia 1.3, we also spilt into four cases. Each case, we calculated the average CPU timing of 10 runs. In all cases, we can see that the speedup is exponential when input size is greater than a few hundreds.





**vs. MATLAB.** For the comparison with MATLAB 2019b, we specify the input as square matrix. Our implementation is still slower than MATLAB. The major reason is due to the significant difference of decomposition discussed in 1.1 and 1.3.





**Profile.** As detailed in 2.1, our algorithm insists of four parts: pre-processing, QR, CSD and post-processing. Here, we measure the CPU time spent in the first three parts and total time, denoted as  $t_{pre}, t_{qr}, t_{csd}$  and  $t_{all}$  and calculated the percentages that each part spent to total time, denoted as  $p_{pre}, p_{qr}, p_{csd}$ . Still, we separate our test into four cases and record the average of 10 test runs. **In most cases, pre-processing dominates the computation effort.** This motivates us to explore time profiling of pre-processing.

	$m$	$p$	$n$	$t_{pre}$	$p_{pre}$	$t_{qr}$	$p_{qr}$	$t_{csd}$	$p_{csd}$	$t_{all}$
$m \geq n$ $p \geq n$	1500	1200	1000	0.6242	41.13%	0.1683	11.09%	0.6011	39.61%	1.5175
	500	500	500	0.0651	26.78%	0.0347	14.29%	0.1191	48.94%	0.2433
	650	310	230	0.0418	54.63%	0.0084	11.08%	0.0195	25.47%	0.0766
	430	610	210	0.0345	47.65%	0.0067	9.25%	0.0247	34.11%	0.0725
$m \geq n > p$	1500	1000	1200	1.500	60.09%	0.1815	7.27%	0.6811	27.28%	2.4963
	720	220	540	0.1182	73.65%	0.0074	4.61%	0.0256	15.94%	0.1605
	440	180	440	0.0651	65.84%	0.0053	5.37%	0.0221	22.41%	0.0989
	370	290	350	0.0659	51.61%	0.0123	9.65%	0.0400	31.34%	0.1278
$p \geq n > m$	1000	1500	1200	0.5234	23.23%	0.2789	12.37%	1.2630	56.06%	2.2529
	250	300	300	0.0205	24.96%	0.0129	15.75%	0.0397	48.25%	0.0822
	360	660	600	0.0645	18.33%	0.0436	12.39%	0.2103	59.72%	0.3521
	130	520	480	0.0311	14.52%	0.0215	10.02%	0.1391	64.79%	0.2146
$n > m$ $n > p$	1000	1200	1500	1.7532	48.51%	0.2038	5.64%	1.4467	40.03%	3.6136
	260	600	770	0.2791	38.86%	0.0441	6.14%	0.3459	48.17%	0.7181
	370	250	700	0.1385	86.69%	0	0%	0	0%	0.1598
	120	120	400	0.0296	96.70%	0	0%	0	0%	0.0307

Table 4: Time profiling for GSVD

**Pre-processing.** To avoid skipping steps in pre-processing, we use rank-deficient matrix as input of  $B$ . Likewise the time profiling of GSVD, we record absolute time spent in each part and the relative percentage to total time. The meaning of subscript in Table 5 is explained below:

1.  $grpB$ : QR decomposition with column pivoting of  $B$ .
2.  $genV$ : Generate  $V$ .
3.  $updateA1st$ : First time to update  $A$ .
4.  $genQ$ : Generate  $Q$ .
5.  $rqB$ : RQ decomposition of  $B$ .
6.  $updateA2nd$ : Second time to update  $A$ .
7.  $updateQ1st$ : First time to update  $Q$ .
8.  $grpA$ : QR decomposition with column pivoting of  $A$ .
9.  $genU$ : Generate  $U$ .
10.  $updateA3rd$ : Third time to update  $A$ .
11.  $updateQ2nd$ : Second time to update  $Q$ .
12.  $rqA$ : RQ decomposition of  $A$ .
13.  $updateQ3rd$ : Third time to update  $Q$ .
14.  $qrA$ : QR decomposition of  $A$ .
15.  $updateU$ : Update  $U$ .

	$m = 1200, p = 1000, n = 900$ $l = 800, k = 100$	$m = 500, p = 500, n = 600$ $l = 400, k = 200$	$m = 250, p = 200, n = 200$ $l = 150, k = 50$
$t_{grpB} (p\text{-by-}n)$	0.036821	0.018432	0.002894
$p_{grpB}$	15.29%	21.59%	11.19%
$t_{genV} (p\text{-by-}p)$	0.022350	0.006850	0.001578
$p_{genV}$	9.28%	8.02%	6.10%
$t_{updateA1st} (m\text{-by-}n)$	0.012765	0.005162	0.000736
$p_{updateA1st}$	5.30%	6.05%	2.84%
$t_{genQ} (n\text{-by-}n)$	0.002553	0.001187	0.000195
$p_{genQ}$	1.06%	1.39%	0.75%
$t_{rqB} (l\text{-by-}n)$	0.024456	0.010305	0.001856
$p_{rqB}$	10.16%	12.07%	7.18%
$t_{updateA2nd} (m\text{-by-}n)$	0.019261	0.005071	0.000781
$p_{updateA2nd}$	8.00%	5.94%	3.02%
$t_{updateQ1st} (n\text{-by-}n)$	0.014279	0.005488	0.000732
$p_{updateQ1st}$	5.93%	6.43%	2.82%
$t_{grpA} (m\text{-by-}n - l)$	0.002878	0.004063	0.000595
$p_{grpA}$	1.20%	4.76%	2.30%
$t_{genU} (m\text{-by-}m)$	0.015431	0.007718	0.001051
$p_{genU}$	6.40%	9.04%	4.06%
$t_{updateA3rd} (m\text{-by-}l)$	0.009105	0.002531	0.000412
$p_{updateA3rd}$	3.78%	2.96%	1.59%
$t_{updateQ2nd} (n\text{-by-}n - l)$	0.000289	0.000871	0.000136
$p_{updateQ2nd}$	0.12%	1.02%	0.53%
$t_{rqA} (k\text{-by-}n - l)$	0	0	0
$p_{rqA}$	0%	0%	0%
$t_{updateQ3rd} (n\text{-by-}n - l)$	0	0	0
$p_{updateQ3rd}$	0%	0%	0%
$t_{qrA} (m - k\text{-by-}l)$	0.022391	0.002823	0.001756
$p_{qrA}$	9.30%	4.76%	6.79%
$t_{updateU} (m\text{-by-}m - k)$	0.022113	0.001799	0.000850
$p_{updateU}$	9.18%	2.11%	3.28%
$t_{all}$	0.240752	0.085373	0.025867

Table 5: Time profiling for Preprocessing

## 5 Applications

### 5.1 Genomic signal processing

The GSVD is applicable for comparative analysis of genome-scale expression datasets of two different organisms [12] and is further extended to tensor [13].

### 5.2 Tikhonov regularization

Tikhonov regularization in general form can be analyzed with the truncated GSVD when we are to solve the ill-posed linear least squares problem. [14] [15] [16] Computerized ionospheric tomography [17] is one of the applications in this regard.

### 5.3 Matrix pencil $A - \lambda B$

The GSVD is also used in the field of the canonical structure of matrix pencil  $A - \lambda B$ . [18] More specifically, the column and row nullities of  $A$  and  $B$  and common null space reveal the information about the Kronecker structure of  $A - \lambda B$ .

### 5.4 Generalized total least squares problem

By making use of the GSVD, one can solve the generalized TLS problem. TLS is also called error-in-variable regression in statistics domain. The great advantage of the GSVD is that it replaces these implicit transformation of data procedures by one, which is numerically reliable and can more easily handle (nearly) singular associated error covariance matrix. [19] [20]

### 5.5 Oriented energy and oriented signal-to-signal ratio

In the context of oriented energy, one of the concerns is to characterize the signal-to-signal ratio of two given sequences of  $m$ -vectors  $\{a_k\}$ ,  $\{b_k\}$ ,  $k = 1, \dots, n$  with associated  $m$ -by- $n$  matrices  $A$  and  $B$ . [21] In other words, we're primarily interested in how to separate the desired signal (for instance  $\{a_k\}$ ) from the undesired one ( $\{b_k\}$ ). More specifically, given that  $\text{rank}(B) = l$ , the question transforms to find the optimal  $l$ -dimensional subspace where the desired signal sequence  $\{a_k\}$  can be optimally distinguished from the corrupting sequence  $\{b_k\}$ .

### 5.6 Subspaces of the $U$ matrix

[2] The  $U$  matrix of the GSVD provides orthonormal bases for three mutually orthogonal subspaces that are powerful in many applications:

$$U = \begin{bmatrix} U_1 = & U_2 = & U_3 = \\ \text{orthogonal basis for} & \text{completion to all of} & \text{orthonormal basis for} \\ \{Ax : Bx = 0\} & \text{col}(A) = \{Ax\} & \text{col}(A)^\perp \end{bmatrix}$$

The "completion" referred to in the above equation means that taken together, the columns of  $U_1$  and  $U_2$  form an orthonormal basis for  $\text{col}(A)$ .

#### 5.6.1 Linear discriminant analysis

Howland and Park [22] [23] applied the GSVD to discriminant analysis to overcome the limitation of nonsingular covariance matrices that are used to represent the scatter within and between clustered text data.

### 5.6.2 One Way ANOVA (Analysis of variance)

A commonly used statistics test is to decide whether a proposed clustering of a vector  $v$  is justified. The test takes the average square component in the  $U_2$  direction and divides it by the average square component in the  $U_3$  direction. [24]

## 5.7 The Jacobi ensemble from random matrix theory is a GSVD

[2] Classical random matrix theory centers are Hermite, Laguerre, and Jacobi ensembles. Historically, they are presented in eigenvalue format, but we have argued that the eigenvalue, SVD, GSVD formats, respectively, are mathematically more natural providing simpler derivations and clearer insights.

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