

# GSVD in Julia

Prepared by Ji Wang (jiiwang@ucdavis.edu)

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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

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

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

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

$$R_0 = \begin{bmatrix} 5.74065 & -7.07986 & -0.125979 & 0.316232 \\ 0.0 & -7.96103 & 2.11852 & 2.98601 \\ 0.0 & 0.0 & -5.72211 & 0.43623 \\ 0.0 & 0.0 & 0.0 & 5.66474 \end{bmatrix}$$

$X = R_0 Q^T$   
 $\uparrow$   
 eigenvalue matrix  
 of  $(A^T A, B^T B)$

The residual norms

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

$$U = \begin{bmatrix} 0.4822 & -0.4489 & -0.4467 & -0.0610 & -0.6023 \\ -0.1159 & 0.4162 & -0.8671 & 0.0905 & 0.2309 \\ -0.4773 & -0.6367 & -0.2125 & -0.4819 & 0.2989 \\ -0.4208 & 0.4107 & 0.0348 & -0.5232 & -0.6159 \\ 0.5909 & 0.2261 & 0.0475 & -0.6943 & 0.3396 \end{bmatrix}$$

$$V = \begin{bmatrix} 0.4946 & -0.3285 & -0.8046 \\ -0.8089 & -0.5125 & -0.2880 \\ -0.3178 & 0.7934 & -0.5192 \end{bmatrix}$$

$$X = \begin{bmatrix} 0.8758 & 4.8394 & -5.1611 & -2.0437 \\ -4.8715 & -1.2203 & -5.5489 & -1.7290 \\ 1.8753 & -2.2244 & -4.2415 & -7.4528 \\ -2.0184 & 1.7541 & -1.1683 & -4.5260 \end{bmatrix}$$

check:  
 — Not an eigenvalue matrix

$X^{-1}$ : Is this an eigenvalue matrix?

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.

---

<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  $A, B$  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 safe diagonalization of a matrix with orthonormal columns that is partitioned into two blocks. [7] The last step is post-processing to get the final products 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.

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

$$BP = V \begin{matrix} & \ell & n - \ell \\ \ell & \begin{pmatrix} B_{11} & B_{12} \\ 0 & 0 \end{pmatrix} \\ p - \ell & \end{matrix} \quad (2.1)$$

Step 1(2) Update  $A := AP$

Step 1(3) Set  $Q := I_n$  and update  $Q := QP$

Step 1(4) If  $n > \ell$ :

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

$$\begin{matrix} \ell & n - \ell & n - \ell & \ell \\ \ell & \begin{pmatrix} B_{11} & B_{12} \end{pmatrix} = \ell \begin{pmatrix} & \\ 0 & B_{13} \end{pmatrix} Z \end{matrix} \quad (2.2)$$

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

Step 1(5) Partition

$$A = \begin{matrix} & n - \ell & \ell \\ m & \begin{pmatrix} A_1 & A_2 \end{pmatrix}, \end{matrix} \quad (2.3)$$

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

$$A_1 P_1 = U \begin{matrix} & k & n - \ell - k \\ m - k & \begin{pmatrix} A_{11} & A_{12} \\ 0 & 0 \end{pmatrix} \end{matrix} \quad (2.4)$$

Step 1(6) Update  $A_2 := U^T A_2$

Step 1(7) Partition:

$$A = \begin{matrix} & k & n - \ell - k & \ell \\ m - k & \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ 0 & 0 & A_{23} \end{pmatrix} \end{matrix} \quad (2.5)$$

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

Step 1(9) If  $n - \ell > k$ :

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

$$k \begin{pmatrix} A_{11} & A_{12} \end{pmatrix} = k \begin{pmatrix} 0 & A_{12} \end{pmatrix} Z_1 \quad (2.6)$$

and it results

$$A = \begin{matrix} & n-\ell-k & k & \ell \\ m-k & \begin{pmatrix} 0 & A_{12} & A_{13} \\ 0 & 0 & A_{23} \end{pmatrix} \end{matrix} \quad (2.7)$$

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

Step 1(10) If  $m > k$ :

Let

$$A_2 = \begin{matrix} & \ell \\ m-k & \begin{pmatrix} A_{13} \\ A_{23} \end{pmatrix} \end{matrix} \quad (2.8)$$

- QR decomposition of  $A_{23}$ :

$$A_{23} = U_1 \begin{matrix} & \ell \\ m-k-\ell & \begin{pmatrix} A_{23} \\ 0 \end{pmatrix} \end{matrix} \quad (2.9)$$

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

In summary, combining (2.1), (2.2), (2.4), (2.6), (2.7) and (2.9), we have the following decomposition at the end of the pre-processing:

$$A = UR_AQ^T, \quad B = VR_BQ^T \quad (2.10)$$

where

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

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

where  $A_{12}$  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  $m - k - \ell < 0$ :

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

where  $A_{12}$  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.

Note:  $R_A$  and  $R_B$  overwrite  $A$  and  $B$ , respectively.

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

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

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

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

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

Thus, (2.10) can be rewritten as:

$$A = U(Q_A \hat{R})Q^T, \quad B = V(Q_B \hat{R})Q^T \quad (2.11)$$

where

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

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

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

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

**Step 3. Safe Diagonalization of  $Q_1$  and  $Q_2$ .** Use the algorithm described in section 2.2, compute the CS decomposition:

$$Q_1 = U_1 \Sigma_1 Z_1^T, \quad Q_2 = V_1 \Sigma_2 Z_1^T \quad (2.12)$$

where

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

$Q_1, Q_2$  are  $\ell$ -by- $\ell$ ,  $U_1, Z_1$  and  $V_1$  are  $\ell$ -by- $\ell$  orthogonal matrices, and  $\Sigma_1$  and  $\Sigma_2$  are  $\ell$ -by- $\ell$  diagonal matrices:

$$\Sigma_1 = \text{diag}(\alpha_1, \alpha_2, \dots, \alpha_\ell), \quad \Sigma_2 = \text{diag}(\beta_1, \beta_2, \dots, \beta_\ell)$$

where  $1 \geq \alpha_1 \geq \alpha_2 \geq \dots \geq \alpha_\ell \geq 0$ ,  $0 \leq \beta_1 \leq \beta_2 \leq \dots \leq \beta_\ell \leq 1$  and  $\Sigma_1^T \Sigma_1 + \Sigma_2^T \Sigma_2 = I_\ell$ .

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

$Q_1$  is  $(m-k)$ -by- $\ell$ ,  $Q_2$  are  $\ell$ -by- $\ell$ ,  $U_1$  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 and  $\Sigma_2$  is  $\ell$ -by- $\ell$  diagonal:

$$\Sigma_1 = \begin{matrix} m-k & \ell-m+k \\ m-k & \ell-m+k \\ 0 & 0 \end{matrix} \begin{pmatrix} \Pi_1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \Sigma_2 = \begin{matrix} m-k & \ell-m+k \\ m-k & \ell-m+k \\ \ell-m+k \end{matrix} \begin{pmatrix} \Pi_2 & 0 \\ 0 & I \end{pmatrix}$$

where  $\Pi_1 = \text{diag}(\alpha_1, \alpha_2, \dots, \alpha_{m-k})$ ,  $\Pi_2 = \text{diag}(\beta_1, \beta_2, \dots, \beta_{m-k})$ , and  $1 \geq \alpha_1 \geq \alpha_2 \geq \dots \geq \alpha_{m-k} \geq \alpha_{m-k+1} = \dots = \alpha_\ell = 0$  and  $0 \leq \beta_1 \leq \beta_2 \leq \dots \leq \beta_{m-k} \leq \beta_{m-k+1} = \dots = \beta_\ell = 1$ .  $\Sigma_1^T \Sigma_1 + \Sigma_2^T \Sigma_2 = I_\ell$ .

Combining (2.11) and (2.12), we have

$$A = U(\hat{U}C\hat{Q}^T)\hat{R}Q^T, \quad B = V(\hat{V}S\hat{Q}^T)\hat{R}Q^T \quad (2.13)$$

where

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

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

and

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

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

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

and

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

#### Step 4. Post-processing to form the desired GSVD (1.1).

- $U := U\hat{U}$ .
- $V := V\hat{V}$ .
- Formulate  $R$  by RQ decomposition:  $\hat{Q}^T \hat{R} = RQ_3$
- $Q := QQ_3^T$
- $C$  and  $S$  defined in (2.13).

## 2.2 GSVD of $Q_1$ and $Q_2$

**Why do we call it GSVD rather than safe diagonalization in the subsection title? typo?** In this section, we detail algorithm of **Step 2 of the GSVD algorithm** for computing the safe diagonalization of  $Q_1$  and  $Q_2$ , where if  $m - k - \ell \geq 0$ ,

$$Q_1, Q_2 \in \mathbb{R}^{\ell \times \ell},$$

and if  $m - k - \ell < 0$ ,

$$Q_1 \in \mathbb{R}^{(m-k) \times \ell} \quad \text{and} \quad Q_2 \in \mathbb{R}^{\ell \times \ell}.$$

This is a special case of the 2-by-1 Cosine-sine decomposition. [9]

Step 2(1). Compute the SVD of  $Q_2$ :

$$Q_2 = V_1 \Sigma_2 Z_1^T, \quad (2.14)$$

where  $V_1$  is  $\ell$ -by- $\ell$  and  $Z_1$  is  $\ell$ -by- $\ell$ , both are orthogonal matrices.  $\Sigma_2 = \text{diag}(\beta_\ell, \dots, \beta_1)$  such that  $1 \geq \beta_\ell \geq \beta_{\ell-1} \geq \dots \geq \beta_1 \geq 0$ .



Step 2(2). Reverse the order of  $\beta_i$  in non-decreasing order:

- Reorder the diagonal entries of  $\Sigma_2$  non-decreasingly:  $\Sigma_2 = \text{diag}(\beta_1, \dots, \beta_\ell)$ ;
- Reverse the columns of  $V_1$ :  $V_1 := V_1(:, \ell : -1 : 1)$ ;
- Reverse the columns of  $Z_1$ :  $Z_1 := Z_1(:, \ell : -1 : 1)$ .

Step 2(3). Determine  $r$  such that  $0 \leq \beta_1 \leq \dots \leq \beta_r \leq \frac{1}{\sqrt{2}} < \beta_{r+1} \leq \dots \leq \beta_\ell \leq 1$ .

The justification for  $r$  see Remark 2.1.

Step 2(4). Matrix-matrix multiply:

$$T = Q_1 Z_1 \quad (2.15)$$

Step 2(5). QR decomposition of  $T$ :

$$T = U_1 R, \quad (2.16)$$

- If  $m - k - \ell \geq 0$ :  
since  $Q_1$  is  $\ell$ -by- $\ell$ ,  $U_1$  is an  $\ell$ -by- $\ell$  orthogonal matrix, and

$$R = \begin{matrix} & r & \ell - r \\ r & \Pi & \epsilon \\ \ell - r & 0 & R_{22} \end{matrix}, \quad (2.17)$$

where  $\Pi = \text{diag}(\alpha_1, \dots, \alpha_r)$ . The bottom  $(\ell - r)$  rows vanish if  $\ell - r \leq 0$ .

For the explanation of why  $R_{22}$  may not be diagonal, see Remark 2.1.

- If  $m - k - \ell < 0$ :  
since  $Q_1$  is  $(m - k)$ -by- $\ell$ ,  $U_1$  is an  $(m - k)$ -by- $(m - k)$  orthogonal matrix, and

$$R = \begin{matrix} & r & m - k - r & \ell - m + k \\ r & \Pi & \epsilon & \epsilon \\ m - k - r & 0 & R_{22} & R_{23} \end{matrix}, \quad (2.18)$$

where  $\Pi = \text{diag}(\alpha_1, \dots, \alpha_r)$ . The bottom  $(m - k - r)$  rows vanish if  $m - k - r \leq 0$ .

For the explanation of why  $\begin{bmatrix} R_{22} & R_{23} \end{bmatrix}$  may not be diagonal, see Remark 2.1.

Combining (2.15) and (2.16), we obtain:

$$Q_1 = U_1 R Z_1^T \quad (2.19)$$

As stated in (2.17) and (2.18), the last few rows of  $R$  might not exist. To be precise,

- If  $m - k - \ell \geq 0$  and  $\ell \leq r$ :  $R = \text{diag}(\alpha_1, \dots, \alpha_\ell)$ .
- If  $m - k - \ell < 0$  and  $m - k \leq r$ :

$$R = \begin{matrix} & m - k & \ell - m + k \\ m - k & \Pi & 0 \end{matrix}, \quad (2.20)$$

where  $\Pi = \text{diag}(\alpha_1, \dots, \alpha_{m-k})$ .

In either case,  $\Sigma_1 = R$ , the algorithm ends here since we already obtain (2.12).

Step 2(6). Refine  $R$  in (2.16) to diagonal if necessary:

- If  $m - k - \ell \geq 0$  and  $\ell - r > 0$ :

- SVD of the block  $R_{22}$  of  $R$  in (2.17):

$$R_{22} = U_r C_r Z_r^T \quad (2.21)$$

where  $U_r$  is an  $(\ell - r)$ -by- $(\ell - r)$  orthogonal matrix,  $Z_r$  is an  $(\ell - r)$ -by- $(\ell - r)$  orthogonal matrix and  $C_r = \text{diag}(\alpha_{r+1}, \dots, \alpha_\ell)$ .

- Update the  $(r + 1)$ -th to  $\ell$ -th columns of  $U_1$ :

$$U_1 := U_1 \begin{matrix} r & \ell - r \\ \ell - r \end{matrix} \begin{pmatrix} I & 0 \\ 0 & U_r \end{pmatrix}$$

- Update the last  $(\ell - r)$  columns of  $Z_1$ :

$$Z_1 := Z_1 \begin{matrix} r & \ell - r \\ \ell - r \end{matrix} \begin{pmatrix} I & 0 \\ 0 & Z_r \end{pmatrix}$$

- Rewrite  $R$  to formulate  $\Sigma_1$ :

$$\Sigma_1 = \begin{matrix} r & \ell - r \\ \ell - r \end{matrix} \begin{pmatrix} \Pi & 0 \\ 0 & C_r \end{pmatrix}$$

- If  $m - k - \ell < 0$  and  $m - k - r > 0$ :

- SVD of the block  $\begin{bmatrix} R_{22} & R_{23} \end{bmatrix}$  of  $R$  in (2.18):

$$\begin{bmatrix} R_{22} & R_{23} \end{bmatrix} = U_r C_r Z_r^T \quad (2.22)$$

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

- Update the  $(r + 1)$ -th to  $(m - k)$ -th columns of  $U_1$ :

$$U_1 := U_1 \begin{matrix} r & m - k - r \\ m - k - r \end{matrix} \begin{pmatrix} I & 0 \\ 0 & U_r \end{pmatrix}$$

- Update the last  $(\ell - r)$  columns of  $Z_1$ :

$$Z_1 := Z_1 \begin{matrix} r & \ell - r \\ \ell - r \end{matrix} \begin{pmatrix} I & 0 \\ 0 & Z_r \end{pmatrix}$$

- Rewrite  $R$  to formulate  $\Sigma_1$ :

$$\Sigma_1 = \begin{matrix} r & \ell - r \\ m - k - r \end{matrix} \begin{pmatrix} \Pi & 0 \\ 0 & C_r \end{pmatrix}$$

Thus, the final decomposition of  $Q_1$  is the following:

$$Q_1 = U_1 \Sigma_1 Z_1^T \quad (2.23)$$

Step 2(7). If  $R$  is refined in Step 2(6), i.e.,  $Z_1$  is modified, we need to update  $V$  as well:

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

$$W = Q_w R_w \quad (2.24)$$

- Update last  $(\ell - r)$  columns of  $V$ :

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

**Remark 2.1.** This algorithm extends the one proposed by Van Loan [10].

First, we briefly justify here why we choose  $\frac{1}{\sqrt{2}}$  as the threshold. 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  $((\frac{1}{\sqrt{2}})^2 + (\frac{1}{\sqrt{2}})^2 = 1)$  so that it nicely separates large singular values from tiny singular values. This theoretical yet empirical choice is first suggested by Van Loan in [10] because the midpoint balances the backward error defined in (4.2) - (4.6) and performance.

We then explain why  $R$  may not be diagonal in finite precision arithmetic.

In Step 2(4), in exact arithmetic, it follows that:

$$\begin{aligned} T^T T &= (Q_1 Z_1)^T Q_1 Z_1 \\ &= Z_1^T Q_1^T Q_1 Z_1 \\ &= Z_1^T (I - Q_2^T Q_2) Z_1 \\ &= Z_1^T (I - Z_1 \Sigma_2^T V_1^T V_1 \Sigma_2 Z_1^T) Z_1 \\ &= Z_1^T (I - Z_1 \Sigma_2^T \Sigma_2 Z_1^T) Z_1 \\ &= I - \Sigma_2^T \Sigma_2 \\ &= \text{diag}(1 - \beta_1^2, 1 - \beta_2^2, \dots, 1 - \beta_\ell^2) \end{aligned} \quad (2.25)$$

Therefore, QR of  $T$  leads to diagonal  $R$ , the reasoning is the follows: by Step 2(5)  $T^T T = (U_1 R)^T U_1 R = R^T R$  is diagonal by (2.25) and  $R$  is upper triangular, thus  $R$  must be diagonal.

But in numerical computation, we cannot ignore the upper-diagonal entries of  $R_{22}$  and  $\begin{bmatrix} R_{22} & R_{23} \end{bmatrix}$  in (2.17) and (2.18) respectively.

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

**Theorem 2.2.** 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:

$$X = QR, \quad (2.26)$$

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

$$|R(i, j)| \leq \min\{\|x_j\|, \frac{\|E\|}{\sigma_{\min}(X_i)}\}. \quad (2.27)$$

*Proof.* This theorem is proved by Van Loan in **Theorem 3.2** [10, 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 the upper-diagonal block matrices of the first  $r$  rows of  $R$  in both (2.17) and (2.18) are effectively zero matrices.

On the contrary, we have:

$$|R_{22}| \simeq \sqrt{1 - \beta_{r+1}} < \frac{1}{\sqrt{2}}, \quad (2.28)$$

$$\left| \begin{bmatrix} R_{22} & R_{23} \end{bmatrix} \right| \simeq \sqrt{1 - \beta_{r+1}} < \frac{1}{\sqrt{2}} \quad (2.29)$$

for (2.17) and (2.18), respectively, both of which suggest that these two submatrices are not well-conditioned and hence their upper-diagonal entries cannot be neglected.

## 2.3 Remarks

**Remark 2.3.** Michael Stewart [11] 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 2.4.** The algorithm presented here is “similar to” that introduced by Golub and Van Loan [6, pp. 502–503] 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 2.5.** 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 (2.10) such that

$$A_{23} = U_1 C R Q_1^T, \quad B_{13} = V_1 S R Q_1^T. \quad (2.30)$$

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.

### 3 Software

The first numerical computing language Fortran, short for “Formula Translating System”, was released in 1957. Over six decades, the landscape of computing has changed dramatically due to the advance of hardware, algorithms, and tremendous increased amount of data, among others. An unfortunate outcome is that the most challenging areas of scientific computing have benefited the least from the enhanced abstraction and productivity offered by higher-level languages. Modern scientific computing environments such as Python (Numpy)[12], R [13], Mathematica [14], and MATLAB [15], to name a few, have grown in popularity and fall under the general category known as dynamic languages or dynamically typed languages. Still, when it comes to performance, C and Fortran remain the de facto for solving computationally intensive problems, especially in large scale.

**Why Julia?** Fortunately, Julia’s innovation lies exactly in the combination of productivity and performance. [16] Julia programming language fulfills much of the Fortran dream: automatic translation of formulas into efficient executable code. This means that by making use of JIT compilation, Julia can generate optimized native code for multiple architectures and can approach the speed of Fortran and C. On top of that, it allows programmers to write clear, high-level, generic and abstract code that closely resembles mathematical formulas, yet produces fast, low-level machine code that has traditionally only been generated by static languages.

In light of this, we implement the algorithm to compute the GSVD described in the previous section in Julia 1.3. In this section, we start with the design of the interface of the algorithm. Then, we show a high-level architecture of the numerical software and present implementation details. Finally, we conclude the features we explored in the process of implementation and some bottlenecks.

#### 3.1 Interface design

The products of the GSVD are six matrices and two integers indicating the rank information. To follow Julia’s convention as an object-oriented language, 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
```

In the nineties, the cost of computer storage was a great concern in computational efforts. Thus, mostly of the LAPACK routines overwrite input matrices or vectors as outputs. Nowadays, computers are made much more cheaper, but the communication cost between memory and cache remains a bottleneck for numerical computing. Functions in Julia, particularly in “LinearAlgebra” package, are two-fold: one makes a copy of the input matrices or vectors, the other overwrite the inputs to save space. Now, we are ready to present the two interfaces.

**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 number of input parameters. Such polymorphism allows a function to be written generically and thus maintain the language’s expressiveness.

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

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

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. It returns a `GeneralizedSVD` factorization object  $F$ , such that  $A = F.U*F.C*F.R*F.Q'$  and  $B = F.V*F.S*F.R*F.Q'$ .

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  $R$ .

### 3.2 Architecture design

The structural unit called `Module` is native in Julia to group relevant functions and definitions. The main module is `GSVD`. Considering that the safe diagonalization 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 safe diagonalization as a standalone module called `SafeDiag`. The high-level architecture of the GSVD software is shown in the UML class diagram below.

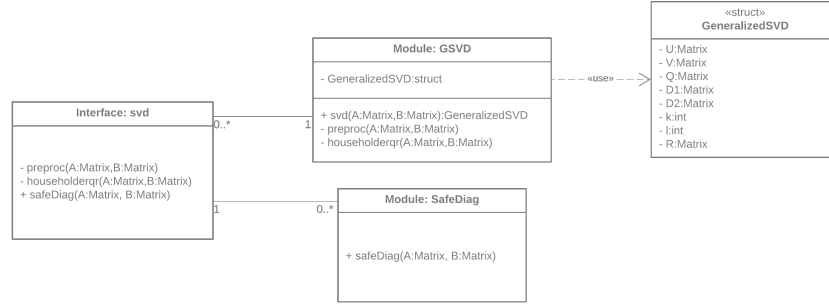


Figure 1: UML class diagram for the GSVD

According to the architecture design, the algorithm thus starts from the main function `svd()` under module `GSVD`. It then calls `preproc()`. Once return, it calls function `safeDiag` intermodularly. Finally, upon return, the main function post-processes to formulate the outputs. The sequence of the major function calls is the following.



### 3.3 Implementation details

We implement the GSVD algorithm described in the previous section in Julia 1.3 using `Float64` data.

#### 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.

- (a) 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})`. Let `tolB` as the tolerance to determine the effective rank of  $B = \ell$ .

$$\text{tol}_B = \max\{p, n\} \|B\|_1 \epsilon$$

where  $\epsilon$  is the machine precision of `Float64`.

We also use QR decomposition with column pivoting again on the leftmost  $n - \ell$  columns of  $A$ . Similarly, by defining

$$\text{tol}_A = \max\{m, n\} \|A\|_1 \epsilon$$

we compute the effective rank of  $[A; B] = k + \ell$ .

- (b) Second is RQ decomposition of the top  $\ell$  rows of  $B$  if  $n > \ell$  via a call to `LAPACK.gerqf!()`. It is called a second time on  $A$  if  $n - \ell > k$ .
- (c) Third is QR decomposition of  $A$  when  $m > k$  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  $\ell$ .

**Step 2** QR decomposition:

This step is to reduce two upper triangular matrices to one and is done by calling `householderqr()`. On entry, two triangular matrices are stacked together and passed as the arguments of `qr()`. On exit,  $Q_1$  and  $Q_2$  overwrites inputs.

**Step 3** Safe diagonalization:

This step calls `safeDiag()` from module `SafeDiag`. This function requires SVD, and QR decomposition. This is done by calls to `svd()`, `qr()` respectively.

- (a) We first compute SVD of  $Q_2$ . To preserve the order of  $\{\cos \theta\}$ , we have to reverse the order of the singular values of  $Q_2$ .
- (b) Since  $\{\cos \theta\}$  are already sorted, we take advantage of binary search to find the threshold  $r$ .
- (c) QR decomposition of the multiply of  $Q_1$  and right singular vectors of  $Q_2$ .  $R$  is not only triangular but diagonal. However, sanitization is necessary to assure the non-negativity of the diagonal entries.

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  $k, \ell$  into the constructor of `GeneralizedSVD` as return.

### 3.4 Julia: features and issues

Through implementation, we exploit advantages of Julia. Meanwhile, we also capture some pitfalls that might be a bottleneck, and thus are worth mentioning.

**Expressiveness.** MATLAB users may find a smooth transition to Julia as a fair amount of syntax of Julia are similar to that of MATLAB, if not the same. To begin with, both Julia and MATLAB use `end` keyword to indicate code block. What's more, thanks to the magic of multiple dispatch, Julia brings ease of use to its programmers. Specifically, elementary operations are intuitive, as simple as math.

Operator	Function	Operand
+	add numbers/vectors/matrices	Int, Float, Vector, Abstract Matrix, Dense Matrix, ...
*	multiply scale or compose	Number, Function

In linear algebra, MATLAB programmers may first find Julia more friendly because the array index in Julia also starts at 1, not 0. Those who are familiar with MATLAB functions should quickly adapt new adventure in Julia. The table below summarizes a list of Julia commands for frequently used matrix decompositions, and their counterparts in MATLAB.



Julia command	MATLAB command	Description
<code>schur(A::StridedMatrix) -&gt; F::Schur</code>	<code>T = schur(A)</code>	Schur decomposition
<code>lu(A, pivot=Val(true); check = true) -&gt; F::LU</code>	<code>[L,U] = lu(A)</code>	LU decomposition
<code>qr(A, pivot=Val(false)) -&gt; F</code>	<code>[Q,R] = qr(A)</code>	QR decomposition
<code>eigen(A; permute::Bool=true, scale::Bool=true, sortby) -&gt; Eigen</code>	<code>[V,D] = eig(A)</code>	Eigenvalues and eigenvectors
<code>svd(A; full::Bool = false) -&gt; SVD</code>	<code>[U,S,V] = svd(A)</code>	Singular value decomposition

Table 1: Interfaces of commonly seen matrix decompositions in Julia and MATLAB

**A powerful approach to linear algebra.** Besides support for multi-dimensional arrays, Julia provides native implementations for many linear algebra operations in the `LinearAlgebra` module. Basic matrix operations are implemented with calls to BLAS and LAPACK routines; the default implementation is OpenBLAS. Optimization efforts are also made in compact storage. For instance, QR decomposition may return a “thin” R matrix, which is stored in a compact blocked format. Furthermore, Julia users can easily write user-extensible wrappers for BLAS and LAPACK on top of the `LinearAlgebra` library. LAPACK wrappers are implemented fully in Julia code, using `ccall`, which does not require a C compiler.

**Some inconsistent interface design.** As a modern programming language, Julia supports multiple dispatch, that is, parametric polymorphism. A good example is that the GSVD interface reuses the name of the SVD of a single matrix  $A$  by taking two matrices as arguments. Unfortunately, this principle is not fully implemented. For instance, when computing the matrix norm, one may intuitively call `norm(A)`. However, this will not produce the desired result as shown below. Instead, one may want to use `opnorm(A)`.

Julia command/result	MATLAB command/result
<code>norm([1 2 3; 4 5 6; 7 8 9])</code> 16.881943016134134	<code>norm([1 2 3; 4 5 6; 7 8 9])</code> 16.8481
<code>opnorm([1 2 3; 4 5 6; 7 8 9])</code> 16.84810335261421	N/A

**Performance relies on “proper” implementation.** Our GSVD algorithm involves many operations with submatrices. We don’t need to pay attention to matrix slicing in other languages. However, in Julia, this could be a significant performance issue since slicing an array creates a copy of the selected subarray, which is computationally expensive. To make things worse, if a sliced matrix is passed as the return value, the result will be inaccurate as it is not overwritten in the original matrix.

An alternative is to create a “view” of the array, which is an array object that actually references the data of the original array in-place, without making a copy. This can be done for individual slices by calling function `view`, or more simply for a whole expression or block of code by putting macro `@views` in front of that expression. One can tell from the following example that by doing so, the speedup is three-fold.

```
julia> fcopy(x) = sum(x[2:end-1]);

julia> @views fview(x) = sum(x[2:end-1]);

julia> x = rand(10^6);

julia> @time fcopy(x);
0.003051 seconds (7 allocations: 7.630 MB)

julia> @time fview(x);
0.001020 seconds (6 allocations: 224 bytes)
```

Many other features have not been studied and explored by the author, most notably, parallelism. This could be a good direction for future work.

### 3.5 GSVD in other languages: a comparison

As we discussed at the beginning of this section, a number of numerical computing platforms feature the Generalized Singular Value decomposition. Here, we list several some of them and the corresponding documentation, shown in Table 2.

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 $A = UD_1[0 \ R]Q^T$ and $B = VD_2[0 \ R]Q^T$ . 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 2: GSVD in different languages

## 4 Testing and Performance

### 4.1 Accuracy (backward stability)

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

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

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

$$orth_{CS} = \frac{\|C^T C + S^T S - I\|_1}{\max(m, n, p) \epsilon} \quad (4.3)$$

$$orth_U = \frac{\|U^T U - I\|_1}{m \epsilon} \quad (4.4)$$

$$orth_V = \frac{\|V^T V - I\|_1}{p \epsilon} \quad (4.5)$$

$$orth_Q = \frac{\|Q^T Q - I\|_1}{n \epsilon} \quad (4.6)$$

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

#### 4.1.1 Numerical examples of small matrices

For the four examples we illustrated in 1.5, we also compute the stability metrics by “JuliaGSVD” and Julia 1.3 in Table 3.

	Version	$res_A$	$res_B$	$orth_{CS}$	$orth_U$	$orth_V$	$orth_Q$
Example 1	JuliaGSVD	0.2956	0.7057	0.4	0.5308	1.0417	1.1790
	Julia 1.3	0.3599	0.5714	0.025	0.9117	1.7083	1.3250
Example 2	JuliaGSVD	0.6173	0.4098	0.625	1.5000	0.5613	1.3998
	Julia 1.3	0.5068	0.5689	0.125	1.4583	0.9245	1.2483
Example 3	JuliaGSVD	0.4181	0.8941	0.375	0.7500	1.3940	1.3277
	Julia 1.3	0.3536	0.5938	0.125	1.4791	1.9540	1.1062
Example 4	JuliaGSVD	0.3600	0.5900	0.9	0.6558	0.5385	1.4362
	Julia 1.3	0.4449	0.3056	0.0	1.3225	0.7205	1.1814

Table 3: 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 six stability metrics for each subcase of a single test run in Table 4. All 320 test runs yield results no greater than 1.5.

	$m$	$p$	$n$	$k+l$	$res_A$	$res_B$	$orth_{CS}$	$orth_U$	$orth_V$	$orth_Q$
$m \geq n$ $p \geq n$	60	50	40	40	0.1140	0.2331	0.2083	0.7117	1.0742	0.4980
	300	250	200	200	0.0372	0.0633	0.0267	0.4815	0.6189	0.3214
	900	750	600	600	0.0151	0.0238	0.0106	0.3254	0.4347	0.2334
	1500	1250	1000	1000	0.0103	0.0157	0.007	0.2751	0.3648	0.1924
$m \geq n > p$	60	40	50	50	0.1254	0.4945	0.1083	0.8612	1.1608	0.5863
	300	200	250	250	0.0397	0.0697	0.035	0.5227	0.7458	0.3262
	900	600	750	750	0.0169	0.0314	0.0128	0.3433	0.5318	0.2478
	1500	1000	1250	1250	0.0107	0.0193	0.01	0.2866	0.4738	0.2028
$p \geq n > m$	40	60	50	50	0.1834	0.1645	0.1417	1.1144	0.9979	0.4617
	200	300	250	250	0.0511	0.0445	0.0333	0.7188	0.5814	0.3294
	600	900	750	750	0.0212	0.0183	0.0133	0.4400	0.3941	0.2111
	1000	1500	1250	1250	0.0173	0.0132	0.012	0.3897	0.3450	0.1772
$n > m$ $n > p$	20	30	60	50	0.0480	0.0392	0.0	0.4960	0.5349	0.3483
	200	300	600	500	0.0114	0.0110	0.0	0.3478	0.2948	0.1958
	400	600	1200	1000	0.0065	0.0065	0.0	0.2564	0.2313	0.1578
	1000	1500	3000	2500	0.0031	0.0032	0.0	0.1901	0.1670	0.1100

Table 4: Stability profiling for random dense matrices

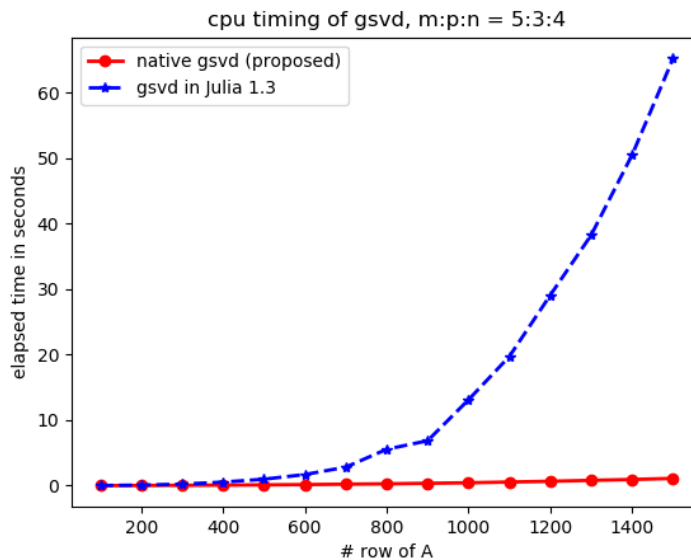
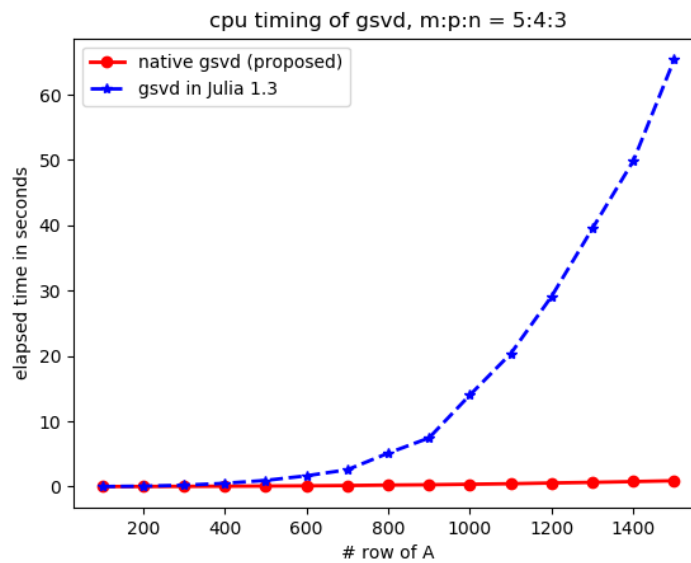
#### 4.1.3 Special types of matrices

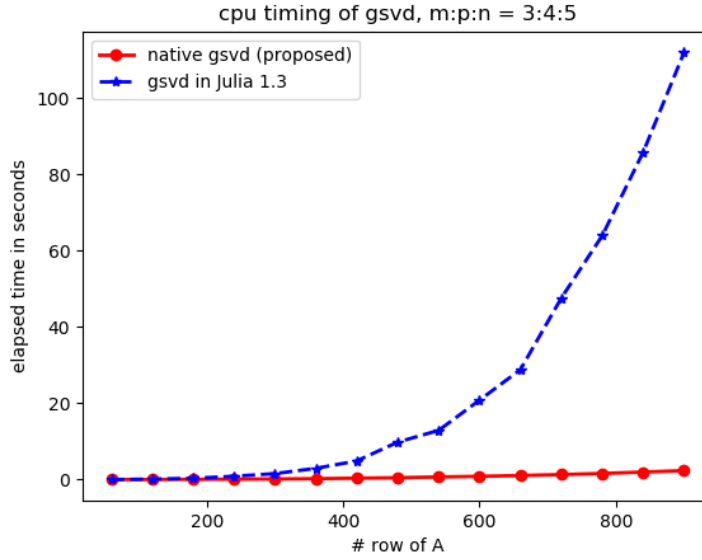
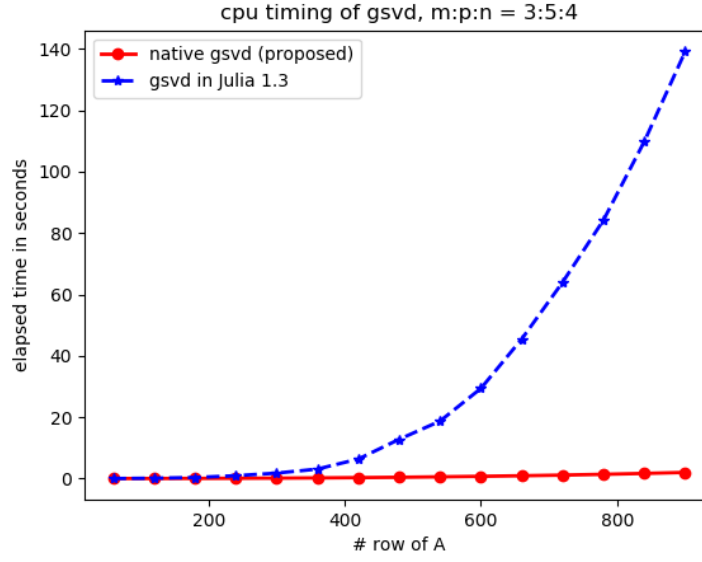
TODO?

## 4.2 Timing

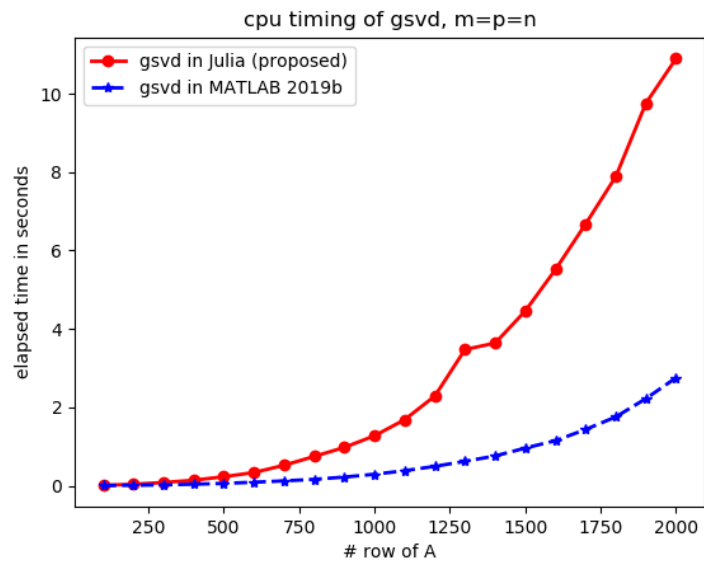
We want to evaluate the timing performance of our implementation between current version in Julia and MATLAB.

**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.**

	$m$	$p$	$n$	$t_{pre}$	$p_{pre}$	$t_{qr}$	$p_{qr}$	$t_{csd}$	$p_{csd}$	$t_{all}$
$m \geq n$ $p \geq n$	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 5: Time profiling for GSVD



## 5 Applications

The Generalized Singular Value Decomposition is powerful in solving many numerical linear algebra problems as well as problems in other disciplines, such as statistics and signal processing. We briefly introduce several prominent applications and highlight one application in genome analysis in this section.

### 5.1 Prominent applications of the GSVD

**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. [17] [18] [19] Computerized ionospheric tomography [20] is one of the applications in this regard.

**Matrix pencil  $A - \lambda B$ .** The GSVD is also used in the field of the canonical structure of matrix pencil  $A - \lambda B$ . [21] More specifically, the column and row nullities of  $A$  and  $B$  and common null space reveal the information about the Kronecker structure of  $A - \lambda B$ .

**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. [22] [23]

**Genome analysis.** The GSVD is applicable for comparative analysis of genome-scale expression datasets of two different organisms [24] and is further extended to tensor [25]. We will elaborate the role of the GSVD in genomes in Section 5.2.

**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  $B$ . [26] 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  $\{b_k\}$ .

**Linear discriminant analysis.** Howland and Park [27] [28] 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.

**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. [29]

### 5.2 GSVD in genome analysis

Modern genomic technology, microarray for instance, facilitates the acquisition of a wide range of molecular biological data, such as DNA-sequence and mRNA-expression, on a genomic scale. With these data, we can apply comparative analysis to understand the universality and specialization of molecular biology mechanisms. Specifically, such analysis helps us to distinguish the similarity and dissimilarity among two or more large-scale data sets. To this end, a mathematical framework is needed to remove the barriers of transferring genetic sequencing results to usable information. Fortunately, the GSVD fits this purpose well:

1. Two data sets are column-matched but row-independent matrices, where rows are genes and columns are samples. They exactly match the type of the input matrix pair of the GSVD.

2. The GSVD simultaneously reduce the two “genes”  $\times$  “samples” spaces to two diagonalized “samplelets”  $\times$  “genelets” spaces. The column space is shared by both datasets. We can interpret the generalized singular values as the significance in one data set relative to that in the other.

We now illustrate this framework with the comparison between yeast and human cell cycle-expression data sets. [30] We also present experimental results, implemented in Julia.

**Why yeast?** The reasons of using yeast are two-fold. First, yeast cells share many basic biological properties with our cells. At least 20 per cent of human genes known to have a role in disease have counterparts in yeast. This suggests that such diseases result from the disruption of very basic cellular processes. Hence, yeast is also used to test new drugs. One may be surprised that antibiotic penicillin is the first of its kind to be made by the yeast *Saccharomyces cerevisiae*. Second, genetic manipulation in yeast is easy and cheap compared to similar experiments in more complex animals such as mice and zebrafish.

**Understanding the data sets.** Invented by Patrick O. Brown [31], DNA microarray is a collection of microscopic DNA spots attached to a solid surface. Scientists use DNA microarrays to measure the expression levels of large numbers of genes simultaneously or to genotype multiple regions of a genome. DNA microarrays can be used to detect DNA (as in comparative genomic hybridization), or detect RNA (most commonly as cDNA after reverse transcription) that may or may not be translated into proteins.

In our experiment, a single microarray probes the relative expression levels of  $m$  genes of yeast in a single sample. A series of  $n$  arrays probes the genome-scale expression levels in  $n$  different samples, i.e., under  $n$  different experimental conditions. Similarly, another set of microarrays probe the relative expression levels of  $p$  genes of human under  $n$  experimental conditions. These two matrices of size  $m$ -by- $n$  and  $p$ -by- $n$  are the input data sets. Notice that both  $m$  and  $p$  are significantly greater than  $n$ .

**Data pre-processing.** Unfortunately, missing data might tabulate into some portion of the data set. One of the methods to impute missing data for genomic expressions is to utilize SVD to approximate the expression of all genes in the data set. [32] [33]

We briefly describe the iterative methods to solve this problem.

1. Set the missing elements as as the mean of the non-missing elements for each row, let the complete matrix be  $X_0$ . Initialize  $i = 0$ .
2. Compute the SVD of  $X_i$ , and use the first 5 singular vectors to approximate  $X_{i+1}$  by replacing the missing values in  $X_i$  with the fitted values from this solution.
3. Increment and repeat Step 2 until  $\frac{\|X_i - X_{i+1}\|_1}{\|X_i\|_1 \max\{m, p\}}$  is below some threshold  $\epsilon$  ( $10^{-6}$ ).

**Mathematical method: GSVD.** Once we have the sanitized data sets, then the GSVD is the simultaneous linear transformation of the two expression data sets  $A$  and  $B$  from  $m$ -genes-by- $n$ -samples and  $p$ -genes-by- $n$ -samples spaces to two reduced  $n$ -genelets-by- $n$ -samplelets spaces.

$$A = UC \begin{bmatrix} 0 & R \end{bmatrix} Q^T, \quad B = VS \begin{bmatrix} 0 & R \end{bmatrix} Q^T \quad (5.1)$$

where  $C^T C = \text{diag}(\alpha_1^2, \dots, \alpha_n^2)$ ,  $S^T S = \text{diag}(\beta_1^2, \dots, \beta_n^2)$ .

We define the antisymmetric angular distance between the data sets:

$$\theta_i = \arctan(\alpha_i / \beta_i) - \pi/4 \quad (5.2)$$

It indicates the relative significance of the  $i$ -th genelet, i.e., its significance in the first data set relative to that in the second. The  $\pi/4$  offset means that an angular distance of 0 indicates a genelet of equal significance in both data sets. The angular distances are arranged in decreasing order of significance in the first data set relative to the second such that  $\pi/4 > \theta_1 > \theta_2 > \dots > \theta_n > -\pi/4$ .

\* 2003-Altner  
\* Edelmann §8.2

**Interpreting biological results.** The heatmap below TODO: will replace with a real one visualizes the simultaneous linear transformation done by the GSVD. Here, statistically, overexpression (red) pixels are data that are above mean plus one standard deviation, underexpression (green) pixels are data that are below mean plus one standard deviation, while no change (black) pixels are data that lie in between.

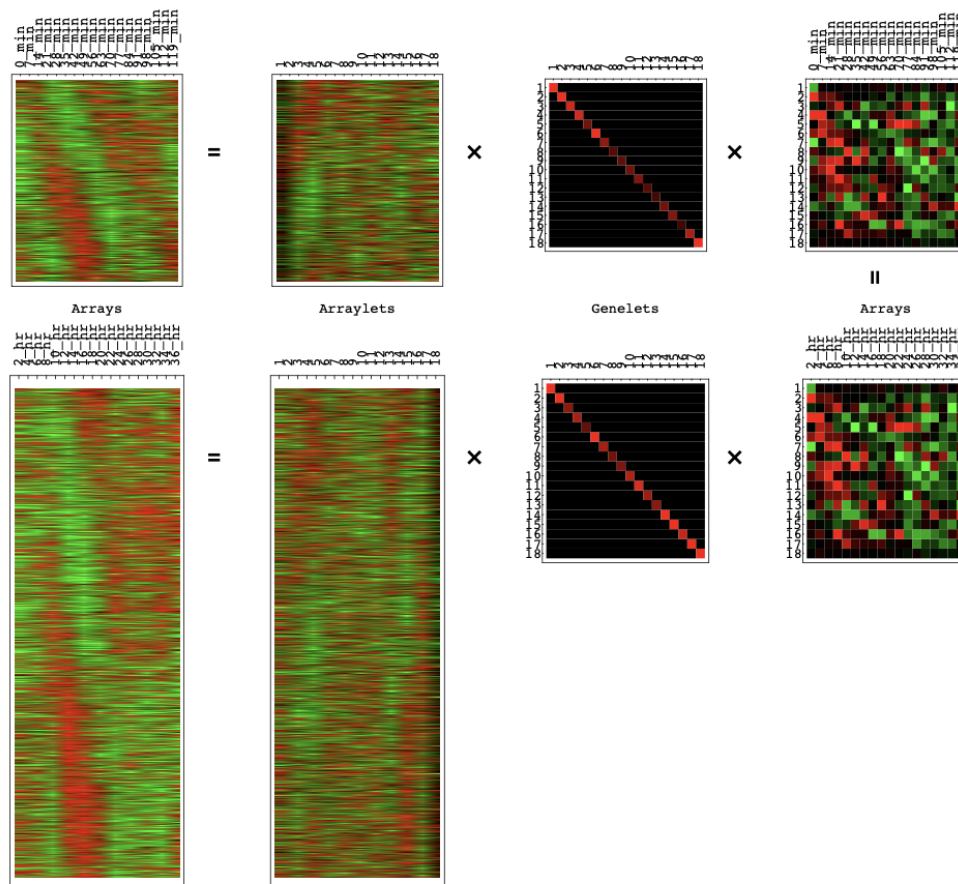


Figure 2: GSVD of the yeast and human cell-cycle expression data sets. Shown is a heatmap with overexpression (red), no change in expression (black), and underexpression (green)

By the bar chart of the angular distance, we know that the first and second genelets are highly significant in the yeast data relative to the human data. The third, fourth, and fifth genelets are almost equally significant in both data sets (slightly more in the yeast data), with  $0 < \theta_3, \theta_4, \theta_5 < \pi/16$ . The 14th, 15th, and 16th genelets, which are also almost equally significant in both data sets (slightly more in the human data), with  $\pi/6 < \theta_{14}, \theta_{15}, \theta_{16} < \pi/4$ . The 17th and 18th genelets are highly significant in the human data relative to the yeast data. All other genelets are significant in neither the yeast data nor the human data.

def?

GSVD

SVD Math/Exact

$A \rightarrow \text{rank}$   $\text{rank} = \text{num. rank}$

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

SVD  $\text{rank}(A) = \text{rank}(\Sigma)$

$A = \begin{bmatrix} \square & \square \end{bmatrix}$

$B = \begin{bmatrix} \square & \square \end{bmatrix}$

$\theta_i$

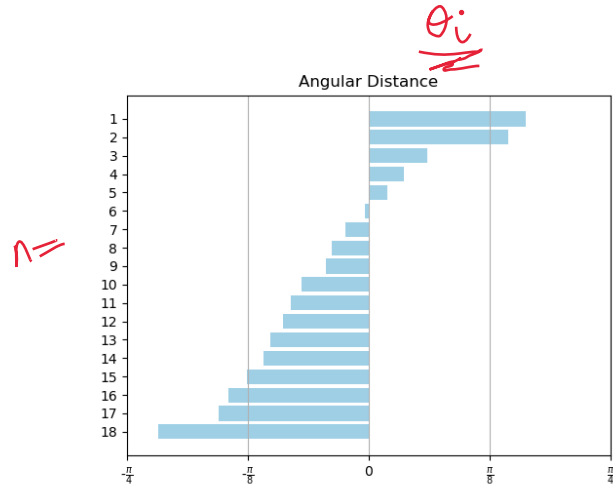


Figure 3: Bar chart of the angular distances

**Conclusion.** The GSVD provides a natural solution by creating a single coherent model from the two datasets recording different aspects of interrelated phenomena by simultaneously identifying the similar and dissimilar between the two corresponding column-matched but row-independent matrices. More recently, research conducted by Alter's lab at the University of Utah dive the GSVD into tensor level [34] and apply it to the study of tumor, e.g. glioblastoma. [35]

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