On a Variational Formulation of QSVD and RSVD

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Abstract

Recently, Chu, Funderlic and Golub [SIAM J. Matrix Anal. Appl., 18:1082–1092, 1997] presented a variational formulation for the quotient singular value decomposition (QSVD) of two matrices $A \in \mathbf{R}^{n\times m}, C \in \mathbf{R}^{p\times m}$ which is a generalization of that one for the ordinary singular value decomposition (OSVD) and characterizes the role of two orthogonal matrices in QSVD. In this paper, we give an alternative derivation of this variational formulation and extend it to establish an analogous variational formulation for the Restricted Singular Value Decomposition (RSVD) of Matrix Triplets $A \in \mathbf{R}^{n\times m}, B \in \mathbf{R}^{n\times l}, C \in \mathbf{R}^{p\times m}$ which provides new understanding of the orthogonal matrices appearing in this decomposition.

Keywords: OSVD, QSVD, RSVD, Generalized Singular Value, Variational Formulation, Stationary Value, Stationary Point.
AMS subject classification: 65F15, 65H15.

1 Introduction

The ordinary singular value decomposition (OSVD) of a given matrix $A \in \mathbf{R}^{n\times m}$ is

$$U^T A V = \begin{array}{c} \\ r_a \\ n-r_a \end{array} \begin{array}{c} \begin{array}{cc} r_a & m-r_a \end{array} \\ \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} \end{array}, \tag{1}$$

with

$$\begin{aligned} U &= n \begin{array}{c} \begin{array}{cc} r_a & n-r_a \end{array} \\ \begin{bmatrix} U_1 & U_2 \end{bmatrix} \end{array}, \quad V = m \begin{array}{c} \begin{array}{cc} r_a & m-r_a \end{array} \\ \begin{bmatrix} V_1 & V_2 \end{bmatrix} \end{array}, \\ \Sigma &= \mathrm{diag}\{\sigma_1, \cdots, \sigma_{r_a}\}, \qquad \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{r_a} > 0, \qquad r_a = \mathrm{rank}(A), \end{aligned}$$

where U, V are orthogonal matrices. The $\sigma_1, \cdots, \sigma_{r_a}$ are the non-trivial singular values of A, and the columns of U_1 and V_1 are, respectively, the non-trivial left and right singular vectors of A. In this paper, $\|\cdot\|$ denotes the $2-$norm of a vector. The following theorem is well-known [4]:

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Theorem 1 *Given $A \in \mathbf{R}^{n\times m}$ with OSVD (1).*

(a) Consider the optimization problem

$$\max_{y=Ax,\ y\neq 0} \frac{\|y\|}{\|x\|}. \tag{2}$$

Then the non-trivial singular values $\sigma_1, \cdots, \sigma_{r_a}$ of A are precisely the stationary values, i.e., the functional evaluations at the stationary points, of (2). And, let the stationary points in (2) corresponding to the stationary values $\sigma_1, \cdots, \sigma_{r_a}$ be $\begin{bmatrix} x_1 \\ y_1 \end{bmatrix}, \cdots, \begin{bmatrix} x_{r_a} \\ y_{r_a} \end{bmatrix}$, then

$$V_1 = \begin{bmatrix} \frac{x_1}{\|x_1\|} & \cdots & \frac{x_{r_a}}{\|x_{r_a}\|} \end{bmatrix}.$$

Moreover, if $n = m = r_a$, then

$$U_1 = \begin{bmatrix} \frac{y_1}{\|y_1\|} & \cdots & \frac{y_{r_a}}{\|y_{r_a}\|} \end{bmatrix}.$$

(b) Consider the dual optimization problem

$$\max_{y^T=x^TA,\ y\neq 0} \frac{\|y\|}{\|x\|}. \tag{3}$$

Then the non-trivial singular values $\sigma_1, \cdots, \sigma_{r_a}$ of A are precisely the stationary values of (3). And, let the stationary points in (3) corresponding to the stationary values $\sigma_1, \cdots, \sigma_{r_a}$ be $\begin{bmatrix} x_1 \\ y_1 \end{bmatrix}, \cdots, \begin{bmatrix} x_{r_a} \\ y_{r_a} \end{bmatrix}$, then

$$U_1 = \begin{bmatrix} \frac{x_1}{\|x_1\|} & \cdots & \frac{x_{r_a}}{\|x_{r_a}\|} \end{bmatrix}.$$

Moreover, if $n = m = r_a$, then

$$V_1 = \begin{bmatrix} \frac{y_1}{\|y_1\|} & \cdots & \frac{y_{r_a}}{\|y_{r_a}\|} \end{bmatrix}.$$

Recently, in Chu, Funderlic and Golub [1] Theorem 1 has been generalized to the Quotient Singular Value Decomposition (QSVD) [3, 5, 6, 7, 8, 9, 10, 11, 13, 14] of two matrices $A \in \mathbf{R}^{n\times m}, C \in \mathbf{R}^{p\times m}$ based on the relationship between QSVD of two matrix A, C and the eigendecomposition of the matrix pencil (A^TA, C^TC).

The purposes of this paper are twofold. Firstly, we present an alternative derivation of the variational formulation in [1] directly based on the QSVD of two matrices A, C. Then we extend this result to the Restricted Singular Value Decomposition (RSVD)[8, 9, 10, 11, 15, 16] of matrix triplets and obtain a analogous variational formulation which provides new understanding of the orthogonal matrices appearing in this decomposition.

In order to prove our main results, we will establish two condensed forms based on orthogonal matrix transformations. The QSVD of two matrices and the RSVD of matrix triplets can be obtained and the variational formulation for QSVD and RSVD can be proved directly based on these two condensed forms.

In this paper, we use the following notation:

- $\mathcal{S}_\infty(M)$ denotes a matrix with orthogonal columns spanning the right nullspace of a matrix M;

- $\mathcal{T}_\infty(M)$ denotes a matrix with orthogonal columns spanning the right nullspace of a matrix M^T;
- $M^\perp$ denotes the orthogonal complement of the space spanned by the columns of M;
- Unless noted, we do not distinguish between a matrix with orthogonal columns and the space spanned by its columns.

We also use the following notation for any given matrices A, B, C with compatible sizes: denote

$$\begin{aligned}
r_a &= \operatorname{rank}(A), \quad r_b = \operatorname{rank}(B), \quad r_c = \operatorname{rank}(C), \\
r_{ab} &= \operatorname{rank}\begin{bmatrix} A & B \end{bmatrix}, \quad \bar{r}_{ac} = \operatorname{rank}\begin{bmatrix} A \\ C \end{bmatrix}, \quad r_{abc} = \operatorname{rank}\begin{bmatrix} A & B \\ C & 0 \end{bmatrix}, \\
k_1 &= r_{abc} - r_b - r_c, \quad k_2 = r_{ab} + r_c - r_{abc}, \\
k_3 &= \bar{r}_{ac} + r_b - r_{abc}, \quad k_4 = r_a + r_{abc} - r_{ab} - \bar{r}_{ac}.
\end{aligned}$$

2 A Variational Formulation for QSVD

Nowadays, several generalizations of the OSVD have been proposed and analysed. One that is well-known is the generalized SVD as introduced by Paige and Saunders in [5], which was proposed by De Moor and Golub [11] to rename as the QSVD. Another one is the RSVD, introduced in its explicit form by Zha [16] and further developed and discussed by De Moor and Golub [8].

In this section we will give an alternative proof for the variational formulation for the QSVD of [1] based directly on QSVD itself. Firstly we present a condensed form to derive QSVD of two matrices.

Lemma 2 *Given matrices $A \in \mathbf{R}^{n\times m}, C \in \mathbf{R}^{p\times m}$. Then there exist three orthogonal matrices $U_a \in \mathbf{R}^{n\times n}, W \in \mathbf{R}^{m\times m}, V_c \in \mathbf{R}^{p\times p}$ such that*

$$\begin{aligned}
U_a^T A W &= \begin{array}{c} \\ \bar{r}_{ac}-r_c \\ r_a+r_c-\bar{r}_{ac} \\ n-r_a \end{array} \begin{array}{c} \begin{array}{cccc} \bar{r}_{ac}-r_c & r_a+r_c-\bar{r}_{ac} & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \begin{bmatrix} A_{11} & A_{12} & 0 & 0 \\ 0 & A_{22} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array}, \\
V_c^T C W &= \begin{array}{c} \\ p-r_c \\ r_a+r_c-\bar{r}_{ac} \\ \bar{r}_{ac}-r_a \end{array} \begin{array}{c} \begin{array}{cccc} \bar{r}_{ac}-r_c & r_a+r_c-\bar{r}_{ac} & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & C_{22} & 0 & 0 \\ C_{31} & C_{32} & C_{33} & 0 \end{bmatrix} \end{array},
\end{aligned} \tag{4}$$

where A_{11}, A_{22}, C_{22} and C_{33} are nonsingular.

Proof. See Appendix A. □

Let the OSVD of $A_{22}C_{22}^{-1}$ be

$$U_{22}^T A_{22} C_{22}^{-1} V_{22} = \operatorname{diag}\{\sigma_1, \cdots, \sigma_s\} =: S_A, \quad s = r_a + r_c - \bar{r}_{ac}, \tag{5}$$

where U_{22}, V_{22} are orthogonal matrices, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_s > 0$. Define

$$\begin{aligned} U &:= U_a \operatorname{diag}\{I_{\bar{r}_{ac}-r_c}, U_{22}, I_{n-r_a}\}, &(6)\\ V &:= V_c \operatorname{diag}\{I_{p-r_c}, V_{22}, I_{\bar{r}_{ac}-r_a}\}. &(7)\end{aligned}$$

$$X = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ -C_{33}^{-1}C_{31} & -C_{33}^{-1}C_{32} & C_{33}^{-1} & 0 \\ 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} A_{11}^{-1} & -A_{11}^{-1}A_{12}C_{22}^{-1}V_{22} & 0 & 0 \\ 0 & C_{22}^{-1}V_{22} & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{bmatrix}, \tag{8}$$

Then, as a direct consequence of the condensed form (4), we have the following well-known QSVD theorem.

Theorem 3 *(***QSVD Theorem***) Let $A \in \mathbf{R}^{n\times m}, C \in \mathbf{R}^{p\times m}$, there exist orthogonal matrices $U \in \mathbf{R}^{n\times n}, V \in \mathbf{R}^{p\times p}$ and nonsingular matrix X such that*

$$U^TAX = \begin{array}{c} \\ \bar{r}_{ac}-r_c \\ r_a+r_c-\bar{r}_{ac} \\ n-r_a \end{array} \begin{array}{c} \begin{array}{cccc} \bar{r}_{ac}-r_c & r_a+r_c-\bar{r}_{ac} & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & S_A & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array},$$

$$V^TCX = \begin{array}{c} \\ p-r_c \\ r_a+r_c-\bar{r}_{ac} \\ \bar{r}_{ac}-r_a \end{array} \begin{array}{c} \begin{array}{cccc} \bar{r}_{ac}-r_c & r_a+r_c-\bar{r}_{ac} & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \end{bmatrix} \end{array}, \tag{9}$$

where S_A is of the form (5), and U, V and X can be chosen to be given by (6), (7) and (8), respectively. $\sigma_i, i = 1, \cdots, s$ are defined to be the non-trivial generalized singular values of two matrices A, C.

According to the uniqueness theorem in [16], we only need to characterize matrices U, V given by (6) and (7) in order to characterize the role of orthogonal matrices in QSVD. Let U, V be given by (6) and (7) and partition these two orthogonal matrices by

$$U = \begin{array}{c} \begin{array}{ccc} \bar{r}_{ac}-r_c & r_a+r_c-\bar{r}_{ac} & n-r_a \end{array} \\ \begin{bmatrix} U_1 & U_2 & U_3 \end{bmatrix} \end{array}, \tag{10}$$

$$V = \begin{array}{c} \begin{array}{ccc} p-r_c & r_a+r_c-\bar{r}_{ac} & \bar{r}_{ac}-r_a \end{array} \\ \begin{bmatrix} V_1 & V_2 & V_3 \end{bmatrix} \end{array}. \tag{11}$$

$$\tag{12}$$

Then, from Lemma 2 we have

$$\begin{aligned} U_3 &= \mathcal{T}_\infty(A), \quad U_1 = \mathcal{T}_\infty^\perp(A\mathcal{S}_\infty(C)), &(13)\\ V_1 &= \mathcal{T}_\infty(C), \quad V_3 = \mathcal{T}_\infty^\perp(C\mathcal{S}_\infty(A)). &(14)\end{aligned}$$

Hence, in order to characterize the role of orthogonal matrices U, V in QSVD, it should only characterize the role of U_2, V_2 in QSVD.

The following variational formulation has been established in [1] to characterize U_2 and V_2.

Theorem 4 *Given $A \in \mathbf{R}^{n\times m}, C \in \mathbf{R}^{p\times m}$. Consider the optimization problem*

$$\max_{\begin{bmatrix} A^T & C^T \\ \mathcal{T}_\infty^T(A) & 0 \\ 0 & \mathcal{T}_\infty^T(C) \end{bmatrix} \begin{bmatrix} x \\ -y \end{bmatrix} = 0,\ x\neq 0} \frac{\|y\|}{\|x\|}. \tag{15}$$

Then the non-trivial generalized singular values $\sigma_1, \cdots, \sigma_s$ of two matrices A, C are precisely the stationary values for the problem (15). Furthermore, let $\begin{bmatrix} x_1 \\ -y_1 \end{bmatrix}, \cdots, \begin{bmatrix} x_s \\ -y_s \end{bmatrix}$ be stationary points of the problem (15) with corresponding stationary values $\sigma_1, \cdots, \sigma_s$, then

$$U_2 = \begin{bmatrix} \frac{x_1}{\|x_1\|} & \cdots & \frac{x_s}{\|x_s\|} \end{bmatrix}, \quad V_2 = \begin{bmatrix} \frac{y_1}{\|y_1\|} & \cdots & \frac{y_s}{\|y_s\|} \end{bmatrix}.$$

Proof. We prove Theorem 4 by the following three arguments.

- Argument 1 Firstly, we characterize orthogonal matrices U_{22}, V_{22} in (5). Consider the optimization problem

$$\max_{x_2^T A_{22} = y_2^T C_{22},\ x_2\neq 0} \frac{\|y_2\|}{\|x_2\|}. \tag{16}$$

  Since A_{22}, C_{22} are both nonsingular, by Theorem 1 the $\sigma_1, \cdots, \sigma_s$, i.e., the singular values of the matrix $A_{22}C_{22}^{-1}$ are precisely the stationary values of the problem (16), and, if $\begin{bmatrix} x_2^1 \\ -y_2^1 \end{bmatrix}, \cdots, \begin{bmatrix} x_2^s \\ -y_2^s \end{bmatrix}$ are the stationary points of the problem (16) with corresponding stationary values $\sigma_1, \cdots, \sigma_s$, then

$$U_{22} = \begin{bmatrix} \frac{x_2^1}{\|x_2^1\|} & \cdots & \frac{x_2^s}{\|x_2^s\|} \end{bmatrix}, \quad V_{22} = \begin{bmatrix} \frac{y_2^1}{\|y_2^1\|} & \cdots & \frac{y_2^s}{\|y_2^s\|} \end{bmatrix}.$$

- Argument 2 Secondly, let

$$\mathcal{F} = \{\begin{bmatrix} x \\ -y \end{bmatrix} | x \in \mathbf{R}^n, y \in \mathbf{R}^p, U_a^T x = \begin{array}{l} \bar{r}_{ac} - r_c \\ r_a + r_c - \bar{r}_{ac} \\ n - r_a \end{array} \begin{bmatrix} 0 \\ x_2 \\ 0 \end{bmatrix},$$

$$V_c^T y = \begin{array}{l} p - r_c \\ r_a + r_c - \bar{r}_{ac} \\ \bar{r}_{ac} - r_a \end{array} \begin{bmatrix} 0 \\ y_2 \\ 0 \end{bmatrix}, \quad x^T A = y^T C, x \neq 0\}.$$

  Consider the optimization problem

$$\max_{\begin{bmatrix} x \\ -y \end{bmatrix} \in \mathcal{F}} \frac{\|y\|}{\|x\|}. \tag{17}$$

Obviously, we have that $\begin{bmatrix} x \\ -y \end{bmatrix}$ is a stationary point of the problem (17) with stationary value σ if and only if $\begin{bmatrix} x_2 \\ -y_2 \end{bmatrix}$ is a stationary point of the problem (16) with the same stationary point σ and furthermore

$$U_a^T x = \begin{array}{c} \bar{r}_{ac} - r_c \\ r_a + r_c - \bar{r}_{ac} \\ n - r_a \end{array} \begin{bmatrix} 0 \\ x_2 \\ 0 \end{bmatrix}, \quad V_c^T y = \begin{array}{c} p - r_c \\ r_a + r_c - \bar{r}_{ac} \\ \bar{r}_{ac} - r_a \end{array} \begin{bmatrix} 0 \\ y_2 \\ 0 \end{bmatrix}.$$

- <u>Argument 3</u> Finally, for any $x \in \mathbf{R}^n, y \in \mathbf{R}^p$, partition

$$U_a^T x = \begin{array}{c} \bar{r}_{ac} - r_c \\ r_a + r_c - \bar{r}_{ac} \\ n - r_a \end{array} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \quad V_c^T y = \begin{array}{c} p - r_c \\ r_a + r_c - \bar{r}_{ac} \\ \bar{r}_{ac} - r_a \end{array} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}.$$

Since

$$U_a^T \mathcal{T}_\infty(A) = \begin{array}{c} \bar{r}_{ac} - r_c \\ r_a + r_c - \bar{r}_{ac} \\ n - r_a \end{array} \begin{bmatrix} 0 \\ 0 \\ I \end{bmatrix}, \quad V_c^T \mathcal{T}_\infty(C) = \begin{array}{c} p - r_c \\ r_a + r_c - \bar{r}_{ac} \\ \bar{r}_{ac} - r_a \end{array} \begin{bmatrix} I \\ 0 \\ 0 \end{bmatrix},$$

it is easy to know that $\begin{bmatrix} x \\ -y \end{bmatrix} \in \mathcal{F}$ if and only if

$$\begin{bmatrix} A^T & C^T \\ \mathcal{T}_\infty^T(A) & 0 \\ 0 & \mathcal{T}_\infty^T(C) \end{bmatrix} \begin{bmatrix} x \\ -y \end{bmatrix} = 0, \quad x \neq 0.$$

Note that

$$U_a^T U_2 = \begin{array}{c} \bar{r}_{ac} - r_c \\ r_a + r_c - \bar{r}_{ac} \\ n - r_a \end{array} \begin{bmatrix} 0 \\ U_{22} \\ 0 \end{bmatrix}, \quad V_c^T V_2 = \begin{array}{c} p - r_c \\ r_a + r_c - \bar{r}_{ac} \\ \bar{r}_{ac} - r_a \end{array} \begin{bmatrix} 0 \\ V_{22} \\ 0 \end{bmatrix},$$

thus, Theorem 4 follows directly from the above Arguments 1, 2 and 3. $\square$

3 A Variational Formulation for RSVD

In Section 2 we have derived the QSVD of two matrices A, C based on the condensed form (4). Now we will establish the RSVD of a matrix triplet (A, B, C) via an analogous condensed form.

Lemma 5 *Given $A \in \mathbf{R}^{n\times m}, B \in \mathbf{R}^{n\times l}, C \in \mathbf{R}^{p\times m}$. Then there exist orthogonal matrices $P \in \mathbf{R}^{n\times n}, Q \in \mathbf{R}^{m\times m}, U_b \in \mathbf{R}^{l\times l}, V_c \in \mathbf{R}^{p\times p}$ such that*

$$
\begin{aligned}
PAQ &= \begin{array}{c} \\ k_1 \\ k_2 \\ k_3 \\ k_4 \\ r_{ab}-r_a \\ n-r_{ab} \end{array} \begin{array}{c} \begin{array}{cccccc} k_1 & k_2 & k_3 & k_4 & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \left[\begin{array}{cccccc} A_{11} & A_{12} & 0 & 0 & 0 & 0 \\ 0 & A_{22} & 0 & 0 & 0 & 0 \\ A_{31} & A_{32} & A_{33} & A_{34} & 0 & 0 \\ A_{41} & A_{42} & 0 & A_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] \end{array}, \\
PBU_b &= \begin{array}{c} \\ k_1 \\ k_2 \\ k_3 \\ k_4 \\ r_{ab}-r_a \\ n-r_{ab} \end{array} \begin{array}{c} \begin{array}{cccc} l-r_b & k_3 & k_4 & r_{ab}-r_a \end{array} \\ \left[\begin{array}{cccc} 0 & 0 & 0 & B_{14} \\ 0 & 0 & 0 & B_{24} \\ 0 & B_{32} & B_{33} & B_{34} \\ 0 & 0 & B_{43} & B_{44} \\ 0 & 0 & 0 & B_{54} \\ 0 & 0 & 0 & 0 \end{array}\right] \end{array}, \\
V_c^TCQ &= \begin{array}{c} \\ p-r_c \\ k_2 \\ k_4 \\ \bar{r}_{ac}-r_a \end{array} \begin{array}{c} \begin{array}{cccccc} k_1 & k_2 & k_3 & k_4 & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \left[\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & C_{22} & 0 & 0 & 0 & 0 \\ C_{31} & C_{32} & 0 & C_{34} & 0 & 0 \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & 0 \end{array}\right] \end{array},
\end{aligned}
\tag{18}
$$

where $A_{11}, A_{22}, A_{33}, A_{44}$, B_{32}, B_{43}, B_{54}, C_{22}, C_{34} and C_{45} are nonsingular.

Proof. See Appendix B. □

Let the OSVD of $B_{43}^{-1}A_{44}C_{34}^{-1}$ be

$$U_{44}^TB_{43}^{-1}A_{44}C_{34}^{-1}V_{44} = \mathrm{diag}\{\sigma_1, \cdots, \sigma_{k_4}\} =: S_A, \tag{19}$$

where U_{44}, V_{44} are orthogonal matrices, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{k_4} > 0$. Define

$$U := U_b \begin{bmatrix} I_{l-r_b} & & & \\ & I_{k_3} & & \\ & & U_{44} & \\ & & & I_{r_{ab}-r_a} \end{bmatrix}, \tag{20}$$

$$V := V_c \begin{bmatrix} I_{p-r_c} & & & \\ & I_{k_2} & & \\ & & V_{44} & \\ & & & I_{\bar{r}_{ac}-r_a} \end{bmatrix}. \tag{21}$$

Similarly to Theorem 3, from Lemma 5 directly, we have

Theorem 6 *(**RSVD Theorem**) Given $A \in \mathbf{R}^{n\times m}, B \in \mathbf{R}^{n\times l}, C \in \mathbf{R}^{p\times m}$. Then there exist nonsingular matrices $X \in \mathbf{R}^{n\times n}, Y \in \mathbf{R}^{m\times m}$ and orthogonal matrices $U \in \mathbf{R}^{l\times l}, V \in \mathbf{R}^{p\times p}$*

such that

$$
\begin{array}{rcl}
X^TAY & = & \begin{array}{c} \\ k_1 \\ k_2 \\ k_3 \\ k_4 \\ r_{ab}-r_a \\ n-r_{ab} \end{array} \begin{array}{c} \begin{array}{cccccc} k_1 & k_2 & k_3 & k_4 & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \left[\begin{array}{cccccc} I & 0 & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 & 0 \\ 0 & 0 & I & 0 & 0 & 0 \\ 0 & 0 & 0 & S_A & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] \end{array}, \\
X^TBU & = & \begin{array}{c} \\ k_1 \\ k_2 \\ k_3 \\ k_4 \\ r_{ab}-r_a \\ n-r_{ab} \end{array} \begin{array}{c} \begin{array}{cccc} l-r_b & k_3 & k_4 & r_{ab}-r_a \end{array} \\ \left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \\ 0 & 0 & 0 & 0 \end{array}\right] \end{array}, \\
V^TCY & = & \begin{array}{c} \\ p-r_c \\ k_2 \\ k_4 \\ \bar{r}_{ac}-r_a \end{array} \begin{array}{c} \begin{array}{cccccc} k_1 & k_2 & k_3 & k_4 & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \left[\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 & I & 0 \end{array}\right] \end{array},
\end{array}
\tag{22}
$$

where S_A is of the form (19), and U, V can be chosen to be given by (20) and (21), respectively, $\sigma_1, \cdots, \sigma_{k_4}$ are defined to be the non-trivial restricted singular values of matrix triplets A, B, C.

From the uniqueness theorem in [16], we only need to consider matrices U, V given by (20) and (21) in order to characterize the role of orthogonal matrices in RSVD. Let U, V be defined by (20) and (21), respectively and partition

$$
\begin{array}{rcl}
U & = & \begin{array}{c} \begin{array}{cccc} l-r_b & k_3 & k_4 & r_{ab}-r_a \end{array} \\ \left[\begin{array}{cccc} U_1 & U_2 & U_3 & U_4 \end{array}\right] \end{array}, \\
V & = & \begin{array}{c} \begin{array}{cccc} p-r_c & k_2 & k_4 & \bar{r}_{ac}-r_a \end{array} \\ \left[\begin{array}{cccc} V_1 & V_2 & V_3 & V_4 \end{array}\right] \end{array}.
\end{array}
$$

We have

$$
\begin{array}{rcl}
U_1 & = & \mathcal{S}_\infty(B), \quad U_4 = \mathcal{S}_\infty^\perp(\mathcal{T}_\infty^T(A)B), \\
V_1 & = & \mathcal{T}_\infty(C), \quad V_4 = \mathcal{T}_\infty^\perp(C\mathcal{S}_\infty(A)).
\end{array}
$$

Furthermore, if we define

$$
\begin{array}{rcl}
\Psi_1 & := & C\mathcal{S}_\infty(\mathcal{T}_\infty^T(B)A), \\
\Psi_2 & := & A\mathcal{S}_\infty(\mathcal{T}_\infty^T(B)A), \\
\Psi_3 & := & (\mathcal{T}_\infty(\Psi_2\mathcal{S}_\infty(\Psi_1)))^TB,
\end{array}
$$

then,

$$
\begin{aligned}
\Psi_1 &= V_c \times \begin{array}{c} \\ p-r_c \\ k_2 \\ k_4 \\ \bar{r}_{ac}-r_a \end{array}
\begin{array}{c} \begin{array}{cccc} k_3 & k_4 & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\
\left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & C_{34} & 0 & 0 \\ C_{43} & C_{44} & C_{45} & 0 \end{array}\right] \end{array}, \\
\Psi_2 &= P^T \times \begin{array}{c} \\ k_1 \\ k_2 \\ k_3 \\ k_4 \\ r_{ab}-r_a \\ n-r_{ab} \end{array}
\begin{array}{c} \begin{array}{cccc} k_3 & k_4 & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\
\left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ A_{33} & A_{34} & 0 & 0 \\ 0 & A_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right] \end{array}, \\
\Psi_3 &= \begin{array}{c} \\ k_1 \\ k_2 \\ k_4 \\ r_{ab}-r_a \\ n-r_{ab} \end{array}
\begin{array}{c} \begin{array}{cccc} l-r_b & k_3 & k_4 & r_{ab}-r_a \end{array} \\
\left[\begin{array}{cccc} 0 & 0 & 0 & B_{14} \\ 0 & 0 & 0 & B_{24} \\ 0 & 0 & B_{43} & B_{44} \\ 0 & 0 & 0 & B_{54} \\ 0 & 0 & 0 & 0 \end{array}\right] \end{array} U_b^T.
\end{aligned}
\tag{23}
$$

Hence, from (23) we have

$$
\left[\begin{array}{cc} U_1 & U_2 \end{array}\right] = \mathcal{S}_\infty(\Psi_3).
$$

Thus, in order to characterize the role of orthogonal matrices U, V in RSVD we only need to characterize the role of U_3, V_3 of U, V in RSVD. This can be done by the following variational formulation.

Theorem 7 *Given matrices $A \in \mathbf{R}^{n\times m}, B \in \mathbf{R}^{n\times l}, C \in \mathbf{R}^{p\times m}$. Consider the optimization problem*

$$
\max_{\left[\begin{array}{cc} A & B \\ \mathcal{S}_\infty^T(\left[\begin{array}{c} A \\ C \end{array}\right]) & 0 \\ \mathcal{S}_\infty^T(A)C^TC & 0 \\ 0 & \mathcal{S}_\infty^T(B) \\ 0 & \mathcal{T}_\infty^T(B\mathcal{S}_\infty^\perp(\Psi_3))B \end{array}\right]\left[\begin{array}{c} x \\ -y \end{array}\right]=0,\ x\neq 0} \frac{\|y\|}{\|Cx\|}. \tag{24}
$$

Then the stationary values for the problem (24) are precisely the non-trivial generalized singular values $\sigma_1, \cdots, \sigma_{k_4}$ of the matrix triplet A, B, C. Moreover, if $\left[\begin{array}{c} x_1 \\ -y_1 \end{array}\right], \cdots, \left[\begin{array}{c} x_{k_4} \\ -y_{k_4} \end{array}\right]$ are the stationary point of the problem (24) corresponding to the stationary values $\sigma_1, \cdots, \sigma_{k_4}$, respectively, then

$$
U_3 = \left[\begin{array}{ccc} \frac{y_1}{\|y_1\|} & \cdots & \frac{y_{k_4}}{\|y_{k_4}\|} \end{array}\right].
$$

Proof. Same as the proof of Theorem 4, we prove part (a) by the following three arguments.

- Argument 1 Firstly, we characterize U_{44} in (19). Consider the optimization problem

$$\max_{A_{44}x_4=B_{43}y_3,\ y_3\neq 0} \frac{\|y_3\|}{\|C_{34}x_4\|}. \tag{25}$$

Since A_{44}, B_{43}, C_{34} are nonsingular, so by Theorem 1, the stationary values of the problem (25) are precisely $\sigma_1, \cdots, \sigma_{k_4}$, i.e., the singular values of the matrix $B_{43}^{-1}A_{44}C_{34}^{-1}$, and, if let the corresponding stationary points be $\begin{bmatrix} x_4^1 \\ -y_3^1 \end{bmatrix}, \cdots, \begin{bmatrix} x_4^{k_4} \\ -y_3^{k_4} \end{bmatrix}$, then

$$U_{44} = \begin{bmatrix} \frac{y_3^1}{\|y_3^1\|} & \cdots & \frac{y_3^{k_4}}{\|y_3^{k_4}\|} \end{bmatrix}.$$

- Argument 2 Secondly, define

$$\mathcal{F} := \left\{ \begin{bmatrix} x \\ -y \end{bmatrix} \| x \in \mathbf{R}^m, y \in \mathbf{R}^l, U_b^T y = \begin{array}{c} l-r_b \\ k_3 \\ k_4 \\ r_{ab}-r_a \end{array} \begin{bmatrix} 0 \\ 0 \\ y_3 \\ 0 \end{bmatrix}, \quad Q^T x = \begin{array}{c} k_1 \\ k_2 \\ k_3 \\ k_4 \\ \bar{r}_{ac}-r_a \\ m-\bar{r}_{ac} \end{array} \begin{bmatrix} 0 \\ 0 \\ x_3 \\ x_4 \\ x_5 \\ 0 \end{bmatrix}, \right.$$

$$\left. C_{43}x_3 + C_{44}x_4 + C_{45}x_5 = 0, Ax = By, y \neq 0 \right\}.$$

Consider the optimization problem

$$\max_{\begin{bmatrix} x \\ -y \end{bmatrix} \in \mathcal{F}} \frac{\|y\|}{\|Cx\|}. \tag{26}$$

Since A_{33}, A_{44}, B_{43} and C_{45} are nonsingular, so a simple calculation yields that the problem (26) are equivalent to the problem (25) in the sense that the stationary values of the problem (26) are precisely the stationary values of the problem (25), i.e., $\sigma_1, \cdots, \sigma_{k_4}$, and, $\begin{bmatrix} x \\ -y \end{bmatrix}$ is the stationary point of the problem (26) if and only if $\begin{bmatrix} x_4 \\ -y_3 \end{bmatrix}$ is the stationary point of the problem (25) with same stationary value.

- Argument 3 Thirdly, for any $x \in \mathbf{R}^m, y \in \mathbf{R}^l$, denote

$$U_b^T y = \begin{array}{c} l-r_b \\ k_3 \\ k_4 \\ r_{ab}-r_a \end{array} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}, \quad Q^T x = \begin{array}{c} k_1 \\ k_2 \\ k_3 \\ k_4 \\ \bar{r}_{ac}-r_a \\ m-\bar{r}_{ac} \end{array} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix}.$$

Since

$$\begin{array}{rcl} \mathcal{S}_\infty^T(\left[\begin{array}{c} A \\ C \end{array}\right])x = 0 & \Longleftrightarrow & x_6 = 0; \\ Ax = By & \Longrightarrow & x_1 = 0,\ x_2 = 0,\ y_4 = 0; \\ \mathcal{S}_\infty^T(A)C^TCx = & \Longleftrightarrow & C_{41}x_1 + C_{42}x_2 + C_{43}x_3 + C_{44}x_4 + C_{45}x_5 = 0; \\ \mathcal{S}_\infty^T(B)y = 0 & \Longleftrightarrow & y_1 = 0. \end{array}$$

From (23), we also know

$$\mathcal{T}_\infty^T(B\mathcal{S}_\infty^\perp(\Psi))By = 0 \quad \Longleftrightarrow y_2 = 0.$$

Therefore, we have that $\left[\begin{array}{c} x \\ -y \end{array}\right] \in \mathcal{F}$ if and only if

$$\left[\begin{array}{cc} A & B \\ \mathcal{S}_\infty^T(\left[\begin{array}{c} A \\ C \end{array}\right]) & 0 \\ \mathcal{S}_\infty^T(A)C^TC & 0 \\ 0 & \mathcal{S}_\infty^T(B) \\ 0 & \mathcal{T}_\infty^T(B\mathcal{S}_\infty^\perp(\Psi_3))B \end{array}\right] \left[\begin{array}{c} x \\ -y \end{array}\right] = 0, \quad y \neq 0.$$

Note that

$$U_b^TU_3 = \begin{array}{c} l - r_b \\ k_3 \\ k_4 \\ r_{ab} - r_a \end{array} \left[\begin{array}{c} 0 \\ 0 \\ U_{44} \\ 0 \end{array}\right],$$

so, Theorem 7 follows directly from the above Arguments 1, 2 and 3. □

Similarily, we also have the dual result of Theorem 7 which characterizes the non-trivial generalized singular values $\sigma_1, \cdots, \sigma_{k_4}$ and the matrix V_3 in (21). For the sake of simplicity, we omit it here.

4 Conclusion

In this paper, we have studied generalized singular value decompositions. We have given an alternative proof of the variational formulation for the QSVD in [1] and established an analogous variational formulation for the RSVD which provides new understanding of the orthogonal matrices appearing in this decomposition.

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Appendix A

In this appendix we prove Lemma 2 constructively.

Proof. We prove Lemma 2 by 4 steps as follows:

Step 1: Perform simulaneous row and column compression:

$$U_1^T A W_1 =: \begin{array}{c} \\ r_a \\ n-r_a \end{array} \begin{array}{c} \begin{array}{ccc} r_a & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \begin{bmatrix} A_{11} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \end{array},$$

$$V_1^T C W_1 =: \begin{array}{c} \\ p-r_c \\ r_a+r_c-\bar{r}_{ac} \\ \bar{r}_{ac}-r_a \end{array} \begin{array}{c} \begin{array}{ccc} r_a & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \begin{bmatrix} 0 & 0 & 0 \\ C_{21} & 0 & 0 \\ C_{31} & C_{33} & 0 \end{bmatrix} \end{array}$$

with A_{11}, C_{33} nonsingular and C_{21} full row rank.

Step 2: Perform a column compression:

$$C_{21} W_2 =: \begin{array}{c} \begin{array}{cc} \bar{r}_{ac}-r_c & r_a+r_c-\bar{r}_{ac} \end{array} \\ \begin{bmatrix} 0 & C_{22} \end{bmatrix} \end{array}$$

with C_{22} nonsingular. Set

$$A_{11} W_2 =: \begin{array}{c} \begin{array}{cc} \bar{r}_{ac}-r_c & r_a+r_c-\bar{r}_{ac} \end{array} \\ \begin{bmatrix} A_{11} & A_{12} \end{bmatrix} \end{array}, \quad C_{31} W_2 =: \begin{array}{c} \begin{array}{cc} \bar{r}_{ac}-r_c & r_a+r_c-\bar{r}_{ac} \end{array} \\ \begin{bmatrix} C_{31} & C_{32} \end{bmatrix} \end{array}.$$

Step 3: Perform a row compression:

$$U_3^T A_{11} =: \begin{array}{c} \bar{r}_{ac}-r_c \\ r_a+r_c-\bar{r}_{ac} \end{array} \begin{bmatrix} A_{11} \\ 0 \end{bmatrix}$$

with A_{11} nonsingular. Set

$$U_3^T A_{12} =: \begin{array}{c} \bar{r}_{ac}-r_c \\ r_a+r_c-\bar{r}_{ac} \end{array} \begin{bmatrix} A_{12} \\ A_{22} \end{bmatrix}.$$

Step 4: Set

$$U_a := U_1 \begin{bmatrix} U_3 & \\ & I \end{bmatrix}, \quad W := W_1 \begin{bmatrix} W_2 & \\ & I \end{bmatrix}, \quad V_c := V_1.$$

Then orthogonal matrices U_a, V_c and W satisfy (4).

Appendix B

Now we prove Lemma 5 constructively.

Proof. We prove Lemma 5 by 5 steps as follows:

Step 1: Compute orthogonal matrices P_1, Q_1 and U_1 based on the dual result of Lemma 2 such that

$$P_1AQ_1 =: \begin{array}{c} \\ r_{ab}-r_b \\ r_a+r_b-r_{ab} \\ r_{ab}-r_a \\ n-r_{ab} \end{array} \begin{array}{c} \begin{array}{ccc} r_{ab}-r_b & r_a+r_b-r_{ab} & m-r_a \end{array} \\ \begin{bmatrix} \Theta_{11} & 0 & 0 \\ \Theta_{21} & \Theta_{22} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \end{array},$$

$$P_1BU_1 =: \begin{array}{c} \\ r_{ab}-r_b \\ r_a+r_b-r_{ab} \\ r_{ab}-r_a \\ n-r_{ab} \end{array} \begin{array}{c} \begin{array}{ccc} l-r_b & r_a+r_b-r_{ab} & r_{ab}-r_a \end{array} \\ \begin{bmatrix} 0 & 0 & \Phi_{14} \\ 0 & \Phi_{32} & \Phi_{34} \\ 0 & 0 & B_{54} \\ 0 & 0 & 0 \end{bmatrix} \end{array}$$

with $\Theta_{11}, \Theta_{22}, \Phi_{32}$ and B_{54} nonsingular. Set

$$CQ_1 =: \begin{array}{c} \begin{array}{ccc} r_{ab}-r_b & r_a+r_b-r_{ab} & m-r_a \end{array} \\ \begin{bmatrix} C_1 & C_2 & C_3 \end{bmatrix} \end{array}.$$

Step 2: Compute orthogonal matrices P_2, Q_2 and V_2 based on Lemma 2 such that

$$P_2 \begin{bmatrix} \Theta_{22} & 0 \end{bmatrix} Q_2 =: \begin{array}{c} \\ k_3 \\ k_4 \end{array} \begin{array}{c} \begin{array}{cccc} k_3 & k_4 & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \begin{bmatrix} A_{33} & A_{34} & 0 & 0 \\ 0 & A_{44} & 0 & 0 \end{bmatrix} \end{array},$$

$$V_2 \begin{bmatrix} C_2 & C_3 \end{bmatrix} Q_2 =: \begin{array}{c} \\ p-k_4-\bar{r}_{ac}-r_a \\ k_4 \\ \bar{r}_{ac}-r_a \end{array} \begin{array}{c} \begin{array}{cccc} k_3 & k_4 & \bar{r}_{ac}-r_a & m-\bar{r}_{ac} \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & C_{34} & 0 & 0 \\ C_{43} & C_{44} & C_{45} & 0 \end{bmatrix} \end{array}$$

with A_{33}, A_{44} and C_{34}, C_{45} nonsingular. Set

$$V_2C_1 =: \begin{array}{c} p-k_4-\bar{r}_{ac}-r_a \\ k_4 \\ \bar{r}_{ac}-r_a \end{array} \begin{bmatrix} C_{11} \\ C_{31} \\ C_{41} \end{bmatrix}.$$

Step 3: Perform a simultaneous row and column compression:

$$V_3C_{11}Q_3 := \begin{array}{c} \\ p-r_c \\ k_2 \end{array} \begin{array}{c} \begin{array}{cc} k_1 & k_2 \end{array} \\ \begin{bmatrix} 0 & 0 \\ 0 & C_{22} \end{bmatrix} \end{array}$$

with C_{22} nonsingular. Set

$$\begin{bmatrix} C_{31} \\ C_{41} \end{bmatrix} Q_3 =: \begin{array}{c} \\ k_4 \\ \bar{r}_{ac}-r_a \end{array} \begin{array}{c} \begin{array}{cc} k_1 & k_2 \end{array} \\ \begin{bmatrix} C_{31} & C_{32} \\ C_{41} & C_{42} \end{bmatrix} \end{array}.$$

Step 4: Perform a row compression and a column compression:

$$P_4\Theta_{11}Q_3 =: \begin{array}{c c} & \begin{array}{cc} k_1 & k_2 \end{array} \\ \begin{array}{c} k_1 \\ k_2 \end{array} & \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix} \end{array}, \quad P_2\Phi_{32}U_4 =: \begin{array}{c c} & \begin{array}{cc} k_3 & k_4 \end{array} \\ \begin{array}{c} k_3 \\ k_4 \end{array} & \begin{bmatrix} B_{32} & B_{33} \\ 0 & B_{43} \end{bmatrix} \end{array},$$

where A_{11}, A_{22} and B_{32}, B_{43} are nonsingular. Set

$$P_2\Theta_{21}Q_4 =: \begin{array}{c c} & \begin{array}{cc} k_1 & k_2 \end{array} \\ \begin{array}{c} k_3 \\ k_4 \end{array} & \begin{bmatrix} A_{31} & A_{32} \\ A_{41} & A_{42} \end{bmatrix} \end{array}, \quad \begin{bmatrix} P_4\Phi_{14} \\ P_2\Phi_{34} \end{bmatrix} =: \begin{array}{c} k_1 \\ k_2 \\ k_3 \\ k_4 \end{array} \begin{bmatrix} B_{14} \\ B_{24} \\ B_{34} \\ B_{44} \end{bmatrix}.$$

Step 5: Set

$$\begin{aligned} P &:= \begin{bmatrix} P_4 & \\ & I \end{bmatrix} \begin{bmatrix} I_{r_{ab}-r_b} & & \\ & P_2 & \\ & & I_{n-r_a} \end{bmatrix} P_1, \quad Q := Q_1 \begin{bmatrix} I & \\ & Q_2 \end{bmatrix} \begin{bmatrix} Q_3 & \\ & I \end{bmatrix}, \\ U_b &:= U_1 \begin{bmatrix} I_{l-r_b} & & \\ & U_4 & \\ & & I_{r_{ab}-r_a} \end{bmatrix}, \quad V_c^T := \begin{bmatrix} V_3 & \\ & I \end{bmatrix} V_2. \end{aligned}$$

Then, the orthogonal matrices P, Q, U_b and V_c satisfy the condensed form (18).

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