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Generalizations of the singular value and QR decompositions*

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Abstract. In this paper, we provide a state-of-the-art survey of a recently discovered set of generalizations of the ordinary singular value decomposition, which contains all existing generalizations for 2 matrices (such as the product SVD and the quotient SVD) and for 3 matrices (such as the restricted SVD), as special cases. We present the main theorem and a discussion on the structural properties of these generalized singular value decompositions. A proposal for a standardized nomenclature is made as well. At the same time, we summarize some recent results on a corresponding generalization for any number of matrices of the QR (or URV) decomposition.

Zusammenfassung. In dieser Arbeit wird eine Übersicht über kürzlich entdeckte Verallgemeinerungen der gewöhnlichen Singularwertzerlegung (SVD) gegeben, die alle vorhandenen Verallgemeinerungen für zwei Matrizen (wie die Produkt SVD und die Quotienten SVD) und für drei Matrizen (wie die eingeschränkte SVD) als Spezialfälle enthält. Wir geben den Hauptsatz an und eine Diskussion der strukturellen Eigenschaften dieser verallgemeinerten SVD. Ein Vorschlag für eine standardisierte Bezeichnungsweise wird ebenfalls gemacht. Gleichzeitig fassen wir einige neue Ergebnisse entsprechender Verallgemeinerungen auf eine beliebige Anzahl von Matrizen der QR (oder URV) Zerlegung zusammen.

Résumé. Nous faisons dans cet article le point sur un ensemble récemment découvert de généralisations de la décomposition en valeurs singulières (SVD) ordinaire, ensemble contenant toutes les généralisations existantes à deux matrices (telle que la SVD produit et la SVD quotient) et à trois matrices (telle que la SVD restreinte) comme cas particuliers. Nous présentons le théorème central et une discussion sur les propriétés structurales de ces décompositions en valeurs singulières généralisées. Nous faisons également une proposition de nomenclature standardisée. Dans le même temps nous résumons certains résultats récents concernant une généralisation correspondante pour la décomposition QR (ou URV) d'un nombre arbitraire de matrices.

Keywords. Ordinary, product, quotient, restricted singular value decomposition, QR decomposition, URV decomposition, complete orthogonal factorization.

1. Introduction

A complete orthogonal factorization of an $m\times n$ matrix A is any factorization of the form

$$A=U\begin{bmatrix}T & 0\\ 0 & 0\end{bmatrix}V^*, \tag{1}$$

where T is $r_a\times r_a$ square nonsingular and $r_a=\operatorname{rank}(A)$. One particular case is the singular value decomposition (SVD), which has become an important tool in the analysis and numerical solution of numerous problems, especially since the development of numerically robust algorithms by Gene Golub and his coworkers [3, 18, 19]. The SVD is a complete orthogonal factorization where the matrix T is diagonal with positive diagonal elements, which are the singular values. In applications where $m\gg n$, it is often a good idea to use the QR-decomposition (QRD) of the matrix as a

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preliminary step in the computation of its SVD. The SVD of A is obtained via the SVD of its triangular factor as

$$A = QR = Q(U_r \Sigma_r V_r^*) = (QU_r)\Sigma_r V_r^*.$$

This idea of combining the QRD and the SVD of the triangular matrix, in order to compute the SVD of the full matrix, is mentioned in [21, p. 119] and was more fully analyzed in [5]. In [20] the method is referred to as R-bidiagonalization. Its flop count is $mn^2 + n^3$ as compared to $2mn^2 - 2/3n^3$ for a bidiagonalization of the full matrix. Hence, whenever $m \geqslant 5/3n$, it is more advantageous to use the R-bidiagonalization algorithm.

There exist still other complete orthogonal factorizations of the form (1) where T is required to be triangular (upper or lower) (see e.g. [20]). Such a factorization has been called an URV-decompositon in [31]. Here

$$A = U \begin{bmatrix} R & 0 \\ 0 & 0 \end{bmatrix} V^*,$$

with $U \in \mathbb{C}^{m \times m}$, $V \in \mathbb{C}^{n \times n}$ are unitary matrices and $R \in \mathbb{C}^{r_a \times r_a}$ is square nonsingular upper triangular.

The ordinary singular value decomposition (OSVD) has become an important tool in the analysis and numerical solution of numerous problems (see e.g. [7, 20, 34] for properties and applications.) Not only does it allow for an elegant problem formulation, but at the same time it provides geometrical and algebraic insight together with an immediate numerically robust implementation [20]. In [24, p. 78], credit for the first proofs of the OSVD is given to Beltrami [2], Jordan [23], Sylvester [33] and Autonne [1].

In the last decade or so, several generalizations for the SVD have been derived. The motivation is basically the necessity to avoid the explicit formation of products and matrix quotients in the computation of the SVD of products and quotients of matrices. Let A and B be nonsingular square matrices and assume that we need the SVD of $AB^{-*} = USV^*$.[1] It is well known that the explicit calculation of B^{-1} followed by the computation of the product may result in loss of numerical precision (digit cancellation), even before any factorization is attempted! The reason is the finite machine precision of any calculator (see the numerical examples in Section 5). Therefore, it seems more appropriate to come up with an implicit combined factorization of A and B separately, such as

$$A = UD_1X^{-1}, \qquad B = X^{-*}D_2V^*, \tag{2}$$

where U and V are unitary and X nonsingular. The matrices D_1 and D_2 are real but 'sparse' (*quasi-diagonal* as we will call them), and the product $D_1D_2^{-\mathrm{T}}$ is diagonal with positive diagonal elements. Then we find

$$AB^{-*} = UD_1X^{-1}XD_2^{-\mathrm{T}}V^* = U(D_1D_2^{-\mathrm{T}})V^*.$$

A factorization as in (2) is always possible for two square non-singular matrices. As a matter of fact, it is always possible for two matrices $A \in \mathbb{C}^{m \times n}$ and $B \in \mathbb{C}^{n \times p}$ (as long as the number of columns of A is the same as the number of rows of B, which we will refer to as a compatibility condition). In general, the matrices A and B may even be rank deficient. The combined factorization (2) is called the quotient singular value decomposition (QSVD) and was first suggested in [37] and refined in [28] (originally it was called the generalized SVD but we have suggested a standardized nomenclature in [10]).

A similar idea might be exploited for the SVD of the product of two matrices $AB = USV^*$, via the so-called product singular value decomposition (PSVD):

$$A = UD_1X^{-1}, \qquad B = XD_2V^*, \tag{3}$$

so that

$$AB = U(D_1D_2)V^*,$$

which is an SVD of AB. The combined factorization (3) was proposed in [16] as a formalization of

[1] The notation B^{-*} refers to the complex conjugate transpose of the inverse of the matrix B.

ideas in [22]. In the general case, for two compatible matrices A and B (that may be rank deficient), the PSVD as in (3) always exists and provides the SVD of AB without the explicit construction of the product. Similarly, if A and B are compatible, the QSVD always exists. However, it does not always deliver the SVD of $AB^{\dagger}$ when B is rank deficient ($B^{\dagger}$ is the pseudo-inverse of B).

Another generalization, this time for three matrices, is the restricted singular value decomposition (RSVD). It was proposed in [39] while numerous applications are reviewed in [11]. Soon after this it was found that all of these generalized SVDs for two or three matrices are special cases of a general theorem, presented in [14]. The main result is that there exist generalized singular value decompositions (GSVD) for any number of matrices $A_1, A_2, \ldots, A_k$ of compatible dimensions. The general structure of these GSVDs is further analysed in [9]. The dimensions of the blocks that occur in any GSVD can be expressed as ranks of the matrices involved and certain products and concatenations of these. We will present a summary of the results below.

As for generalizations of the QRD, it is mainly Paige in [27] who pointed out the importance of generalized QRDs for two matrices as a basic conceptual and mathematical tool. The motivation is that in some applications one needs the QRD of a product of two matrices AB where $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times p}$. For general matrices A and B such a computation avoids forming the product explicitly and transforms A and B separately to obtain the desired results. Paige [27] refers to such a factorization as a product QR factorization. Similarly, in some applications one needs the QR-factorization of AB^{-1} where B is square and nonsingular. A general numerically robust algorithm would not compute the inverse of B nor the product explicitly, but would transform A and B separately. Paige in [27] proposed to call such a combined decomposition of two matrices a generalized QR factorization, following [16]. We propose here to reserve the name generalized QRD for the complete set of generalizations of the QR-decompositions, which will be developed in this paper. We will also propose a novel nomenclature in a similar way as we have done for the generalizations of the SVD in [10].

Stoer [30] appears to be the first to have given a reliable computation of this type of generalized QR-factorization for two matrices (see [17]). Computational methods for producing the two types of generalized QR-factorizations for two matrices as described above, have appeared regularly in the literature as (intermediate) steps in the solution of some problems. A constructive proof of generalizations of the QRD for any number of matrices can be found in [13]. As we will see below, our generalized QRDs can also be considered as the appropriate generalization of the URV-decomposition of a matrix.

This paper is organized as follows. In Section 2, we present the main theorem for generalized singular value decompositions, while the corresponding generalized QR decompositions are explored in Section 3. The structural properties are summarized in Section 4, while in Section 5 we discuss the potential numerical advantages of the GSVDs with some small examples. We also give a brief survey of possible applications.

2. A tree of generalizations of the OSVD

In this section, we present a general theorem which can be considered as the appropriate generalization for any number of matrices of the SVD of one matrix. It contains the existing generalizations of the SVD for two (i.e. the PSVD and the QSVD) and three matrices (i.e. the RSVD) as special cases. A constructive proof can be found in [14].

THEOREM 1. Generalized Singular Value Decompositions for k matrices. Consider a set of k matrices with compatible dimensions: $A_1(n_0 \times n_1)$, $A_2(n_1 \times n_2), \ldots, A_{k-1}(n_{k-2} \times n_{k-1})$, $A_k(n_{k-1} \times n_k)$. *Then there exist*

- *Unitary matrices* $U_1(n_0 \times n_0)$ *and* $V_k(n_k \times n_k)$.
- *Matrices* $D_j, j = 1, 2, \ldots, k-1$ *of the form*

$$\underset{n_{j-1}\times n_j}{D_j} = \begin{array}{c} \\ r_j^1 \\ r_{j-1}^1-r_j^1 \\ r_j^2 \\ r_{j-1}^2-r_j^2 \\ r_j^3 \\ \vdots \\ \vdots \\ r_j^j \\ n_{j-1}-r_{j-1}-r_j^j \end{array} \begin{array}{c} \begin{array}{cccccc} r_j^1 & r_j^2 & r_j^3 & \cdots\cdots & r_j^j & n_j-r_j \end{array} \\ \begin{bmatrix} I & 0 & 0 & \cdots\cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots\cdots & 0 & 0 \\ 0 & I & 0 & \cdots\cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots\cdots & 0 & 0 \\ 0 & 0 & I & \cdots\cdots & 0 & 0 \\ 0 & \vdots & \vdots & \cdots\cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \cdots\cdots & \vdots & \vdots \\ 0 & \vdots & \vdots & \cdots\cdots & I & 0 \\ 0 & 0 & \cdots & \cdots\cdots & 0 & 0 \end{bmatrix} \end{array}, \tag{4}$$

where the integers r_j are the rank of the matrices A_j, satisfying

$$r_j = \operatorname{rank}(A_j) = \sum_{i=1}^{j} r_j^i. \tag{5}$$

– *A matrix S_k of the form*

$$\underset{n_{k-1}\times n_k}{S_k} = \begin{array}{c} \\ r_k^1 \\ r_{k-1}^1-r_k^1 \\ r_k^2 \\ r_{k-1}^2-r_k^2 \\ r_k^3 \\ \vdots \\ \vdots \\ r_k^k \\ n_{k-1}-r_{k-1}-r_k^k \end{array} \begin{array}{c} \begin{array}{cccccc} r_k^1 & r_k^2 & r_k^3 & \cdots\cdots & r_k^k & n_k-r_k \end{array} \\ \begin{bmatrix} S_k^1 & 0 & 0 & \cdots\cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots\cdots & 0 & 0 \\ 0 & S_k^2 & 0 & \cdots\cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots\cdots & 0 & 0 \\ 0 & 0 & S_k^3 & \cdots\cdots & 0 & 0 \\ 0 & \vdots & \vdots & \cdots\cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \cdots\cdots & \vdots & \vdots \\ 0 & \vdots & \vdots & \cdots\cdots & S_k^k & 0 \\ 0 & 0 & \cdots & \cdots\cdots & 0 & 0 \end{bmatrix} \end{array}. \tag{6}$$

The $r_k^i \times r_k^i$ matrices S_k^i are diagonal with positive diagonal elements. Expressions for the integers r_j^i are given in Section 3. They are ranks of certain matrices in the constructive proof of this Theorem [14].

– *Nonsingular matrices $X_j (n_j \times n_j)$ and Z_j, $j = 1, 2, \dots, k-1$ where Z_j is either $Z_j = X_j^{-*}$ or either $Z_j = X_j$ (i.e. both choices are always possible),*

such that the given matrices can be factorized as

$$A_1 = U_1 D_1 X_1^{-1},$$
$$A_2 = Z_1 D_2 X_2^{-1},$$
$$A_3 = Z_2 D_3 X_3^{-1},$$
$$\vdots$$
$$A_i = Z_{i-1} D_i X_i^{-1},$$
$$\vdots$$
$$A_k = Z_{k-1} S_k V_k^*.$$

Observe that the matrices D_j in (4) and S_k in (6) are in general not diagonal. Their only non-zero blocks however are diagonal block matrices. We propose to label them as quasi-diagonal matrices. The matrices D_j, $j = 1, \dots, k-1$ are quasi-diagonal, their only nonzero blocks being identity matrices. The matrix S_k is quasi-diagonal and its nonzero blocks are diagonal matrices with positive diagonal elements. Observe that we always take the last factor in every factorization as the inverse of a nonsingular matrix, which is only a matter of convention (another convention would result in a modified definition of the matrices Z_i). As to the name of a certain GSVD, we propose to adopt the following convention.

DEFINITION 1. The nomenclature for GSVDs. If $k = 1$ in Theorem 1, then the corresponding factorization of the matrix A_1 will be called the ordinary singular value decomposition.

If for a matrix pair A_i, A_{i+1}, $1 \leqslant i \leqslant k-1$ in Theorem 1, we have that

$$Z_i = X_i,$$

then the factorization of the pair will be said to be of P-type.

If on the other hand, for a matrix pair A_i, A_{i+1}, $1 \leqslant i \leqslant k-1$ in Theorem 1, we have that

$$Z_i = X_i^{-*},$$

the factorization of the pair will be said to be of Q-type.

The name of a GSVD of the matrices A_i, $i = 1, 2, \ldots, k > 1$ as in Theorem 1 is then obtained by simply enumerating the different factorization types.

Let us give some examples.

EXAMPLE 1. Consider two matrices A_1 $(n_0 \times n_1)$ and A_2 $(n_1 \times n_2)$. Then, we have two possible GSVDs:

	P-type	Q-type
A_1	$U_1 D_1 X_1^{-1}$	$U_1 D_1 X_1^{-1}$
A_2	$X_1 S_2 V_2^*$	$X_1^{-*} S_2 V_2^*$

The P-type factorization corresponds to the PSVD as in [16] (called ΠSVD there) and [8, 10], while the Q-type factorization is nothing else than the QSVD in [20, 28, 37] (called generalized SVD there). This justifies the choice of names for the factorization of pairs: A P-type factorization is precisely the kind of transformation that occurs in the PSVD while a Q-type factorization occurs in the QSVD.

EXAMPLE 2. The RSVD for three matrices (A_1, A_2, A_3) as introduced and analyzed in [11, 39] has the form

$$A_1 = U_1 S_1 X_1^{-1},$$
$$A_2 = X_1^{-*} S_2 X_2^{-1},$$
$$A_3 = X_2^{-*} S_3 V_3^*,$$

where S_1, S_2, S_3 are certain quasi-diagonal matrices. It can be verified that this RSVD can be rearranged into a QQ–SVD that is conform with the structure of Theorem 1.

EXAMPLE 3. Let us write down the PQQP–SVD for 5 matrices:

$$A_1 = U_1 D_1 X_1^{-1},$$
$$A_2 = X_1 D_2 X_2^{-1},$$
$$A_3 = X_2^{-*} D_3 X_3^{-1},$$
$$A_4 = X_3^{-*} D_4 X_4^{-1},$$
$$A_5 = X_4 S_5 V_5^*.$$

We also introduce the following notation, using powers, which symbolize a certain repetition of a letter or of a sequence of letters:

- P^3Q^2–SVD = PPPQQ–SVD,
- $(PQ)^2Q^3(PPQ)^2$–SVD = PQPQQQQPPQPPQ–SVD.

Despite the fact that there are 2^{k-1} different sequences of letters P and Q at level $k > 1$, not all of these sequences correspond to different GSVDs. The reason for this is that for instance the QP–SVD of (A^1, A^2, A^3) can be obtained from the PQ–SVD of $((A^3)^*, (A^2)^*, (A^1)^*)$. Similarly, the $P^2(QP)^3$–SVD of $(A^1, \ldots, A^9)$ is essentially the same as the $(PQ)^3P^2$–SVD of $((A^9)^*, \ldots, (A^1)^*)$. The following table gives the number of different factorizations for k matrices.

	k even	k odd
number of different GSVDs	$\frac{1}{2}(2^{k-1} + 2^{k/2})$	$\frac{1}{2}(2^{k-1} + 2^{(k-1)/2})$

Finally, we shall spend some words on the proof of the main Theorem, a detailed exposition of which can be found in [14]. It is based on two basic ideas: First, there is an inductive argument which allows us to construct the GSVD of k matrices $A_1, \ldots, A_k$ from a corresponding one for $k-1$ matrices $A_1, \ldots, A_{k-1}$. A key result here is a certain block factorization lemma for partitioned matrices. Next, the already obtained GSVD of the $k-1$ matrices $A_1, \ldots, A_{k-1}$ has to be modified according to a certain algorithm, which we have called the ripple-through-phenomenon in [14]. For all details of the constructive proof, the interested reader is referred to [14].

3. Generalized QR (URV) decompositions

In [13], we have derived the following generalization of the QR-decomposition for a chain of k matrices.

THEOREM 2. Generalized URV-decompositions. Given k complex matrices A_1 $(n_0 \times n_1)$, A_2 $(n_1 \times n_2), \ldots, A_k$ $(n_{k-1} \times n_k)$. *There always exist unitary matrices* $Q_0, Q_1, \ldots, Q_k$ *such that*

$$\tilde{T}_i = Q_{i-1}^* A_i Q_i,$$

where $\tilde{T}_i$ *is a lower triangular or upper triangular matrix (both cases are always possible) with the following structure:*

- *Lower triangular (which will be denoted by a superscript* l*):*

$$\tilde{T}_i^l = \begin{array}{cc} & \begin{array}{ccccc} r_i^1 & r_i^2 & \cdots & r_i^i & r_i^{i+1} \end{array} \\ \begin{array}{c} r_{i-1}^1 \\ r_{i-1}^2 \\ \vdots \\ r_{i-1}^i \end{array} & \begin{bmatrix} R_{i,1} & 0 & \cdots & 0 & 0 \\ * & R_{i,2} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ * & * & \cdots & R_{i,i} & 0 \end{bmatrix} \end{array},$$

where

$$R_{i,j} = \begin{bmatrix} 0 \\ R_{i,j}^l \end{bmatrix}$$

and $R_{i,j}^l$ *is a square nonsingular lower triangular matrix.*

- *Upper triangular (which will be denoted by a superscript* u*):*

$$\tilde{T}_i^u = \begin{array}{cc} & \begin{array}{ccccc} r_i^{i+1} & r_i^1 & \cdots & r_i^{i-1} & r_i^i \end{array} \\ \begin{array}{c} r_{i-1}^1 \\ r_{i-1}^2 \\ \vdots \\ r_{i-1}^i \end{array} & \begin{bmatrix} 0 & R_{i,1} & * & \cdots & * \\ 0 & 0 & R_{i,2} & \cdots & * \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & R_{i,i} \end{bmatrix} \end{array},$$

where

$$R_{i,j} = \begin{bmatrix} 0 \\ R_{i,j}^u \end{bmatrix}$$

and $R_{i,j}^u$ *is a square nonsingular upper triangular matrix.*

The block dimensions coincide with those of Theorem 1.

As to the nomenclature of these generalized URV-decompositions, we propose the following definition.

DEFINITION 2. Nomenclature for generalized URV. The name of a generalized URV-decomposition of k matrices of compatible dimensions is generated by enumerating the letters L (for lower) and U (for upper), according to the lower or upper triangularity of the matrices T_i, $i = 1, \ldots, k$ in the decomposition of Theorem 2.

For k matrices, there are 2^k different sequences with two letters. For instance, for $k = 3$, there are 8 generalized URV decompositions (LLL, LLU, LUL, LLU, ULL, ULU, UUL, UUU).

4. On the structure of the GSVD and the GQRD

In this section, we first point out how for each GSVD there are two generalized URV-decompositions and we clarify the correspondence between the two types of generalized decompositions. Next we give a summary of expressions for the block dimensions r_i^j in Theorem 1 and 2, in terms of the ranks of the matrices $A_1, \ldots, A_k$ and concatenations and products thereof. These expressions were derived in [9].

Recall the nomenclature for the generalized URV-decompositions (Definition 2) and the generalized singular value decompositions (Definition 1). The relation between these two definitions is the following:

- A pair of identical letters, i.e. L–L or U–U that occurs in the factorization of A_i, A_{i+1} corresponds to a P-type factorization of the pair.
- A pair of alternating letters, i.e. L–U or U–L that occurs in the factorization of A_i, A_{i+1} corresponds to a Q-type factorization of the pair.

As an example, for a PQP–SVD of 4 matrices, there are two possible corresponding generalized URV-decompositions, namely an LLUL-decomposition and an UULU-decomposition. As with the GSVD, we can also introduce the convention to use powers of (a sequence of) letters. For instance, for a P^3Q^2–SVD, there are two GURVs, namely an L^4UL–URV and an U^4LU–URV.

We now derive expressions for the block dimensions r_i^j.[2]

Let us first consider the case of a GSVD that consists only of P-type factorizations. Denote the rank of the product of the matrices A_i, $A_{i+1}, \ldots, A_j$ with $i \leqslant j$ by

$$r_{i(i+1)\cdots(j-1)j} = \operatorname{rank}(A_i A_{i+1} \cdots A_{j-1} A_j).$$

THEOREM 3. On the structure of the P^{k-l}–SVD, the L^k–URV and the U^k–URV. Consider any of the factorizations above for the matrices $A_1, A_2, \ldots, A_k$. Then, the block dimensions r_j^i that appear in Theorems 1 and 2 are given by

$$r_j^1 = r_{(1)(2)\cdots(j)}, \tag{7}$$

$$r_j^i = r_{i(i+1)\cdots(j)} - r_{(i-1)(i)\cdots(j)}, \tag{8}$$

with $r_j^i = r_i$ if $i = j$.

Next, consider the case of a GSVD that only consists of Q-type factorizations. Denote the rank of the block bidiagonal matrix

$$\begin{bmatrix} A_i & 0 & 0 & \cdots & 0 & 0 & 0 \\ A_{i+1}^* & A_{i+2} & 0 & \cdots & 0 & 0 & 0 \\ 0 & A_{i+3}^* & A_{i+4} & \cdots & 0 & 0 & 0 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & \cdots & \cdots & \cdots & A_{j-3}^* & A_{j-2} & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & A_{j-1}^* & A_j \end{bmatrix} \tag{9}$$

by $r_{i|i+1|\cdots|j-1|j}$.

THEOREM 4. On the structure of the Q^{k-l}–SVD, the $(LU)^{k/2}$–URV (k even), the $(UL)^{k/2}$–URV (k even), the $(UL)^{(k-1)/2}U$–URV (k odd) and the $(LU)^{(k-1)/2}L$–URV (k odd). Consider any of the above factorizations for the matrices $A_1, A_2, \ldots, A_k$. Then

– If $j-i$ even:

$$r_{i|\cdots|j} = r_{i|\cdots|j-1} + (r_j^1 + r_j^2 + \cdots + r_j^i) + r_j^{i+2} + r_j^{i+4} + \cdots + r_j^{j-2} + r_j^j;$$

– If $j-i$ odd:

$$r_{i|\cdots|j} = r_{i|\cdots|j-1} + (r_j^{i+1} + r_j^{i+3} + \cdots + r_j^{j-2} + r_j^j).$$

For the general case, we shall need a mixture of the two proceding notations for block bidiagonal matrices, the blocks of which can be products of matrices, such as

$$\begin{bmatrix} A_{i_0}A_{i_0+1}\cdots A_{i_1-1} & 0 & 0 & \cdots & 0 \\ (A_{i_1}\cdots A_{i_2-1})^* & A_{i_2}\cdots A_{i_3-1} & 0 & \cdots & 0 \\ 0 & (A_{i_3}\cdots A_{i_4-1})^* & A_{i_4}\cdots A_{i_5-1} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & \cdots & A_{i_l}\cdots A_j \end{bmatrix},$$

where $1 \leqslant i_0 < i_1 < i_2 < i_3 < \cdots < i_l \leqslant j \leqslant k$. Their rank will be denoted by

$$r_{(i_0)\cdots(i_1-1)|i_1\cdots(i_2-1)|\cdots|i_l\cdots(j)}.$$

For instance, the rank of the matrix

$$\begin{bmatrix} A_2A_3 & 0 & 0 \\ A_4^* & A_5A_6A_7 & 0 \\ 0 & (A_8A_9)^* & A_{10} \end{bmatrix}$$

will be represented by

$$r_{(2)(3)|4|(5)(6)(7)|(8)(9)|(10)}.$$

THEOREM 5. On the structure of a GSVD and a GURV. The rank $r_{(i_0)(i_0+1)\cdots(i_1-1)|i_1\cdots(i_2-1)|\cdots|i_l\cdots j}$ can be derived as follows:

[2] Recall that the subscript i refers to the ith matrix, while the superscript j refers to the jth block in that matrix.

1. *Calculate the following* $l+1$ *integers* s_j^i, $i=1,2,\ldots,l+1$:

$$s_j^1 = r_j^1 + r_j^2 + \cdots + r_j^{i_0},$$

$$s_j^2 = r_j^{i_0+1} + r_j^{i_0+2} + \cdots + r_j^{i_1},$$

$$\vdots$$

$$s_j^{l+1} = r_j^{i_{l-1}+1} + r_j^{i_{l-1}+2} + \cdots + r_j^{i_l}.$$

2. *Depending on l even or odd there are two cases*:
   - l even:

$$r_{i_0\cdots i_1-1|i_1\cdots i_2-1|\cdots|i_l\cdots j} = r_{i_0\cdots i_1-1|i_1\cdots i_2-1|\cdots|i_{l-1}\cdots i_l-1} + s_j^1 + s_j^3 + \cdots + s_j^{l+1},$$

   - l *odd*:

$$r_{i_0\cdots i_1-1|i_1\cdots i_2-1|\cdots|i_l\cdots j} = r_{i_0\cdots i_1-1|i_1\cdots i_2-1|\cdots|i_{l-1}\cdots i_l-1} + s_j^2 + s_j^4 + \cdots + s_j^{l+1}.$$

Observe that Theorems 3 and 4 are special cases of Theorem 5.

While Theorem 3 provides a direct expression of the dimensions r_j^i in terms of differences of ranks of products, Theorems 4 and 5 do so only implicitly. Let us illustrate this with a couple of examples.

EXAMPLE 4. Let us determine the block dimensions of the quasi-diagonal matrix S_4 in a QPP–SVD of the matrices A_1, A_2, A_3, A_4 (which will also be the block dimensions of an LUUU or a ULLL-decomposition). From Theorem 5 we find

$$r_4^4 = r_4 - r_{34}, \qquad r_3^4 = r_{34} - r_{234}.$$

From Theorem 5, we find

$$s_4^1 = r_4^1, \qquad s_4^2 = r_4^2$$

and

$$r_{(1)|(2)(3)(4)} = r_1 + s_4^2,$$

so that

$$r_4^2 = r_{1|(2)(3)(4)} - r_1.$$

Finally, since $r_4 = r_4^1 + r_4^2 + r_4^3 + r_4^4$, we find

$$r_4^1 = r_1 + r_{(2)(3)(4)} - r_{1|(2)(3)(4)}.$$

Observe that this last relation can be interpreted geometrically as the dimension of the intersection between the row spaces of A_1 and $A_2A_3A_4$:

$$r_4^1 = \dim \operatorname{span}_{\text{row}}(A_1) + \dim \operatorname{span}_{\text{row}}(A_2A_3A_4) - \dim \operatorname{span}_{\text{row}}\begin{bmatrix} A_1 \\ (A_2A_3A_4)^* \end{bmatrix}.$$

EXAMPLE 5. Consider the determination of r_5^1, r_5^2, r_5^3, r_5^4, r_5^5 in a PQ^3–SVD of 5 matrices A_1, A_2, A_3, A_4, A_5 with Theorem 5, which will coincide with the structure of a UULUL–URV or an LLULU–URV:

	s_5^i
$r_{4\|5}$	$s_5^1 = r_5^1 + r_5^2 + r_5^3 + r_5^4$ $s_5^2 = r_5^5$
$r_{3\|4\|5}$	$s_5^1 = r_5^1 + r_5^2 + r_5^3$ $s_5^2 = r_5^4$ $s_5^3 = r_5^5$
$r_{2\|3\|4\|5}$	$s_5^1 = r_5^1 + r_5^2$ $s_5^2 = r_5^3$ $s_5^3 = r_5^4$ $s_5^4 = r_5^5$
$r_{(1)(2)\|3\|4\|5}$	$s_5^1 = r_5^1$ $s_5^2 = r_5^2 + r_5^3$ $s_5^3 = r_5^4$ $s_5^4 = r_5^5$

These relations can be used to set up a set of equations for the unknowns $r_5^1, r_5^2, r_5^3, r_5^4, r_5^5$, using Theorem 5 as

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} r_5^1 \\ r_5^2 \\ r_5^3 \\ r_5^4 \\ r_5^5 \end{bmatrix}$$

$$= \begin{bmatrix} r_5 \\ r_{4|5} - r_4 \\ r_{3|4|5} - r_{3|4} \\ r_{2|3|4|5} - r_{2|3|4} \\ r_{(1)(2)|3|4|5} - r_{(1)(2)|3|4} \end{bmatrix},$$

the solution of which is

$$r_5^1 = r_{3|4|5} - r_{3|4} + r_{(1)(2)|3|4} - r_{(1)(2)|3|4|5},$$

$$r_5^2 = r_{(1)(2)|3|4|5} - r_{(1)(2)|3|4} - r_{2|3|4|5} + r_{2|3|4},$$

$$r_5^3 = r_{2|3|4|5} - r_{2|3|4} - r_{4|5} + r_4,$$

$$r_5^4 = r_5 - r_{3|4|5} + r_{3|4},$$

$$r_5^5 = r_{4|5} - r_4.$$

5. Applications

Most of the problems for which the OSVD, PSVD, QSVD, etc. provide an answer, can in principle be solved via a (generalized) eigenvalue problem. However, this always requires the explicit calculation of products or quotients of matrices, which can given raise to severe loss of numerical accuracy. Even if the eigenvalue algorithms would be numerically robust, it is in most cases the explicit formation of matrix products (which consists essentially of inner products) that causes loss of numerical accuracy. As an example, consider the computation of the P^3-SVD of 4 matrices A_1, A_2, A_3, A_4, where

$$A_1 = \begin{bmatrix} 1 & \mu & 0 \\ 1 & 0 & \mu \end{bmatrix}, \quad A_2 = \begin{bmatrix} 1 & 1 \\ \mu & 0 \\ 0 & \mu \end{bmatrix},$$

$$A_3 = \begin{bmatrix} -1 & \mu & 0 \\ 1 & 0 & \mu \end{bmatrix}, \quad A_4 = \begin{bmatrix} -1 & 1 \\ \mu & 0 \\ 0 & \mu \end{bmatrix}.$$

Assume that $\mu^2 < \varepsilon_m < \mu$, where ε_m is the machine precision. Let fl( ) represent the effect of performing a calculation on a finite precision machine so that $\mathrm{fl}(1+\mu^2) = 1$. Then, it is easy to illustrate that matrix multiplication on a finite precision machine is not associative:

$$\mathrm{fl}[\mathrm{fl}(A_1A_2)\mathrm{fl}(A_3A_4)] = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix},$$

$$\mathrm{fl}[\mathrm{fl}(\mathrm{fl}(A_1A_2)A_3)A_4] = \begin{bmatrix} \mu^2 & \mu^2 \\ \mu^2 & \mu^2 \end{bmatrix},$$

$$\mathrm{fl}[\mathrm{fl}(A_1\mathrm{fl}(A_2A_3))A_4] = \begin{bmatrix} 2\mu^2 & 0 \\ 0 & 2\mu^2 \end{bmatrix}.$$

The first result has rank 0, the second result has rank 1 and the third result has rank 2! The correct result would be

$$A_1A_2A_3A_4 = \begin{bmatrix} \mu^2(\mu^2+2) & 0 \\ 0 & \mu^2(\mu^2+2) \end{bmatrix}$$

and is of rank 2. Obviously, it is only a direct explicit factorization of every matrix separately that can preserve the fine numerical details that otherwise get irreversibly lost in matrix products.

For another example, suppose we want to compute the QSVD of a pair of matrices

$$A_1 = \begin{bmatrix} 1 & 1 \\ -1 & 1 \\ \varepsilon & \varepsilon \end{bmatrix}, \quad A_2 = \begin{bmatrix} 1 & \mu & 0 \\ 1 & 0 & \mu \end{bmatrix},$$

where $\mu^2 < \varepsilon_m < \mu$ and $\varepsilon^2 < \varepsilon_m < \varepsilon$. The theoretically correct QSVD of this matrix pair is

$$A_1 = U_1 D_1 X_1^{-1}$$

$$= \begin{bmatrix} \frac{1}{\sqrt{1+\varepsilon^2}} & 0 & -\frac{\varepsilon}{\sqrt{1+\varepsilon^2}} \\ 0 & -1 & 0 \\ \frac{\varepsilon}{\sqrt{1+\varepsilon^2}} & 0 & \frac{1}{\sqrt{1+\varepsilon^2}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$\times \begin{bmatrix} \frac{1}{2\sqrt{1+\varepsilon^2}} & \frac{1}{2} \\ \frac{1}{2\sqrt{1+\varepsilon^2}} & -\frac{1}{2} \end{bmatrix}^{-1},$$

$$A_2 = X_1^{-\mathrm{T}} S_2 V_2^{\mathrm{T}}$$

$$= \begin{bmatrix} \dfrac{1}{2\sqrt{1+\varepsilon^2}} & \dfrac{1}{2} \\ \dfrac{1}{2\sqrt{1+\varepsilon^2}} & -\dfrac{1}{2} \end{bmatrix}^{-\mathrm{T}} \begin{bmatrix} \dfrac{\sqrt{4+2\mu^2}}{2\sqrt{1+\varepsilon^2}} & 0 & 0 \\ 0 & \dfrac{\mu}{\sqrt{2}} & 0 \end{bmatrix}$$

$$\times \begin{bmatrix} \dfrac{2}{\sqrt{4+2\mu^2}} & \dfrac{\mu}{\sqrt{4+2\mu^2}} & \dfrac{\mu}{\sqrt{4+2\mu^2}} \\ 0 & \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \\ -\dfrac{\mu}{\sqrt{\mu^2+2}} & \dfrac{1}{\sqrt{\mu^2+2}} & \dfrac{1}{\sqrt{\mu^2+2}} \end{bmatrix}.$$

Now, in many applications [12, 26, 29], one is interested in the extrema of the so-called oriented signal-to-signal ratio of two vector sequences in the direction of a vector x, which is defined as

$$E_x[A_1^{\mathrm{T}}, A_2] = (x^{\mathrm{T}} A_1^{\mathrm{T}} A_1 x)/(x^{\mathrm{T}} A_2 A_2^{\mathrm{T}} x). \qquad (10)$$

It is easy to verify that the extremal values of this quotient for our example, are given by the inverses of the diagonal elements of $S_2 S_2^{\mathrm{T}}$:

$$\min(E_x[A_1^{\mathrm{T}}, A_2]) = \frac{4(1+\varepsilon^2)}{(4+2\mu^2)},$$

$$\max(E_x[A_1^{\mathrm{T}}, A_2]) = \frac{2}{\mu^2}.$$

If the vector sequence in the matrix A_1^{T} is considered to be signal + noise, and the one in A_2 contains the noise (disturbances), then it can be verified that the 'signal energy' [12] in the direction $x = [1 \ \ -1]^{\mathrm{T}}$ is 1 while the noise energy is $\mu/\sqrt{2}$. On the other hand, if we would first calculate explicitly the matrix products $A_1^{\mathrm{T}} A_1$ and $A_2 A_2^{\mathrm{T}}$ and optimize (10) as a generalized eigenvalue problem of the matrix pair $(A_1^{\mathrm{T}} A_1, A_2 A_2^{\mathrm{T}})$, then the extremal values of

$$x^{\mathrm{T}}(\mathrm{fl}[A_1^{\mathrm{T}} A_1])x/(x^{\mathrm{T}}(\mathrm{fl}[A_2 A_2^{\mathrm{T}}])x)$$

are 1 and ∞! In this case, the signal energy in the direction $x = [1 \ \ -1]^{\mathrm{T}}$ is 1 while the noise energy is 0. This would lead to the conclusion that this direction is noiseless, while in fact it is not!

The OSVD is so frequently used in signal processing and systems and control theory that we shall not even attempt here to give a complete survey of all its applications. The interested reader may wish to consult [7, 20, 34] in order to get a survey of applications and algorithms. A system identification application is treated in [25]. It is the dynamic counterpart of solving overdetermined sets of linear equations via total linear least squares using the OSVD [20]. The use of the QSVD is advocated in signal processing applications where strong 'desired' signals have to be separated from weak 'disturbing' signals. Typically, the frequency domain spectra are overlapping which complicates the use of frequency domain filtering techniques. The concept behind this separation technique is the oriented signal-to-signal ratio which coincides with the concept of prewhitening if noise covariance matrices are known [12]. Typical applications can be found in [4, 26, 29, 35]. In [26, 32], QSVD based system identification algorithms are explored, which give unbiased results as compared to the OSVD version, when data are first treated prior to identification with some filter, as often happens in practice. Applications of the PSVD are mentioned in [8, 15, 22], including the computation of the Kalman decomposition of a linear system. Typically, the PSVD can be invoked whenever so-called contragredient transformations are involved as is the case in open (observability and controllability Lyapunov equations) and closed loop balancing (via the filter and control algebraic Riccati equation). Applications of the RSVD (=QQ–SVD) are treated in [11]. A typical problem concerns the minimization of the rank of the matrix $A + BDC$ where A, B, C are given matrices, over all possible matrices D, such that a unitarily invariant norm of D is minimal. The answer is given in terms of the QQ–SVD of the matrix triplet (B, A, C). Relationships with the shorted operator, generalized Schur complements, generalized Gauss–Markov estimation problems and a generalization of total linear least squares are also pointed out in [11] (see also [36]). It is interesting to note that our QQ–SVD can be used to calculate the minimal rank matrix in a matrix ball, which is the solution set of a completion problem [6]. In [38], it is shown how the PP–SVD can increase the numerical robustness of the solution of matrix approximation problems of the form

$$\min_{\mathrm{rank}(X)=r} \|A(B-X)C\|_F^2,$$

where A, B, C are given rectangular and possibly rank deficient matrices and X is to be found. The closeness of the approximation is measured by the semi-matrix norm with row weighting matrix A and column weighting matrix C. In [38] not only consistency conditions are derived for the problem but it is also shown how a subspace can be found using the PP–SVD so that the semi-norm becomes a matrix norm.

Finally, let us conclude by pointing out that GSVDs might prove useful in designing robust algorithms for the stochastic realization problem, a subject which is actually under investigation.

6. Conclusions

In this paper, we have stated the generalization of two well known matrix factorizations for any number of matrices: the singular value and the QR decomposition. We have also pointed out an interesting bijection between the two sets of decompositions. For each GSVD there is a GQRD and vice versa. This opens interesting perspectives for algorithms. Despite the fact that the proof in [14] is constructive, it is probably not the best algorithm to compute a certain GSVD. The constructive proof of the GQRD [13] is already more elegant and uses the SVD as its basic building block. Just as the QR-decomposition can be used as a preprocessing step in computing the SVD of a matrix (especially when it is very 'rectangular', e.g. many more columns than rows, as occurs in most signal processing applications), a GQRD could be used as a preprocessing step in the computation of a GSVD. In most applications however, we expect that the GQRD alone will be sufficient since it contains already the complete structure of the corresponding GSVD.

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