# GSVD in Julia

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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:

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

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 $C^TC + S^TS = I_{k+\ell}$. $C$ and $S$ have the following detailed structures:

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

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

  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,

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

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

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

  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,

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

  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 $i = 1, ..., k+\ell$. The ratios

$$\sigma_i \equiv \alpha_i / \beta_i \tag{1.2}$$

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

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

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

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

then $A^TA$ and $B^TB$ are simultaenously diagonalized:

$$X^TA^TAX = \begin{array}{c} \\ n-k-\ell \\ k+\ell \end{array} \begin{array}{c} \begin{array}{cc} n-k-\ell & k+\ell \end{array} \\ \begin{pmatrix} 0 & 0 \\ 0 & C^TC \end{pmatrix} \end{array}, \tag{1.4a}$$

$$X^TB^TBX = \begin{array}{c} \\ n-k-\ell \\ k+\ell \end{array} \begin{array}{c} \begin{array}{cc} n-k-\ell & k+\ell \end{array} \\ \begin{pmatrix} 0 & 0 \\ 0 & S^TS \end{pmatrix} \end{array}. \tag{1.4b}$$

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

$$A^TAX_{i+n-k-\ell} = \lambda_i B^TBX_{i+n-k-\ell}$$

for $i = 1, \cdots, k+\ell$, where $\lambda_i = (\alpha_i/\beta_i)^2$ are "non-trivial" eigenvalues of $(A^TA, B^TB)$. $X_{i+n-k-\ell}$ 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 $(A^T,\ B^T)^T$:

$$A = UCQ^T, \quad B = VSQ^T \tag{1.5}$$

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:

$$A = UCH, \quad B = VSH \tag{1.6}$$

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 $C^TC + S^TS = I$. $C$ and $S$ are of the following detailed structures:

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

  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

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

- $H$ 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-$n$ orthgonal matrix, then
$$\text{null}(A) \cap \text{null}(B) = \text{span}\{Q(:, 1 : n-k-\ell)\}.$$
In addition, let $X = Q \begin{array}{c} \\ n-k-\ell \\ k+\ell \end{array} \begin{array}{c} \begin{array}{cc} n-k-\ell & k+\ell \end{array} \\ \begin{pmatrix} I & 0 \\ 0 & R_0^{-1} \end{pmatrix} \end{array}$, then the "non-trivial" eigenvalues of the generalized eigenvalue problem $A^TAx = \lambda B^TBx$ are the square of the generalized singular values of $A$ and $B$, and 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:

$$A = UCX^T, \quad B = VSX^T \tag{1.7}$$

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 diagaonl $\mathrm{diag}(C, \max(0, q-m))$. If $m \geq q$, this is the main diagonal of $C$.

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

  Furthermore, $C^TC = \mathrm{diag}(\alpha_1^2, \cdots, \alpha_q^2)$, $S^TS = \mathrm{diag}(\beta_1^2, \cdots, \beta_q^2)$, where $\alpha_i$, $\beta_i \in [0,1]$ for $i = 1, \cdots, q$. 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) $n > m, n \leq p$:
   $$C = \begin{array}{c} \\ m \\ \end{array} \begin{array}{c} \begin{array}{cc} n-m & m \end{array} \\ \begin{pmatrix} 0 & \Sigma_1 \end{pmatrix} \end{array}, \quad S = \begin{array}{c} \\ n \\ p-n \end{array} \begin{array}{c} \begin{array}{c} n \end{array} \\ \begin{pmatrix} \Sigma_2 \\ 0 \end{pmatrix} \end{array}$$
   where $\Sigma_1 = \mathrm{diag}(\alpha_{n-m+1}, \cdots, \alpha_n)$ and $\Sigma_2 = \mathrm{diag}(\beta_1, \cdots, \beta_n)$.
   (b) $n \leq m, n > p$:
   $$C = \begin{array}{c} \\ m-n \\ n \end{array} \begin{array}{c} \begin{array}{c} n \end{array} \\ \begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix} \end{array}, \quad S = \begin{array}{c} \\ p \end{array} \begin{array}{c} \begin{array}{cc} p & n-p \end{array} \\ \begin{pmatrix} \Sigma_2 & 0 \end{pmatrix} \end{array}$$
   where $\Sigma_1 = \mathrm{diag}(\alpha_1, \cdots, \alpha_n)$ and $\Sigma_2 = \mathrm{diag}(\beta_1, \cdots, \beta_p)$.
   (c) $n \leq m, n \leq p$:
   $$C = \begin{array}{c} \\ m-n \\ n \end{array} \begin{array}{c} \begin{array}{c} n \end{array} \\ \begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix} \end{array}, \quad S = \begin{array}{c} \\ p-n \\ n \end{array} \begin{array}{c} \begin{array}{c} n \end{array} \\ \begin{pmatrix} \Sigma_2 \\ 0 \end{pmatrix} \end{array}$$
   where $\Sigma_1 = \mathrm{diag}(\alpha_1, \cdots, \alpha_n)$ and $\Sigma_2 = \mathrm{diag}(\beta_1, \cdots, \beta_n)$.
   (d) $n > m, n > p$:
   $$C = \begin{array}{c} \\ m \\ \end{array} \begin{array}{c} \begin{array}{cc} n-m & m \end{array} \\ \begin{pmatrix} 0 & \Sigma_1 \end{pmatrix} \end{array}, \quad S = \begin{array}{c} \\ p \end{array} \begin{array}{c} \begin{array}{cc} p & n-p \end{array} \\ \begin{pmatrix} \Sigma_2 & 0 \end{pmatrix} \end{array}$$
   where $\Sigma_1 = \mathrm{diag}(\alpha_{n-m+1}, \cdots, \alpha_n)$ and $\Sigma_2 = \mathrm{diag}(\beta_1, \cdots, \beta_p)$.
2. $m + p < n$, thus $q = m + p$:
   $$C = \begin{array}{c} \\ m \\ \end{array} \begin{array}{c} \begin{array}{cc} p & m \end{array} \\ \begin{pmatrix} 0 & \Sigma_1 \end{pmatrix} \end{array}, \quad S = \begin{array}{c} \\ p \end{array} \begin{array}{c} \begin{array}{cc} p & m \end{array} \\ \begin{pmatrix} \Sigma_2 & 0 \end{pmatrix} \end{array}$$
   where $\Sigma_1 = \mathrm{diag}(\alpha_{p+1}, \cdots, \alpha_{p+m})$ and $\Sigma_2 = \mathrm{diag}(\beta_1, \cdots, \beta_p)$.

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 $B^T B$:

$$A^T A = X C^T C X^T, \quad B^T B = X S^T S X^T. \tag{1.8}$$

   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 inproperly 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:

$$A = UCX^{-1}, \quad B = VSX^{-1} \tag{1.9}$$

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-$n$:

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

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

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

  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 $\mu(A, B) = \{\alpha_i/\beta_i \mid i = 1, \cdots, r\}$.
3. rank($[A; B]$) is the number of "non-trivial???" diagonal entries of $C$ and $S$.
4. By the definition (1.9), $A^TA$ and $B^TB$ are simultaneously diagonalized:

$$X^TA^TAX = C^TC, \quad X^TB^TBX = S^TS,$$

   Therefore, the first $r$ quotients of the diagonal entries of $C^TC$ and $S^TS$ are the "non-trivial" eigenvalues of the matrix pairs $(A^TA, B^TB)$, 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

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

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

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

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

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

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

$$R0 = \begin{bmatrix} 5.74065 & -7.07986 & -0.125979 & 0.316232 \\ 0.0 & -7.96103 & 2.11852 & 2.98601 \\ 0.0 & 0.0 & -5.72211 & 0.43623 \\ 0.0 & 0.0 & 0.0 & 5.66474 \end{bmatrix}$$

The residual norms

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

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

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

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

Consequently, the generalized singular values computed are:

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

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

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

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

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

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 $(A^TA, B^TB)$ computed by MATLAB's function `eig(A'*A, B'*B)` are

$$0.08343777448439993, \quad 0.5636963529903901, \quad 4.011557310890648, \quad \texttt{Inf}.$$

The square roots are

$$0.2888559753309596, \quad 0.7507971450334572, \quad 2.002887243678647, \quad \texttt{Inf}.$$

These values are equal to the gsvs computed by LAPACK-GSVD and MATLAB-GSVD.
Note: the "inf" eigenvalue is due to the fact $B^TB$ is rank deficient.

(e) The eigenvalues of $(A^TA, B^TB)$ computed by MATLAB function `dsygvic(n, A'*A, B'*B, tol)` [1] are

$$4.0116, \quad 0.0834, \quad 0.5637.$$

The square roots are

$$2.0029, \quad 0.2889, \quad 0.7508.$$

[1] 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 $\tilde{R}$.

| | |
|---|---|
| $res_A = \frac{\|\tilde{U}^T A\tilde{Q} - \tilde{C}\tilde{R}\|_1}{max(m,n)\|A\|_1 \varepsilon}$ | 0.6172649988387877 |
| $res_B = \frac{\|\tilde{V}^T B\tilde{Q} - \tilde{S}\tilde{R}\|_1}{max(p,n)\|B\|_1 \varepsilon}$ | 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 $(A^TA, B^TB)$ 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+0.1892281406434339`im`, **0.06991284853891447**, 0.3476443465695792, **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 $A^TA - \lambda B^TB$ is singular, i.e., $A^TA$ and $B^TB$ have a non-trivial common null space. The function "dsygvic.m" should return only two "corrected" eigenvalues.
The computation of the eigenvalues of $(A^TA, B^TB)$ 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:

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

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

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

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

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

$$R0 = \begin{bmatrix} 0.0 & 0.0 & -12.2133 & 8.28663 \\ 0.0 & 0.0 & 0.0 & -18.1154 \end{bmatrix}$$

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 $\tilde{U}, \tilde{V}, \tilde{Q}, \tilde{D1}, \tilde{D2}$ and $\tilde{R0}$.

| | |
|---|---|
| $res_A = \frac{\|\tilde{U}^T A\tilde{Q} - \tilde{D1}\tilde{R0}\|_1}{max(m,n)\|A\|_1 \varepsilon}$ | 0.5068000688771875 |
| $res_B = \frac{\|\tilde{V}^T B\tilde{Q} - \tilde{D2}\tilde{R0}\|_1}{max(p,n)\|B\|_1 \varepsilon}$ | 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 $(A^TA, B^TB)$ computed by MATLAB's function `eig(A'*A,B'*B)` are

$-1.8035125057805033e^{-15}$, **0.028991708031064364**, **0.8651279673000131**, **57.659486562484965**.

The square roots are

$0.0+4.2467781973874066e^{-8}$`im`, **0.17026951585960526**, **0.930122554989402**, **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 $(A^TA, B^TB)$ 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 $\tilde{U}, \tilde{V}, \tilde{Q}, \tilde{D1}, \tilde{D2}$ and $\tilde{R0}$.

| | |
|---|---|
| $res_A = \frac{\|\tilde{U}^T A\tilde{Q} - \tilde{D1}\tilde{R0}\|_1}{max(m,n)\|A\|_1 \varepsilon}$ | 0.3536371804643456 |
| $res_B = \frac{\|\tilde{V}^T B\tilde{Q} - \tilde{D2}\tilde{R0}\|_1}{max(p,n)\|B\|_1 \varepsilon}$ | 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

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

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 $\tilde{R}$.

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

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

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 $(A^TA, B^TB)$ computed by MATLAB's function `eig(A'*A,B'*B)` are

$-0.34554912453318243, 1.3025318975863486e^{-16}$, **0.5798671184339763**, **2.586799548232693**, `Inf`.

The square roots are

0.0+0.5878342662121547`im`, $1.1412851955520796e^{-8}$, **0.7614900645668178**, **1.6083530545973708**, `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 $(A^TA, B^TB)$ 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 $\tilde{U}, \tilde{V}, \tilde{Q}, \tilde{D1}, \tilde{D2}$ and $\tilde{R0}$.

| | |
|---|---|
| $res_A = \frac{\|\tilde{U}^T A\tilde{Q} - \tilde{D1}\tilde{R0}\|_1}{max(m,n)\|A\|_1 \varepsilon}$ | 0.4449492156962062 |
| $res_B = \frac{\|\tilde{V}^T B\tilde{Q} - \tilde{D2}\tilde{R0}\|_1}{max(p,n)\|B\|_1 \varepsilon}$ | 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 $B$:

$$BP = V \begin{array}{c} \\ \ell \\ p-\ell \end{array} \begin{array}{c} \begin{array}{cc} \ell & n-\ell \end{array} \\ \begin{pmatrix} B_{11} & B_{12} \\ 0 & 0 \end{pmatrix} \end{array} \tag{2.1}$$

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 $(B_{11} \;\; B_{12})$:

$$\begin{array}{c} \\ \ell \end{array} \begin{array}{c} \begin{array}{cc} \ell & n-\ell \end{array} \\ \begin{pmatrix} B_{11} & B_{12} \end{pmatrix} \end{array} = \begin{array}{c} \\ \ell \end{array} \begin{array}{c} \begin{array}{cc} n-\ell & \ell \end{array} \\ \begin{pmatrix} 0 & B_{13} \end{pmatrix} \end{array} Z \tag{2.2}$$

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

Step 1(5) Partition

$$A = \begin{array}{c} \\ m \end{array} \begin{array}{c} \begin{array}{cc} n-\ell & \ell \end{array} \\ \begin{pmatrix} A_1 & A_2 \end{pmatrix} \end{array}, \tag{2.3}$$

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

$$A_1 P_1 = U \begin{array}{c} \\ k \\ m-k \end{array} \begin{array}{c} \begin{array}{cc} k & n-\ell-k \end{array} \\ \begin{pmatrix} A_{11} & A_{12} \\ 0 & 0 \end{pmatrix} \end{array} \tag{2.4}$$

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

Step 1(7) Partition:

$$A = \begin{array}{c} \\ k \\ m-k \end{array} \begin{array}{c} \begin{array}{ccc} k & n-\ell-k & \ell \end{array} \\ \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ 0 & 0 & A_{23} \end{pmatrix} \end{array} \tag{2.5}$$

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

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

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

$$\begin{array}{c} \\ k \end{array} \begin{array}{c} \begin{array}{cc} k & n-\ell-k \end{array} \\ \begin{pmatrix} A_{11} & A_{12} \end{pmatrix} \end{array} = \begin{array}{c} \\ k \end{array} \begin{array}{c} \begin{array}{cc} n-\ell-k & k \end{array} \\ \begin{pmatrix} 0 & A_{12} \end{pmatrix} \end{array} Z_1 \tag{2.6}$$

  and it results

$$A = \begin{array}{c} \\ k \\ m-k \end{array} \begin{array}{c} \begin{array}{ccc} n-\ell-k & k & \ell \end{array} \\ \begin{pmatrix} 0 & A_{12} & A_{13} \\ 0 & 0 & A_{23} \end{pmatrix} \end{array} \tag{2.7}$$

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

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

Let

$$A_2 = \begin{array}{c} \\ k \\ m-k \end{array} \begin{array}{c} \begin{array}{c} \ell \end{array} \\ \begin{pmatrix} A_{13} \\ A_{23} \end{pmatrix} \end{array} \tag{2.8}$$

- QR decomposition of $A_{23}$:

$$A_{23} = U_1 \begin{array}{c} \\ \ell \\ m-k-\ell \end{array} \begin{array}{c} \begin{array}{c} \ell \end{array} \\ \begin{pmatrix} A_{23} \\ 0 \end{pmatrix} \end{array} \tag{2.9}$$

- 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:

$$A = UR_AQ^T, \quad B = VR_BQ^T \tag{2.10}$$

where

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

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

  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 $m-k-\ell < 0$:

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

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

$$\begin{array}{c} \\ \ell \\ \ell \end{array}\!\!\begin{array}{c} \ell \\ \begin{pmatrix} A_{23} \\ B_{23} \end{pmatrix} \end{array} = \begin{array}{c} \ell \\ \ell \end{array}\!\!\begin{array}{c} \ell \\ \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} \end{array} R_{23}$$

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

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

Thus, (2.10) can be rewritten as:

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

where

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

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

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

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

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

$$Q_1 = U_1 \Sigma_1 Z_1^T, \quad Q_2 = V_1 \Sigma_2 Z_1^T \tag{2.12}$$

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:

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

  where $1 \geq \alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_\ell \geq 0$, $0 \leq \beta_1 \leq \beta_2 \leq \cdots \leq \beta_\ell \leq 1$ 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:

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

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

Combining (2.11) and (2.12) , we have

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

where

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

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

  and

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

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

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

  and

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

**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 $Q_2$:

$$Q_2 = V_1\Sigma_2 Z_1^T, \tag{2.14}$$

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

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

- Reorder the diagonal entries of $\Sigma_2$ non-decreasingly: $\Sigma_2 = \mathrm{diag}(\beta_1, \cdots, \beta_\ell)$;
- 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 $0 \le \beta_1 \le \cdots \le \beta_r \le \frac{1}{\sqrt{2}} < \beta_{r+1} \le \cdots \le \beta_\ell \le 1$.
The justification for $r$ see Remark 2.1.

Step 2(4). Matrix-matrix multiply:

$$T = Q_1 Z_1 \tag{2.15}$$

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

$$T = U_1 R, \tag{2.16}$$

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

$$R = \begin{array}{c} \\ r \\ \ell - r \end{array} \begin{array}{c} \begin{array}{cc} r & \ell - r \end{array} \\ \begin{pmatrix} \Pi & \epsilon \\ 0 & R_{22} \end{pmatrix} \end{array}, \tag{2.17}$$

  where $\Pi = \mathrm{diag}(\alpha_1, \cdots, \alpha_r)$. The bottom $(\ell - r)$ rows vanish if $\ell - r \le 0$.
  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

$$R = \begin{array}{c} \\ r \\ m - k - r \end{array} \begin{array}{c} \begin{array}{ccc} r & m - k - r & \ell - m + k \end{array} \\ \begin{pmatrix} \Pi & \epsilon & \epsilon \\ 0 & R_{22} & R_{23} \end{pmatrix} \end{array}, \tag{2.18}$$

  where $\Pi = \mathrm{diag}(\alpha_1, \cdots, \alpha_r)$. The bottom $(m - k - r)$ rows vanish if $m - k - r \le 0$.
  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:

$$Q_1 = U_1 R Z_1^T \tag{2.19}$$

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

- If $m - k - \ell \ge 0$ and $\ell \le r$: $R = \mathrm{diag}(\alpha_1, \cdots, \alpha_\ell)$.
- If $m - k - \ell < 0$ and $m - k \le r$:

$$R = \begin{array}{c} \\ m - k \end{array} \begin{array}{c} \begin{array}{cc} m - k & \ell - m + k \end{array} \\ \begin{pmatrix} \Pi & 0 \end{pmatrix} \end{array}, \tag{2.20}$$

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

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 $m - k - \ell \ge 0$ and $\ell - r > 0$:

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

$$R_{22} = U_r C_r Z_r^T \tag{2.21}$$

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

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

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

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

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

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

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

- 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):

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

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 $\alpha_{r+1}, \cdots, \alpha_{m-k}$.

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

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

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

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

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

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

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

$$Q_1 = U_1 \Sigma_1 Z_1^T \tag{2.23}$$

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

$$W = Q_w R_w \tag{2.24}$$

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

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

**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 arithemetic, it follows that:

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

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 $D = diag(\|x_1\|, \|x_2\|, \cdots, \|x_n\|)$ and $x_i$ denotes the $i$-th column of $X$.*

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

$$X = QR, \tag{2.26}$$

*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*

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

*Proof.* This theorem is proved by Van Loan in **Theorem 3.2** [10, pp. 484–485]. □

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

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

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:

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

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

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 matrice $C$, $p$-by-$n$ diagonal matrice $S$ such that $U^TAX = C$ and $V^TBX = S$.

*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 $Q_2$:
$U^TQ_1Z = C = \text{diag}(\alpha_i, \cdots, \alpha_n)$, $V^TQ_2Z = S = \text{diag}(\beta_i, \cdots, \beta_n)$.

*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 trangular matrices, namely, $A_{23}$ and $B_{13}$ in (2.10) such that

$$A_{23} = U_1CRQ_1^T, \quad B_{13} = V_1SRQ_1^T. \tag{2.30}$$

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

# 3 Software

## 3.1 Interface design

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

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

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

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

Compute the generalized SVD of `A` and `B`, returning a `GeneralizedSVD` factorization object `F`, such that `A = F.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+l) diagonal matrix with 1s in the first K entries,
- `S` is a p-by-(k+l) matrix whose top right L-by-L block is diagonal,
- `R` is a (k+l)-by-n matrix whose rightmost (k+l)-by-(k+l) block is nonsingular upper block triangular,
- `k+l` is the effective numerical rank of the matrix `[A; B]`.

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

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

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

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

## 3.2 Architecture

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

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

`svd()` → `preproc()` → `csd()` → `svd():postproc`

## 3.3 Implementation details

*Step* 1 Pre-processing:

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

*Step* 2 QR decomposition:

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

*Step* 3 CS decomposition:

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

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

## 3.4 GSVD in other languages: a comparison

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

| Language | GSVD Documentation |
|---|---|
| Native Julia (proposed) | `svd(A, B) -> GeneralizedSVD`<br>Computes the generalized SVD of `A` and `B`, returning a `GSVD` factorization object `F`, such that<br>`A = F.U*F.C*F.R*F.Q'` and `B = F.V*F.S*F.R*F.Q'`. |
| Julia 1.3 (LAPACK wrapper) | `svd(A, B) -> GeneralizedSVD`<br>Computes the generalized SVD of `A` and `B`, returning a `GeneralizedSVD` factorization object `F`, such that<br>`A = F.U*F.D1*F.R0*F.Q'` and `B = F.V*F.D2*F.R0*F.Q'`. |
| MATLAB (2019b) | `[U,V,X,C,S] = gsvd(A,B)`<br>Returns unitary matrices `U` and `V`, a (usually) square matrix `X`, and nonnegative diagonal matrices `C` and `S` so that<br>`A = U*C*X', B = V*S*X', C'*C + S'*S = I`. |
| Mathematica | `SingularValueDecomposition[m,a]`<br>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) | `z <- gsvd(A, B)`<br>Computes The Generalized Singular Value Decomposition of matrices $A$ and $B$ such that $A = UD_1[0\ R]Q^T$ and $B = VD_2[0R]Q^T$. 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:<br>Given two $M_i$-by-$N$ column-matched but row-independent matrices $D_i$, each with full column rank and $N \leq Mi$, the GSVD is an exact simultaneous factorization $Di = Ui\Sigma_i V^T, i = 1, 2$. $U_i$ is $M_i$-by-$N$ and are column-wise orthonormal and $V$ is $N$-by-$N$ nonsingular matrix with normalized rows. $diag(\Sigma_i)$ returns two lists of $N$ positive values and the ratios are called the generalized singular values. |

Table 1: GSVD in different languages

# 4 Testing and Performance

## 4.1 Accuracy (backward stability)

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

$$res_A = \frac{\|U^T AQ - CR\|_1}{max(m,n)\|A\|_1\epsilon} \tag{4.1}$$

$$res_b = \frac{\|V^T BQ - SR\|_1}{max(p,n)\|B\|_1\epsilon} \tag{4.2}$$

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

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

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

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

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 2.

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

Table 2: Stability profiling for small matrices

### 4.1.2 Random dense matrices

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

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

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

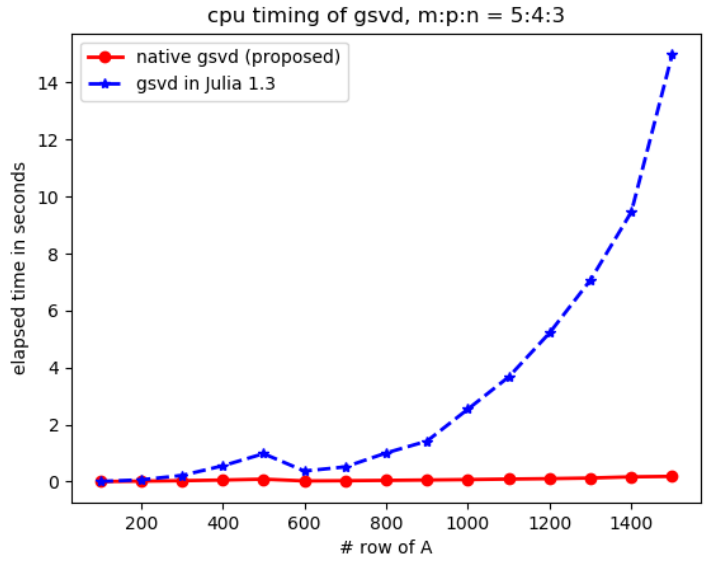
Table 3: Stability profiling for random dense matrices

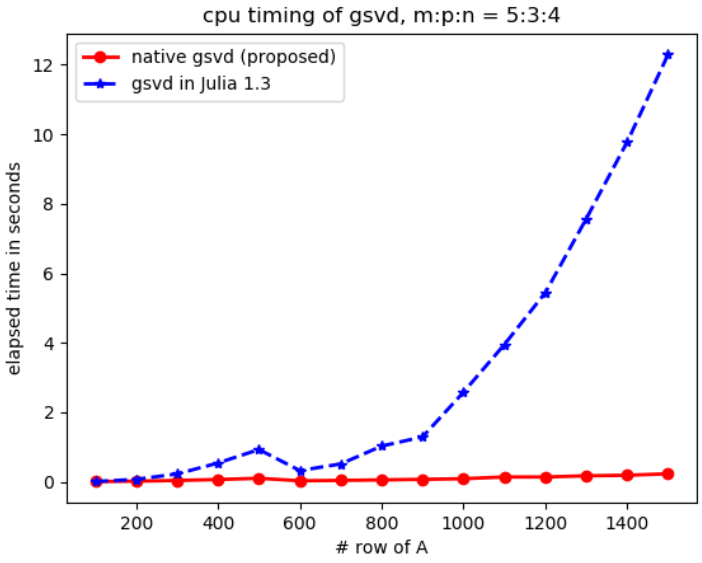
#### 4.1.3 Special types of matrices

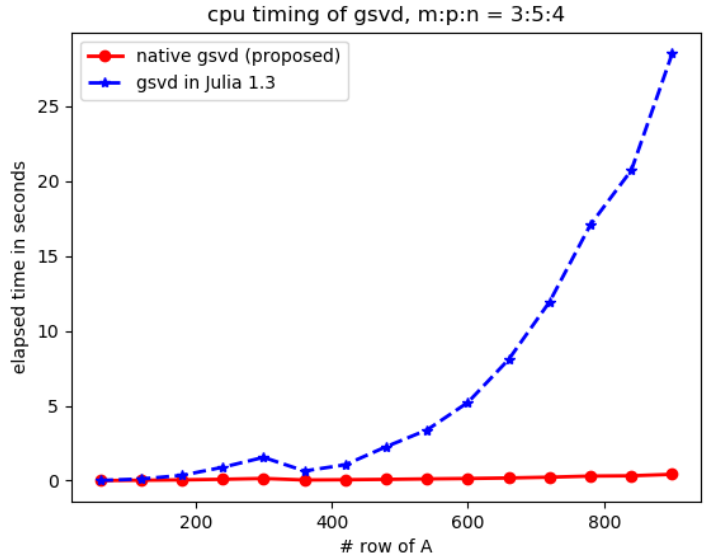
## 4.2 Timing

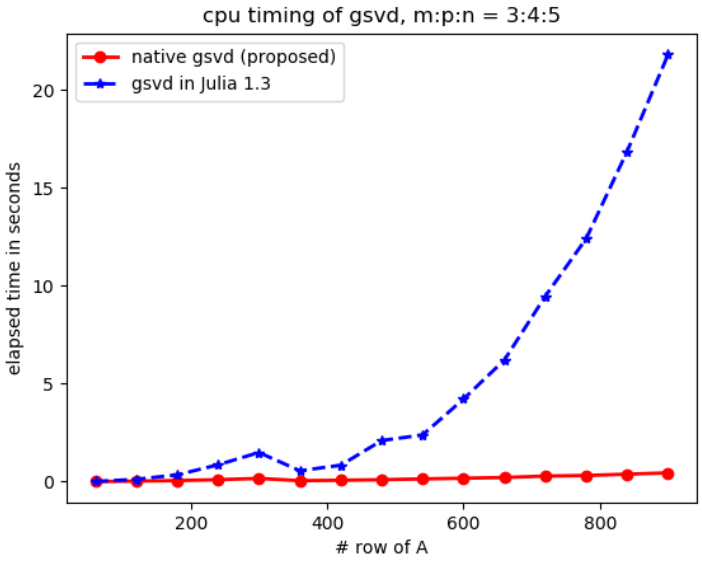
We want to evaluate the timing performance of our implementation between current version in Julia and MATLAB.

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

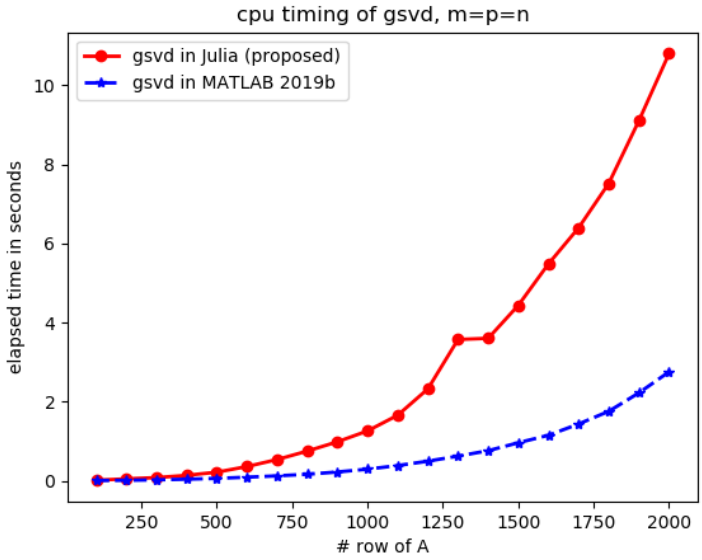





**vs. MATLAB.** For the comparison with MATLAB 2019b, we specify the input as square matrix. Our implementation is still slower than MATLAB. The major reason is due to the significant difference of decomposition discussed in 1.1 and 1.3.


cpu timing of gsvd, m=p=n
gsvd in Julia (proposed)
gsvd in MATLAB 2019b
elapsed time in seconds
# row of A
0
2
4
6
8
10
250
500
750
1000
1250
1500
1750
2000

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

| | $m$ | $p$ | $n$ | $t_{pre}$ | $p_{pre}$ | $t_{qr}$ | $p_{qr}$ | $t_{csd}$ | $p_{csd}$ | $t_{all}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| | 1500 | 1200 | 1000 | 0.6242 | 41.13% | 0.1683 | 11.09% | 0.6011 | 39.61% | 1.5175 |
| $m \geq n$ | 500 | 500 | 500 | 0.0651 | 26.78% | 0.0347 | 14.29% | 0.1191 | 48.94% | 0.2433 |
| $p \geq n$ | 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 |
| | 1500 | 1000 | 1200 | 1.500 | 60.09% | 0.1815 | 7.27% | 0.6811 | 27.28% | 2.4963 |
| $m \geq n > p$ | 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 |
| | 1000 | 1500 | 1200 | 0.5234 | 23.23% | 0.2789 | 12.37% | 1.2630 | 56.06% | 2.2529 |
| $p \geq n > m$ | 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 |
| | 1000 | 1200 | 1500 | 1.7532 | 48.51% | 0.2038 | 5.64% | 1.4467 | 40.03% | 3.6136 |
| $n > m$ | 260 | 600 | 770 | 0.2791 | 38.86% | 0.0441 | 6.14% | 0.3459 | 48.17% | 0.7181 |
| $n > p$ | 370 | 250 | 700 | 0.1385 | 86.69% | 0 | 0% | 0 | 0% | 0.1598 |
| | 120 | 120 | 400 | 0.0296 | 96.70% | 0 | 0% | 0 | 0% | 0.0307 |

Table 4: Time profiling for GSVD

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

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

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

Table 5: Time profiling for Preprocessing

# 5 Applications

## 5.1 Genomic signal processing

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

## 5.2 Tikhonov regularization

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

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

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

## 5.4 Generalized total least squares problem

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

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

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

## 5.6 Subspaces of the $U$ matrix

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

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

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

### 5.6.1 Linear discriminant analysis

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

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

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

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

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

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