

## ON THE STRUCTURE OF GENERALIZED SINGULAR VALUE AND QR DECOMPOSITIONS\*

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**Abstract.** This paper analyzes in detail the structure of generalizations of the singular value decomposition and the QR decomposition for any number of matrices. The structure is completely determined as a function of the ranks of the matrices or their products and concatenations.

**Key words.** ordinary, product, quotient, restricted singular value decomposition, QR decomposition, complete orthogonal factorization

**AMS subject classifications.** 15A09, 15A18, 15A21, 15A24, 65F20

**1. Introduction.** In a previous paper [4], we introduced an infinite tree of generalizations of the ordinary singular value decomposition (OSVD) and we derived a constructive proof of it. All decompositions in this tree are considered as generalized singular value decompositions (GSVDs) and it was shown in [4] how all of them can be labeled with a sequence of the letters P and Q, where P stands for *product* and Q stands for *quotient*. In [5], we introduced a corresponding set of generalizations of the QR decomposition, which could be denoted by appropriate enumerations of the letters L (lower) and U (upper). It is the purpose of this paper to discuss in more detail the structure of these generalizations. In particular, we shall derive formulas for the dimensions of the blocks in the quasi-diagonal matrices of the GSVDs of [4] (Theorem 1.1 of this paper), or the triangular matrices in the GQRDs (generalized QR decompositions) of [5] (Theorem 1.2 of this paper), in terms of the ranks of the matrices involved and concatenations and products of these matrices.

This paper is organized as follows. In the remainder of this section, we summarize the main results on generalized SVDs and QRDs obtained in [4] and [5]. Since there is a one-to-one correspondence between these two generalizations, we will concentrate on the generalizations of the SVD, while the results will apply for the GQRDs as well. In §2, we analyze in detail the structure of a GSVD that only consists of P-steps. In §3, we analyze GSVDs that only contain Q-steps. In §4, we discuss the general case where we exploit the obtained insights from §§2 and 3. Instead of providing rigorous proofs, we have chosen to indicate our methods of deriving these results with illustrative examples.

Let us first state the main result of [4] in the following theorem.

**THEOREM 1.1 (GSVDs for  $k$  matrices).** *Consider a set of  $k$  matrices with compatible dimensions:  $A_1$  ( $n_0 \times n_1$ ),  $A_2$  ( $n_1 \times n_2$ ),  $\dots$ ,  $A_{k-1}$  ( $n_{k-2} \times n_{k-1}$ ),  $A_k$  ( $n_{k-1} \times n_k$ ). Then there exist*

- *unitary matrices  $U_1$  ( $n_0 \times n_0$ ) and  $V_k$  ( $n_k \times n_k$ );*

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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** (Nomenclature for GSVDs). If  $k = 1$  in Theorem 1.1, then the corresponding factorization of the matrix  $A_1$  will be called the OSVD. If for a matrix pair  $A_i, A_{i+1}, 1 \leq i \leq k - 1$  in Theorem 1.1, 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  $A_i, A_{i+1}, 1 \leq i \leq k - 1$  in Theorem 1.1, 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  $A_i, i = 1, 2, \dots, k > 1$  as in Theorem 1.1, is then obtained by simply enumerating the different factorization types.

We now 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 the following 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 (product singular value decomposition) as in [9] (called IISVD there) and in [1] and [3], while the Q-type factorization is nothing else than the QSVD (quotient singular value decomposition) in [8], [10], and [11] (called generalized SVD there). 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.* Let us write down the PQQP-SVD for five matrices:

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

In [5], we derived the following generalization of the QR decomposition for a chain of  $k$  matrices.

**THEOREM 1.2** (Generalized QR decompositions for  $k$  matrices). *Given  $k$  complex matrices  $A_1 (n_0 \times n_1), A_2 (n_1 \times n_2), \dots, A_k (n_{k-1} \times n_k)$ . There always exist unitary matrices  $Q_0, Q_1, \dots, Q_k$  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  $l$ ):*

$$\tilde{T}_i^l = \begin{matrix} & r_i^1 & r_i^2 & \dots & r_i^i & r_i^{i+1} \\ \begin{matrix} r_{i-1}^1 \\ r_{i-1}^2 \\ \vdots \\ r_{i-1}^i \end{matrix} & \left( \begin{matrix} R_{i,1} & 0 & \dots & 0 & 0 \\ * & R_{i,2} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ * & * & \dots & R_{i,i} & 0 \end{matrix} \right), & \text{where } R_{i,j} = \begin{pmatrix} 0 \\ R_{i,j}^l \end{pmatrix},
 \end{matrix}$$

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

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

$$\tilde{T}_i^u = \begin{matrix} & r_i^{i+1} & r_i^1 & \dots & r_i^{i-1} & r_i^i \\ \begin{matrix} r_{i-1}^1 \\ r_{i-1}^2 \\ \vdots \\ r_{i-1}^i \end{matrix} & \begin{pmatrix} 0 & R_{i,1} & * & \dots & * \\ 0 & 0 & R_{i,2} & \dots & * \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & R_{i,i} \end{pmatrix} \end{matrix}, \quad \text{where } R_{i,j} = \begin{pmatrix} R_{i,j}^u \\ 0 \end{pmatrix},$$

and  $R_{i,j}^u$  is a square nonsingular upper triangular matrix. The block dimensions  $r_i^j$  coincide with those of Theorem 1.1.

As to the nomenclature of these GQRDs, we propose the following definition.

**DEFINITION 2 (Nomenclature for GQRD).** The name of a GQRD 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  $\tilde{T}_i, i = 1, \dots, k$  in the decomposition of Theorem 1.2.

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

The relation between the two generalizations, the GSVDs and the GQRDs, is the following:

- (i) 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;
- (ii) 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 four matrices, there are two possible corresponding GQRDs, 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 (which is short for a PPPQQ-SVD), there are two QR decompositions, namely, an  $L^4UL$ -QR and an  $U^4LU$ -QR.

**2. Structure of a GSVD with only P-steps.** The main purpose of this section is to derive expressions for the block dimensions  $r_p^q$  when all steps in the GSVD are P-steps. These block dimensions will be expressed as a function of the ranks of products of the form

$$\text{rank}(A_i A_{i+1}, \dots, A_{j-1} A_j),$$

which will be denoted by  $r_{i(i+1)\dots(j-1)j}$ . This will be done in two steps. First, we derive an implicit characterization of the block dimensions. This leads directly to an explicit determination of these block dimensions.

**LEMMA 2.1.** *The rank of the product of the matrices  $D_i, D_{i+1}, \dots, D_j$  that appears in a  $P^{k-1}$ -SVD (or the rank of the product  $A_i A_{i+1}, \dots, A_j$  in an  $L^k$ -QR or a  $U^k$ -QR) is given by*

$$\text{rank}(D_i D_{i+1} \dots D_j) = r_{(i)(i+1)\dots(j)} = r_j^1 + r_j^2 + \dots + r_j^i.$$

As the examples will reveal, the following theorem follows directly from this lemma.

**THEOREM 2.2.** *Consider a  $P^{k-1}$ -SVD of the matrices  $A_1, A_2, \dots, A_k$ . Then, the block dimensions  $r_p^q, p = 1, \dots, k, q = 1, \dots, p$  are given by*

$$\begin{aligned} r_j^1 &= r_{(1)(2)\dots(j)}, \\ r_j^i &= r_{i(i+1)\dots(j)} - r_{(i-1)(i)\dots(j)}, \end{aligned}$$



We see by inspection that

$$\begin{aligned} r_{(1)(2)(3)(4)} &= r_4^1, \\ r_{(2)(3)(4)} &= r_4^1 + r_4^2, \\ r_{(3)(4)} &= r_4^1 + r_4^2 + r_4^3, \\ r_4 &= r_4^1 + r_4^2 + r_4^3 + r_4^4, \end{aligned}$$

from which it follows that

$$\begin{aligned} r_4^1 &= r_{(1)(2)(3)(4)}, \\ r_4^2 &= r_{(2)(3)(4)} - r_{(1)(2)(3)(4)}, \\ r_4^3 &= r_{(3)(4)} - r_{(2)(3)(4)}, \\ r_4^4 &= r_4 - r_{(3)(4)}. \end{aligned}$$

The same expressions apply for the blocks in the corresponding  $U^4$ - or  $L^4$ -QR.

Observe that in the product  $D_3$  and  $S_4$ , only the diagonal blocks of  $S_4$  with dimensions  $r_4^1, r_4^2, r_4^3$  survive. In the product  $D_2 D_3 S_4$  only the blocks with dimensions  $r_4^1$  and  $r_4^2$  survive, and in  $D_1 D_2 D_3 S_4$  only the block with dimension  $r_4^1$  survives. This observation can easily be generalized to the following survival rule for a pure PSVD, which is the essence of the proof of Lemma 2.1.

In a product of matrices  $D_i, D_{i+1}, \dots, D_j$  (or  $S_k$ ) only the blocks with block dimensions  $r_j^1, r_j^2, \dots, r_j^i$  survive.

Once this observation has been established, a proof of Theorem 3.2 is straightforward.

**3. A GSVD with only Q-steps.** Let us now look closer at the structure of a GSVD with only Q-steps. We will see that we can derive expressions for the block dimensions  $r_p^q, p = 1, \dots, k, q = 1, \dots, p$  in two steps. First, we obtain an implicit formula where the required block dimensions are unknowns in a set of linear equations. In a second step, these are solved to obtain an expression for the block dimensions  $r_p^q$  in terms of the ranks of the block matrices

$$\begin{pmatrix} A_i & 0 & 0 & \dots & 0 & 0 & 0 \\ A_{i+1}^* & A_{i+2} & 0 & \dots & 0 & 0 & 0 \\ 0 & A_{i+3}^* & A_{i+4} & \dots & 0 & 0 & 0 \\ 0 & \dots & \dots & \dots & \dots & \dots & 0 \\ 0 & \dots & \dots & \dots & A_{j-3}^* & A_{j-2} & 0 \\ 0 & \dots & \dots & \dots & 0 & A_{j-1}^* & A_j \end{pmatrix}.$$

Their rank is denoted by  $r_{i|i+1|\dots|j-1|j}$ .

We will proceed in the same way as in §2. Instead of proving our results rigorously, we prefer to reveal the mechanisms by some clarifying examples. First, we obtain the following implicit characterization.

**LEMMA 3.1.** *Consider a  $Q^{k-1}$ -SVD of the matrices  $A_1, A_2, \dots, A_k$ . Then if  $j - i$  even*

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

*if  $j - i$  odd*

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



The left and right factors are nonsingular. Hence, we can obtain expressions for all dimensions involved by analyzing the block bidiagonal matrix

$$\left( \begin{array}{c|c} D_1 & 0 \\ \hline D_2^t & S_3 \end{array} \right) = \begin{array}{c} r_3^1 \\ r_2^1 - r_3^1 \\ r_1 - r_2^1 \\ n_0 - r_1 \\ \hline r_3^1 \\ r_2^1 - r_3^1 \\ r_3^2 \\ r_2^2 - r_3^2 \\ r_3^3 \\ n_2 - r_2 - r_3^3 \end{array} \left( \begin{array}{ccc|ccc} I & 0 & 0 & & & \\ 0 & I & 0 & & & \\ 0 & 0 & I & & & \\ 0 & 0 & 0 & & & \\ \hline I & 0 & 0 & S_3^1 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 & 0 & 0 \\ & & & I & 0 & 0 & 0 \\ & & & 0 & I & 0 & 0 \\ & & & 0 & 0 & S_3^2 & 0 & 0 \\ & & & 0 & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 & S_3^3 & 0 \\ & & & 0 & 0 & 0 & 0 & 0 \end{array} \right),$$

where we have used the finest possible subdivision of matrices (i.e., a partitioning based upon the block dimensions  $r_3^1, r_3^2, r_3^3$ ). All nonzero blocks are diagonal. Elements not shown are zero. First, it is straightforward to see that  $r_3 = r_3^1 + r_3^2 + r_3^3$ . Next, we concentrate on the submatrix  $(D_2^t \ S_3)$ . In this matrix, the block columns with the matrices  $S_3^1$  and  $S_3^2$  are linearly dependent on the previous ones. The block column with  $S_3^3$  is linearly independent. Hence  $\text{rank}(D_2^t \ S_3) = r_{2|3} = r_2 + r_3^3$ . Next, we will relate the rank  $r_{1|2} = \text{rank}(D_1^t \ D_2)^t$  to

$$r_{1|2|3} = \text{rank} \left( \begin{array}{cc} D_1 & 0 \\ \hline D_2^t & S_3 \end{array} \right).$$

It can be seen that when the block column with  $S_3^1$  is appended to  $(D_1^t \ D_2)^t$ , the rank will increase with

$$r_3^1 \times \left[ \text{rank} \left( \begin{array}{cc} 1 & 0 \\ 1 & 1 \end{array} \right) - \text{rank} \left( \begin{array}{c} 1 \\ 1 \end{array} \right) \right] = r_3^1.$$

If the block column with  $S_3^2$  is appended to  $(D_1^t \ D_2)^t$ , the rank will not increase. Finally, if the block column with  $S_3^3$  is appended, then the rank will increase with  $r_3^3 \times [\text{rank}(0 \ 1) - \text{rank}(0)] = r_3^3$ . Hence

$$\begin{aligned} r_{1|2|3} &= r_{1|2} + r_3^1 \times \left[ \text{rank} \left( \begin{array}{cc} 1 & 0 \\ 1 & 1 \end{array} \right) - \text{rank} \left( \begin{array}{c} 1 \\ 1 \end{array} \right) \right] \\ &\quad + r_3^2 \times [\text{rank}(1 \ 1) - \text{rank}(1)] \\ &\quad + r_3^3 \times [\text{rank}(0 \ 1) - \text{rank}(0)] = r_{1|2} + r_3^1 + r_3^3. \end{aligned}$$

We can now set up a set of linear equations as

$$\begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} r_3^1 \\ r_3^2 \\ r_3^3 \end{pmatrix} = \begin{pmatrix} r_3 \\ r_{2|3} - r_2 \\ r_{1|2|3} - r_{1|2} \end{pmatrix},$$

which can be solved as

$$\begin{pmatrix} r_3^1 \\ r_3^2 \\ r_3^3 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} r_3 \\ r_{2|3} - r_2 \\ r_{1|2|3} - r_{1|2} \end{pmatrix} = \begin{pmatrix} r_{1|2|3} - r_{1|2} + r_2 - r_{2|3} \\ r_3 + r_{1|2} - r_{1|2|3} \\ r_{2|3} - r_2 \end{pmatrix}.$$



The same expressions will appear in the ULU- or LUL-QR.

*Example 5* ( $Q^7$ -SVD). The courageous reader may wish to verify that for  $k = 7$ , the following set of linear equations needs to be solved:

$$\begin{pmatrix} r_7 \\ r_{6|7} - r_6 \\ r_{5|6|7} - r_{5|6} \\ r_{4|5|6|7} - r_{4|5|6} \\ r_{3|4|5|6|7} - r_{3|4|5|6} \\ r_{2|3|4|5|6|7} - r_{2|3|4|5|6} \\ r_{1|2|3|4|5|6|7} - r_{1|2|3|4|5|6} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} r_7^1 \\ r_7^2 \\ r_7^3 \\ r_7^4 \\ r_7^5 \\ r_7^6 \\ r_7^7 \end{pmatrix}.$$

This set of equations can be solved as

$$\begin{pmatrix} r_7^1 \\ r_7^2 \\ r_7^3 \\ r_7^4 \\ r_7^5 \\ r_7^6 \\ r_7^7 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} r_7 \\ r_{6|7} - r_6 \\ r_{5|6|7} - r_{5|6} \\ r_{4|5|6|7} - r_{4|5|6} \\ r_{3|4|5|6|7} - r_{3|4|5|6} \\ r_{2|3|4|5|6|7} - r_{2|3|4|5|6} \\ r_{1|2|3|4|5|6|7} - r_{1|2|3|4|5|6} \end{pmatrix}.$$

The pattern of the inverse matrix now becomes clear. We have a triantidiagonal matrix with a sequence of alternating 1 and  $-1$ , ending in a 1 in the top right-hand corner. As a matter of fact, this observation constitutes the essence of a proof of Theorem 3.2.

**4. On the structure of a GSVD.** For the analysis of the structure of a completely general GSVD, in which the letters P and Q can appear in any order, we need a mixture of the two preceding notations for block bidiagonal matrices, the blocks of which can be products of matrices, such as

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

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

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

For instance, the rank of the matrix

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

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

In the following theorem, we derive an implicit expression of the block dimensions  $r_p^q, p = 1, \dots, k, q = 1, \dots, p$  of a GSVD of  $A_1, A_2, \dots, A_k$ . We proceed in two steps. The first part of the theorem is based on the survival rule described in Lemma 2.1, and the second part is then an application of the pure Q-step SVD in Lemma 3.1.





and other matrices that are formed from products and concatenations of these matrices. Some more examples and details can be found in the technical report [6] and the papers [2]–[5], and [7].

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