

A QR-type reduction for computing the SVD of a general matrix product/quotient

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Summary. In this paper, a QR-type reduction technique is developed for the computation of the SVD of a general matrix product/quotient $A = A_1^{s_1} A_2^{s_2} \cdots A_m^{s_m}$ with $A_i \in \mathbf{R}^{n \times n}$ and $s_i = 1$ or $s_i = -1$. First the matrix A is reduced by at most m QR-factorizations to the form $Q_{11}^{(1)} (Q_{21}^{(1)})^{-1}$, where $Q_{11}^{(1)}, Q_{21}^{(1)} \in \mathbf{R}^{n \times n}$ and $(Q_{11}^{(1)})^T Q_{11}^{(1)} + (Q_{21}^{(1)})^T Q_{21}^{(1)} = I$. Then the SVD of A is obtained by computing the CSD (Cosine-Sine Decomposition) of $Q_{11}^{(1)}$ and $Q_{21}^{(1)}$ using the Matlab command *gsvd*. The performance of the proposed method is verified by some numerical examples.

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1 Introduction

This paper deals with a new method for the computation of the Singular Value Decomposition (SVD) of a sequence of matrices in product/quotient form. The simplest forms of these Generalized SVD's (GSVD), for two matrices, are the well-known Quotient SVD (QSVD) (introduced in [17] and refined in [14]) and Product SVD (PSVD) (proposed in [9], refining ideas introduced in [13]). One of the three possible forms involving three matrices, is the so-called Restricted SVD (RSVD) (introduced in its explicit form in [20] and further developed and discussed in [5]). General schemes have been discussed in e.g. [6, 7].

The GSVD is one of the essential numerical linear algebraic tools in signal processing and identification. Possible applications include source separation, stochastic realization, generalized Gauss-Markov estimation problems, generalized total linear least squares, open and closed loop balancing, etc.

Like the QSVD, PSVD and RSVD, the SVD of a general matrix product/quotient has many applications. For example, it is important for the estimation of Lyapunov exponents for dynamic systems [12]. Consider difference equations

$$(1) \quad \Theta_{k+1} = \Phi_k^{s_k} \Theta_k, \quad \Theta_0 = I, \quad \Phi_k \in \mathbf{R}^{n \times n}, \quad s_k = 1 \text{ or } s_k = -1.$$

The i th Lyapunov exponent is then defined by

$$\lambda_i = \lim_{k \rightarrow \infty} \log(\sigma_i(\Theta_k))/k,$$

where $\sigma_i(\Theta_k)$ is the i th biggest singular value of Θ_k . Discretizations of ordinary differential equations may also lead to sequences of matrix products/quotients [11].

Up to now, the calculation of the QSVD has been extensively studied. The fact that the Cosine-Sine Decomposition (CSD) of a partitioned column-orthogonal matrix $\begin{bmatrix} A \\ C \end{bmatrix}$ corresponds to the QSVD of the couple (A, C) , forms the basis for two backward stable algorithms, proposed in [16] and [18]. Recently, the computation of the QSVD via the CSD and the Lanczos bidiagonalization process has been studied in [21]. The Kogbetliantz algorithm has been generalized in [15] for the computation of the QSVD. In [15], the elegant implementation initially transforms A and C into a pair of triangular matrices and preserves the triangular form in the iterative phase by using suitable plane rotations. A variation of the algorithm in [15], also backward stable, is given in [2]. This technique is implemented as the LAPACK procedure STGSJA() [2].

The Kogbetliantz algorithm has also been generalized for the computation of the RSVD [19]. However, Jacobi-type algorithms typically have a (moderately) higher complexity than QR-type algorithms. Moreover, the Jacobi

approach has so far only been followed for problems involving at most three matrices; generalizing the scheme for long matrix sequences proves to be hard. Recently an implicit bidiagonalization QR-type algorithm for the computation of the SVD of a general matrix product/quotient has been proposed in [11]. For quotient factors this scheme requires solving a series of upper triangular systems of linear equations during the bidiagonalization.

In this paper, we generalize the idea in [4] for computing the RSVD to propose a QR-type *reduction* technique for computing the SVD of a general matrix product/quotient

$$A = A_1^{s_1} A_2^{s_2} \cdots A_m^{s_m}$$

with $A_i \in \mathbf{R}^{n \times n}$, $s_i = 1$ or $s_i = -1$. We will show that, if not all s_i are the same, the matrix A can be reduced by $m - 1$ QR-factorizations to the form $Q_{11}^{(1)} (Q_{21}^{(1)})^{-1}$ with $Q_{11}^{(1)}, Q_{21}^{(1)} \in \mathbf{R}^{n \times n}$, $(Q_{11}^{(1)})^T Q_{11}^{(1)} + (Q_{21}^{(1)})^T Q_{21}^{(1)} = I$; if all s_i are equal, then we need m QR-factorizations. The main advantage of this QR-type reduction is the way in which quotients are dealt with. Finally the SVD of A can be found by resorting, e.g., to Van Loan's CSD method [18].

The next section describes how the QR-type reduction can be realized. Section 3 contains a number of numerical experiments. Section 4 presents the conclusions.

2 QR-Type reduction

Consider a matrix A of the following form:

$$(2) \quad \begin{cases} A = A_1^{s_1} A_2^{s_2} \cdots A_m^{s_m}, & m \geq 2, \quad A_i \in \mathbf{R}^{n \times n}, \quad s_i = 1 \text{ or } s_i = -1, \\ A_i \text{ is nonsingular if } s_i = -1. \end{cases}$$

Like in [11], we assume for simplicity that the matrices A_i in (2) are square; as was pointed out in [7], this does not affect the generality of what follows. The purpose of this section is to show how the matrix A can be reduced to the form $Q_{11}^{(1)} (Q_{21}^{(1)})^{-1}$ with $Q_{11}^{(1)}, Q_{21}^{(1)} \in \mathbf{R}^{n \times n}$, $(Q_{11}^{(1)})^T Q_{11}^{(1)} + (Q_{21}^{(1)})^T Q_{21}^{(1)} = I$, by performing at most m QR-factorizations. Section 2.1 explains how the problem can be solved for a sequence of 2 or 3 matrices. Section 2.2 subsequently describes how the sequence can be expanded, once the result for a subsequence of three matrices is known. Section 2.3 presents the overall algorithm. Section 2.4 proves backward stability for the procedure.

2.1 Basic lemmas

First, the following three lemmas describe the cases $m = 2$ and $m = 3$:

Lemma 1 [14, 15] Assume that $A_1, A_2 \in \mathbf{R}^{n \times n}$ and A_2 is nonsingular. Let the QR factorization of $\begin{bmatrix} A_1 \\ A_2 \end{bmatrix}$ be

$$\begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} Q_{11}^{(1)} & Q_{12}^{(1)} \\ Q_{21}^{(1)} & Q_{22}^{(1)} \end{bmatrix} \begin{bmatrix} R^{(1)} \\ 0 \end{bmatrix}, \quad R^{(1)}, Q_{11}^{(1)}, Q_{12}^{(1)}, Q_{21}^{(1)}, Q_{22}^{(1)} \in \mathbf{R}^{n \times n}.$$

Then $Q_{21}^{(1)}$ is nonsingular and

$$A_1 A_2^{-1} = Q_{11}^{(1)} (Q_{21}^{(1)})^{-1}.$$

Lemma 2 Given matrices $A_i \in \mathbf{R}^{n \times n}$, $i = 1, 2, 3$.

(a) Assume A_3 is nonsingular. Let the QR factorization of $\begin{bmatrix} A_2 \\ A_3 \end{bmatrix}$ be

$$(3) \quad \begin{bmatrix} A_2 \\ A_3 \end{bmatrix} = \begin{bmatrix} Q_{11}^{(2)} & Q_{12}^{(2)} \\ Q_{21}^{(2)} & Q_{22}^{(2)} \end{bmatrix} \begin{bmatrix} R^{(2)} \\ 0 \end{bmatrix}, \quad R^{(2)}, Q_{11}^{(2)}, Q_{12}^{(2)}, Q_{21}^{(2)}, Q_{22}^{(2)} \in \mathbf{R}^{n \times n}.$$

Then $Q_{21}^{(2)}$ is nonsingular. Furthermore, let the QR factorization of $\begin{bmatrix} A_1 Q_{11}^{(2)} \\ Q_{21}^{(2)} \end{bmatrix}$ be

$$(4) \quad \begin{bmatrix} A_1 Q_{11}^{(2)} \\ Q_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(1)} & Q_{12}^{(1)} \\ Q_{21}^{(1)} & Q_{22}^{(1)} \end{bmatrix} \begin{bmatrix} R^{(1)} \\ 0 \end{bmatrix}, \quad R^{(1)}, Q_{11}^{(1)}, Q_{12}^{(1)}, Q_{21}^{(1)}, Q_{22}^{(1)} \in \mathbf{R}^{n \times n}.$$

We have that $Q_{21}^{(1)}$ is nonsingular and

$$A_1 A_2 A_3^{-1} = Q_{11}^{(1)} (Q_{21}^{(1)})^{-1}.$$

(b) Assume A_1 and A_3 nonsingular. Let the QR factorization of $\begin{bmatrix} A_2 \\ A_3 \end{bmatrix}$ be

$$(5) \quad \begin{bmatrix} A_2 \\ A_3 \end{bmatrix} = \begin{bmatrix} Q_{11}^{(2)} & Q_{12}^{(2)} \\ Q_{21}^{(2)} & Q_{22}^{(2)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(2)} \end{bmatrix}, \quad R^{(2)}, Q_{11}^{(2)}, Q_{12}^{(2)}, Q_{21}^{(2)}, Q_{22}^{(2)} \in \mathbf{R}^{n \times n},$$

and the QR factorization of $\begin{bmatrix} A_1^T Q_{11}^{(2)} \\ Q_{21}^{(2)} \end{bmatrix}$ be

$$(6) \quad \begin{bmatrix} A_1^T Q_{11}^{(2)} \\ Q_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(1)} & Q_{12}^{(1)} \\ Q_{21}^{(1)} & Q_{22}^{(1)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(1)} \end{bmatrix}, \quad R^{(1)}, Q_{11}^{(1)}, Q_{12}^{(1)}, Q_{21}^{(1)}, Q_{22}^{(1)} \in \mathbf{R}^{n \times n}.$$

Then $Q_{11}^{(2)}$ and $Q_{21}^{(2)}$ are nonsingular, and

$$A_1^{-1} A_2 A_3^{-1} = Q_{11}^{(1)} (Q_{21}^{(1)})^{-1}.$$

Proof. (a) This part follows directly from Lemma 1:

$$A_2 A_3^{-1} = Q_{11}^{(2)} (Q_{21}^{(2)})^{-1}, \quad (A_1 Q_{11}^{(2)}) (Q_{21}^{(2)})^{-1} = Q_{11}^{(1)} (Q_{21}^{(1)})^{-1}.$$

(b) As A_1 and A_3 are nonsingular, $Q_{11}^{(2)}$, $Q_{22}^{(2)}$, $R^{(2)}$ and $Q_{12}^{(1)}$, $Q_{21}^{(1)}$, $R^{(1)}$ are nonsingular as well. Since

$$\left[(Q_{11}^{(2)})^T \quad (Q_{21}^{(2)})^T \right] \begin{bmatrix} A_1 Q_{11}^{(1)} \\ Q_{21}^{(1)} \end{bmatrix} = 0,$$

we have that

$$\begin{bmatrix} A_1 Q_{11}^{(1)} \\ Q_{21}^{(1)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(2)} & Q_{12}^{(2)} \\ Q_{21}^{(2)} & Q_{22}^{(2)} \end{bmatrix} \begin{bmatrix} 0 \\ \tilde{R}^{(1)} \end{bmatrix}, \quad \text{for some } \tilde{R}^{(1)} \in \mathbf{R}^{n \times n};$$

$\tilde{R}^{(1)}$ is nonsingular because $Q_{21}^{(1)}$ is nonsingular. Hence,

$$\begin{bmatrix} A_1 Q_{11}^{(1)} \\ Q_{21}^{(1)} \end{bmatrix} = \begin{bmatrix} A_2 \\ A_3 \end{bmatrix} (R^{(2)})^{-1} \tilde{R}^{(1)},$$

i.e.,

$$\begin{bmatrix} Q_{11}^{(1)} \\ Q_{21}^{(1)} \end{bmatrix} = \begin{bmatrix} A_1^{-1} A_2 \\ A_3 \end{bmatrix} (R^{(2)})^{-1} \tilde{R}^{(1)}.$$

Therefore, we have that

$$A_1^{-1} A_2 A_3^{-1} = Q_{11}^{(1)} (Q_{21}^{(1)})^{-1}. \quad \square$$

Lemma 2 describes how a matrix A_1 or A_1^{-1} can be added to the left of $A_2 A_3^{-1}$. The next lemma is the equivalent for working from left to right.

Lemma 3 Given matrices $A_i \in \mathbf{R}^{n \times n}$, $i = 1, 2, 3$.

(a) Assume A_2 and A_3 are nonsingular. Let the QR factorization of $\begin{bmatrix} A_1 \\ A_2 \end{bmatrix}$ be given by

$$(7) \quad \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} Q_{11}^{(2)} & Q_{12}^{(2)} \\ Q_{21}^{(2)} & Q_{22}^{(2)} \end{bmatrix} \begin{bmatrix} R^{(2)} \\ 0 \end{bmatrix}, \quad R^{(2)}, Q_{11}^{(2)}, Q_{12}^{(2)}, Q_{21}^{(2)}, Q_{22}^{(2)} \in \mathbf{R}^{n \times n}$$

and let the QR factorization of $\begin{bmatrix} Q_{11}^{(2)} \\ A_3 Q_{21}^{(2)} \end{bmatrix}$ be given by

$$(8) \quad \begin{bmatrix} Q_{11}^{(2)} \\ A_3 Q_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(1)} & Q_{12}^{(1)} \\ Q_{21}^{(1)} & Q_{22}^{(1)} \end{bmatrix} \begin{bmatrix} R^{(1)} \\ 0 \end{bmatrix}, \quad R^{(1)}, Q_{11}^{(1)}, Q_{12}^{(1)}, Q_{21}^{(1)}, Q_{22}^{(1)} \in \mathbf{R}^{n \times n}.$$

Then we have that

$$A_1 A_2^{-1} A_3^{-1} = Q_{11}^{(1)} (Q_{21}^{(1)})^{-1},$$

in which $Q_{21}^{(1)}$ is nonsingular.

(b) Assume A_2 is nonsingular. Let the QR factorization of $\begin{bmatrix} A_1 \\ A_2 \end{bmatrix}$ be given by

$$(9) \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} Q_{11}^{(2)} & Q_{12}^{(2)} \\ Q_{21}^{(2)} & Q_{22}^{(2)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(2)} \end{bmatrix}, \quad R^{(2)}, Q_{11}^{(2)}, Q_{12}^{(2)}, Q_{21}^{(2)}, Q_{22}^{(2)} \in \mathbf{R}^{n \times n},$$

and let the QR factorization of $\begin{bmatrix} Q_{11}^{(2)} \\ A_3^T Q_{21}^{(2)} \end{bmatrix}$ be given by

$$(10) \begin{bmatrix} Q_{11}^{(2)} \\ A_3^T Q_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(1)} & Q_{12}^{(1)} \\ Q_{21}^{(1)} & Q_{22}^{(1)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(1)} \end{bmatrix}, \quad R^{(1)}, Q_{11}^{(1)}, Q_{12}^{(1)}, Q_{21}^{(1)}, Q_{22}^{(1)} \in \mathbf{R}^{n \times n}.$$

Then we have that

$$A_1 A_2^{-1} A_3 = Q_{11}^{(1)} (Q_{21}^{(1)})^{-1},$$

in which $Q_{21}^{(1)}$ is nonsingular.

Proof. The proof is similar to that of Lemma 2 and hence is omitted here. \square

2.2 Taking more matrices into account

Assume a matrix $A = A_1^{s_1} A_2^{s_2} A_3^{s_3}$, reduced to the form $Q_{11}^{(1)} (Q_{21}^{(1)})^{-1}$ with $Q_{11}^{(1)}, Q_{21}^{(1)} \in \mathbf{R}^{n \times n}$, $(Q_{11}^{(1)})^T Q_{11}^{(1)} + (Q_{21}^{(1)})^T Q_{21}^{(1)} = I$, as shown in Lemma 2/ Lemma 3. Now we explain how the matrix $\hat{A}^{\hat{s}} A$ or $A \hat{A}^{\hat{s}}$, in which $\hat{A} \in \mathbf{R}^{n \times n}$, $\hat{s} \in \{\pm 1\}$, and \hat{A} is nonsingular if $\hat{s} = -1$, can be reduced to the form $\hat{Q}_{11}^{(1)} (\hat{Q}_{21}^{(1)})^{-1}$ with $\hat{Q}_{11}^{(1)}, \hat{Q}_{21}^{(1)} \in \mathbf{R}^{n \times n}$, $(\hat{Q}_{11}^{(1)})^T \hat{Q}_{11}^{(1)} + (\hat{Q}_{21}^{(1)})^T \hat{Q}_{21}^{(1)} = I$, by performing at most one extra QR-decomposition.

We consider the reduction of $\hat{A}^{\hat{s}} A$ first. The case $\hat{s} = 1$ is trivial: compute the QR factorization of $\begin{bmatrix} \hat{A} Q_{11}^{(1)} \\ Q_{21}^{(1)} \end{bmatrix}$ to get

$$\begin{bmatrix} \hat{A} Q_{11}^{(1)} \\ Q_{21}^{(1)} \end{bmatrix} = \begin{bmatrix} \hat{Q}_{11}^{(1)} & \hat{Q}_{12}^{(1)} \\ \hat{Q}_{21}^{(1)} & \hat{Q}_{22}^{(1)} \end{bmatrix} \begin{bmatrix} \hat{R}^{(1)} \\ 0 \end{bmatrix}, \quad \hat{R}^{(1)}, \hat{Q}_{11}^{(1)}, \hat{Q}_{12}^{(1)}, \hat{Q}_{21}^{(1)}, \hat{Q}_{22}^{(1)} \in \mathbf{R}^{n \times n}.$$

In the case $\hat{s} = -1$, application of Lemma 2 to the matrix product $\hat{A}^{-1} Q_{11}^{(1)} (Q_{21}^{(1)})^{-1}$ would lead to the following definition of orthogonal matrix $\begin{bmatrix} \hat{Q}_{11}^{(1)} & \hat{Q}_{12}^{(1)} \\ \hat{Q}_{21}^{(1)} & \hat{Q}_{22}^{(1)} \end{bmatrix}$:

(11)

$$\begin{bmatrix} Q_{11}^{(1)} \\ Q_{21}^{(1)} \end{bmatrix} = \begin{bmatrix} \hat{Q}_{11}^{(2)} & \hat{Q}_{12}^{(2)} \\ \hat{Q}_{21}^{(2)} & \hat{Q}_{22}^{(2)} \end{bmatrix} \begin{bmatrix} 0 \\ \hat{R}^{(2)} \end{bmatrix}, \quad \hat{R}^{(2)}, \hat{Q}_{11}^{(2)}, \hat{Q}_{12}^{(2)}, \hat{Q}_{21}^{(2)}, \hat{Q}_{22}^{(2)} \in \mathbf{R}^{n \times n},$$

(12)

$$\begin{bmatrix} \hat{A}^T \hat{Q}_{11}^{(2)} \\ \hat{Q}_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} \hat{Q}_{11}^{(1)} & \hat{Q}_{12}^{(1)} \\ \hat{Q}_{21}^{(1)} & \hat{Q}_{22}^{(1)} \end{bmatrix} \begin{bmatrix} 0 \\ \hat{R}^{(1)} \end{bmatrix}, \quad \hat{R}^{(1)}, \hat{Q}_{11}^{(1)}, \hat{Q}_{12}^{(1)}, \hat{Q}_{21}^{(1)}, \hat{Q}_{22}^{(1)} \in \mathbf{R}^{n \times n}.$$

However, this would impose the calculation of two kernels. On the other hand, one QR-factorization can always be avoided by combining Eq. (11) with the computation in the preceding step. If $s_1 = 1$, then Eqs. (4) and (11) can be combined to

$$\begin{bmatrix} A_1 Q_{11}^{(2)} \\ Q_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} \hat{Q}_{11}^{(2)} & \hat{Q}_{12}^{(2)} \\ \hat{Q}_{21}^{(2)} & \hat{Q}_{22}^{(2)} \end{bmatrix} \begin{bmatrix} 0 \\ \hat{\mathcal{R}}^{(2)} \end{bmatrix}, \quad \hat{\mathcal{R}}^{(2)}, \hat{Q}_{11}^{(2)}, \hat{Q}_{12}^{(2)}, \hat{Q}_{21}^{(2)}, \hat{Q}_{22}^{(2)} \in \mathbf{R}^{n \times n}.$$

If $s_1 = -1$, then Eqs. (6) and (11) can be combined to

$$\begin{bmatrix} A_1^T Q_{11}^{(2)} \\ Q_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} \hat{Q}_{11}^{(2)} & \hat{Q}_{12}^{(2)} \\ \hat{Q}_{21}^{(2)} & \hat{Q}_{22}^{(2)} \end{bmatrix} \begin{bmatrix} \hat{\mathcal{R}}^{(1)} \\ 0 \end{bmatrix}, \quad \hat{\mathcal{R}}^{(1)}, \hat{Q}_{11}^{(2)}, \hat{Q}_{12}^{(2)}, \hat{Q}_{21}^{(2)}, \hat{Q}_{22}^{(2)} \in \mathbf{R}^{n \times n}.$$

Now, we consider the reduction of $A \hat{A}^{\hat{s}}$. The case $\hat{s} = -1$ is trivial: compute the QR factorization of $\begin{bmatrix} Q_{11}^{(1)} \\ \hat{A} Q_{21}^{(1)} \end{bmatrix}$ to get

$$\begin{bmatrix} Q_{11}^{(1)} \\ \hat{A} Q_{21}^{(1)} \end{bmatrix} = \begin{bmatrix} \hat{Q}_{11}^{(1)} & \hat{Q}_{12}^{(1)} \\ \hat{Q}_{21}^{(1)} & \hat{Q}_{22}^{(1)} \end{bmatrix} \begin{bmatrix} \hat{R}^{(1)} \\ 0 \end{bmatrix}, \quad \hat{R}^{(1)}, \hat{Q}_{11}^{(1)}, \hat{Q}_{12}^{(1)}, \hat{Q}_{21}^{(1)}, \hat{Q}_{22}^{(1)} \in \mathbf{R}^{n \times n}.$$

In the case $\hat{s} = 1$, application of Lemma 3 to the matrix product $Q_{11}^{(1)} (Q_{21}^{(1)})^{-1} \hat{A}$ would lead to the following definition of orthogonal matrix $\begin{bmatrix} \hat{Q}_{11}^{(1)} & \hat{Q}_{12}^{(1)} \\ \hat{Q}_{21}^{(1)} & \hat{Q}_{22}^{(1)} \end{bmatrix}$:

(13)

$$\begin{bmatrix} Q_{11}^{(1)} \\ Q_{21}^{(1)} \end{bmatrix} = \begin{bmatrix} \hat{Q}_{11}^{(2)} & \hat{Q}_{12}^{(2)} \\ \hat{Q}_{21}^{(2)} & \hat{Q}_{22}^{(2)} \end{bmatrix} \begin{bmatrix} 0 \\ \hat{R}^{(2)} \end{bmatrix}, \quad \hat{R}^{(2)}, \hat{Q}_{11}^{(2)}, \hat{Q}_{12}^{(2)}, \hat{Q}_{21}^{(2)}, \hat{Q}_{22}^{(2)} \in \mathbf{R}^{n \times n},$$

(14)

$$\begin{bmatrix} \hat{Q}_{11}^{(2)} \\ \hat{A}^T \hat{Q}_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} \hat{Q}_{11}^{(1)} & \hat{Q}_{12}^{(1)} \\ \hat{Q}_{21}^{(1)} & \hat{Q}_{22}^{(1)} \end{bmatrix} \begin{bmatrix} 0 \\ \hat{R}^{(1)} \end{bmatrix}, \quad \hat{R}^{(1)}, \hat{Q}_{11}^{(1)}, \hat{Q}_{12}^{(1)}, \hat{Q}_{21}^{(1)}, \hat{Q}_{22}^{(1)} \in \mathbf{R}^{n \times n}.$$

Fortunately, one QR-factorization can be avoided by combining Eq. (13) with the computation in the preceding step: If $s_2 = -1$, we compute the QR

factorization of $\begin{bmatrix} Q_{11}^{(2)} \\ A_2 Q_{21}^{(2)} \end{bmatrix}$ to get

$$\begin{bmatrix} Q_{11}^{(2)} \\ A_2 Q_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} \hat{Q}_{11}^{(2)} & \hat{Q}_{12}^{(2)} \\ \hat{Q}_{21}^{(2)} & \hat{Q}_{22}^{(2)} \end{bmatrix} \begin{bmatrix} 0 \\ \hat{\mathcal{R}}^{(2)} \end{bmatrix}, \quad \hat{\mathcal{R}}^{(2)}, \hat{Q}_{11}^{(2)}, \hat{Q}_{12}^{(2)}, \hat{Q}_{21}^{(2)}, \hat{Q}_{22}^{(2)} \in \mathbf{R}^{n \times n}.$$

If $s_2 = 1$, then we compute the QR factorization of $\begin{bmatrix} Q_{11}^{(2)} \\ A_2^T Q_{21}^{(2)} \end{bmatrix}$ to get

$$\begin{bmatrix} Q_{11}^{(2)} \\ A_2^T Q_{21}^{(2)} \end{bmatrix} = \begin{bmatrix} \hat{Q}_{11}^{(2)} & \hat{Q}_{12}^{(2)} \\ \hat{Q}_{21}^{(2)} & \hat{Q}_{22}^{(2)} \end{bmatrix} \begin{bmatrix} \hat{\mathcal{R}}^{(1)} \\ 0 \end{bmatrix}, \quad \hat{\mathcal{R}}^{(1)}, \hat{Q}_{11}^{(2)}, \hat{Q}_{12}^{(2)}, \hat{Q}_{21}^{(2)}, \hat{Q}_{22}^{(2)} \in \mathbf{R}^{n \times n}.$$

For $m > 3$, the global reduction of A to the form $Q_{11}^{(1)}(Q_{21}^{(1)})^{-1}$ can then be realized by first applying Lemma 2 to a subsequence $A_{j-2}^{s_{j-2}} A_{j-1}^{s_{j-1}} A_j^{s_j}$, of the form required in that lemma, and subsequently taking into account the matrices $A_{j-3}, A_{j-4}, \dots, A_1$ and $A_{j+1}, A_{j+2}, \dots, A_m$.

2.3 Overall algorithm

The overall algorithm is presented as Alg. 1. First we give two examples.

Example 1 Let $A = A_1^{-1} A_2^{-1} A_3^{-1} A_4 A_5^{-1}$ in which $A_i \in \mathbf{R}^{n \times n}$, $i = 1, \dots, 5$ and A_1, A_2, A_3 and A_5 are nonsingular. For $i = 1, \dots, 4$, let orthogonal

matrices $\begin{bmatrix} Q_{11}^{(i)} & Q_{12}^{(i)} \\ Q_{21}^{(i)} & Q_{22}^{(i)} \end{bmatrix}$ with $Q_{11}^{(i)}, Q_{12}^{(i)}, Q_{21}^{(i)}, Q_{22}^{(i)} \in \mathbf{R}^{n \times n}$ satisfy

$$\begin{aligned} \begin{bmatrix} A_4 \\ A_5 \end{bmatrix} &= \begin{bmatrix} Q_{11}^{(4)} & Q_{12}^{(4)} \\ Q_{21}^{(4)} & Q_{22}^{(4)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(4)} \end{bmatrix}, \quad R^{(4)} \in \mathbf{R}^{n \times n}, \\ \begin{bmatrix} A_3^T Q_{11}^{(4)} \\ Q_{21}^{(4)} \end{bmatrix} &= \begin{bmatrix} Q_{11}^{(3)} & Q_{12}^{(3)} \\ Q_{21}^{(3)} & Q_{22}^{(3)} \end{bmatrix} \begin{bmatrix} R^{(3)} \\ 0 \end{bmatrix}, \quad R^{(3)} \in \mathbf{R}^{n \times n}, \\ \begin{bmatrix} A_2^T Q_{11}^{(3)} \\ Q_{21}^{(3)} \end{bmatrix} &= \begin{bmatrix} Q_{11}^{(2)} & Q_{12}^{(2)} \\ Q_{21}^{(2)} & Q_{22}^{(2)} \end{bmatrix} \begin{bmatrix} R^{(2)} \\ 0 \end{bmatrix}, \quad R^{(2)} \in \mathbf{R}^{n \times n}, \\ \begin{bmatrix} A_1^T Q_{11}^{(2)} \\ Q_{21}^{(2)} \end{bmatrix} &= \begin{bmatrix} Q_{11}^{(1)} & Q_{12}^{(1)} \\ Q_{21}^{(1)} & Q_{22}^{(1)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(1)} \end{bmatrix}, \quad R^{(1)} \in \mathbf{R}^{n \times n}. \end{aligned}$$

Then we have that

$$A = Q_{11}^{(1)}(Q_{21}^{(1)})^{-1}.$$

Example 2 Let $A = A_1^{-1}A_2A_3^{-1}A_4^{-1}A_5A_6^{-1}$ in which $A_i \in \mathbf{R}^{n \times n}$, $i = 1, \dots, 6$ and A_1, A_3, A_4 and A_6 are nonsingular. For $i = 1, \dots, 5$, let orthogonal matrices $\begin{bmatrix} Q_{11}^{(i)} & Q_{12}^{(i)} \\ Q_{21}^{(i)} & Q_{22}^{(i)} \end{bmatrix}$ with $Q_{11}^{(i)}, Q_{12}^{(i)}, Q_{21}^{(i)}, Q_{22}^{(i)} \in \mathbf{R}^{n \times n}$

$$\begin{aligned} \begin{bmatrix} A_5 \\ A_6 \end{bmatrix} &= \begin{bmatrix} Q_{11}^{(5)} & Q_{12}^{(5)} \\ Q_{21}^{(5)} & Q_{22}^{(5)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(5)} \end{bmatrix}, \quad R^{(5)} \in \mathbf{R}^{n \times n}, \\ \begin{bmatrix} A_4^T Q_{11}^{(5)} \\ Q_{21}^{(5)} \end{bmatrix} &= \begin{bmatrix} Q_{11}^{(4)} & Q_{12}^{(4)} \\ Q_{21}^{(4)} & Q_{22}^{(4)} \end{bmatrix} \begin{bmatrix} R^{(4)} \\ 0 \end{bmatrix}, \quad R^{(4)} \in \mathbf{R}^{n \times n}, \\ \begin{bmatrix} A_3^T Q_{11}^{(4)} \\ Q_{21}^{(4)} \end{bmatrix} &= \begin{bmatrix} Q_{11}^{(3)} & Q_{12}^{(3)} \\ Q_{21}^{(3)} & Q_{22}^{(3)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(3)} \end{bmatrix}, \quad R^{(3)} \in \mathbf{R}^{n \times n}, \\ \begin{bmatrix} A_2 Q_{11}^{(3)} \\ Q_{21}^{(3)} \end{bmatrix} &= \begin{bmatrix} Q_{11}^{(2)} & Q_{12}^{(2)} \\ Q_{21}^{(2)} & Q_{22}^{(2)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(2)} \end{bmatrix}, \quad R^{(2)} \in \mathbf{R}^{n \times n}, \\ \begin{bmatrix} A_1^T Q_{11}^{(2)} \\ Q_{21}^{(2)} \end{bmatrix} &= \begin{bmatrix} Q_{11}^{(1)} & Q_{12}^{(1)} \\ Q_{21}^{(1)} & Q_{22}^{(1)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(1)} \end{bmatrix}, \quad R^{(1)} \in \mathbf{R}^{n \times n}. \end{aligned}$$

Then we have that

$$A = Q_{11}^{(1)}(Q_{21}^{(1)})^{-1}.$$

Algorithm 1

Input: Matrix A of the form (2).

Output: Matrices $Q_{11}^{(1)}, Q_{21}^{(1)} \in \mathbf{R}^{n \times n}$ such that $(Q_{11}^{(1)})^T Q_{11}^{(1)} + (Q_{21}^{(1)})^T Q_{21}^{(1)} = I$ and $A = Q_{11}^{(1)}(Q_{21}^{(1)})^{-1}$.

Init:

$\begin{cases} \text{If all } s_i = 1, \text{ set } A_{m+1} := I, s_{m+1} := -1; m := m + 1, \\ \text{If all } s_i = -1, \text{ set } A_{m+1} := A_m, A_m := I, s_m = 1, s_{m+1} := -1; m := m + 1, \\ \text{If } -s_1 = \dots = -s_j = s_{j+1} = \dots = s_m = 1, \text{ apply procedure to } A^T. \end{cases}$

Determine maximal j such that $s_j = 1$ and $s_{j+1} = -1$. Set $s_{m+1} := -1$, $s_0 = -s_{j+2}$, $Q_{11}^{(j+1)} = I$, $Q_{21}^{(j+1)} = A_{j+1}$.

Loop: for $i = j, j - 1, \dots, 1$, do:

- Case $s_i = 1$ and $s_{i-1} = 1$. Compute the QR factorization of $\begin{bmatrix} A_i Q_{11}^{(i+1)} \\ Q_{21}^{(i+1)} \end{bmatrix}$:

$$\begin{bmatrix} A_i Q_{11}^{(i+1)} \\ Q_{21}^{(i+1)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(i)} & Q_{12}^{(i)} \\ Q_{21}^{(i)} & Q_{22}^{(i)} \end{bmatrix} \begin{bmatrix} R^{(i)} \\ 0 \end{bmatrix}, \quad R^{(i)}, Q_{11}^{(i)}, Q_{12}^{(i)}, Q_{21}^{(i)}, Q_{22}^{(i)} \in \mathbf{R}^{n \times n}.$$

- *Case $s_i = 1$ and $s_{i-1} = -1$. Compute the QR factorization of $\begin{bmatrix} A_i Q_{11}^{(i+1)} \\ Q_{21}^{(i+1)} \end{bmatrix}$:*

$$\begin{bmatrix} A_i Q_{11}^{(i+1)} \\ Q_{21}^{(i+1)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(i)} & Q_{12}^{(i)} \\ Q_{21}^{(i)} & Q_{22}^{(i)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(i)} \end{bmatrix}, \quad R^{(i)}, Q_{11}^{(i)}, Q_{12}^{(i)}, Q_{21}^{(i)}, Q_{22}^{(i)} \in \mathbf{R}^{n \times n}.$$

- *Case $s_i = -1$ and $s_{i-1} = 1$. Compute the QR factorization of $\begin{bmatrix} A_i^T Q_{11}^{(i+1)} \\ Q_{21}^{(i+1)} \end{bmatrix}$:*

$$\begin{bmatrix} A_i^T Q_{11}^{(i+1)} \\ Q_{21}^{(i+1)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(i)} & Q_{12}^{(i)} \\ Q_{21}^{(i)} & Q_{22}^{(i)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(i)} \end{bmatrix}, \quad R^{(i)}, Q_{11}^{(i)}, Q_{12}^{(i)}, Q_{21}^{(i)}, Q_{22}^{(i)} \in \mathbf{R}^{n \times n}.$$

- *Case $s_i = -1$ and $s_{i-1} = -1$. Compute the QR factorization of $\begin{bmatrix} A_i^T Q_{11}^{(i+1)} \\ Q_{21}^{(i+1)} \end{bmatrix}$:*

$$\begin{bmatrix} A_i^T Q_{11}^{(i+1)} \\ Q_{21}^{(i+1)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(i)} & Q_{12}^{(i)} \\ Q_{21}^{(i)} & Q_{22}^{(i)} \end{bmatrix} \begin{bmatrix} R^{(i)} \\ 0 \end{bmatrix}, \quad R^{(i)}, Q_{11}^{(i)}, Q_{12}^{(i)}, Q_{21}^{(i)}, Q_{22}^{(i)} \in \mathbf{R}^{n \times n}.$$

End loop.

Set $Q_{11}^{(j+1)} := Q_{11}^{(1)}$, $Q_{21}^{(j+1)} := Q_{21}^{(1)}$. Loop: for $i = j + 2, j + 3, \dots, m$ do:

- *Case $s_i = 1$ and $s_{i+1} = 1$. Compute the QR factorization of $\begin{bmatrix} Q_{11}^{(i-1)} \\ A_i^T Q_{21}^{(i-1)} \end{bmatrix}$:*

$$\begin{bmatrix} Q_{11}^{(i-1)} \\ A_i^T Q_{21}^{(i-1)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(i)} & Q_{12}^{(i)} \\ Q_{21}^{(i)} & Q_{22}^{(i)} \end{bmatrix} \begin{bmatrix} R^{(i)} \\ 0 \end{bmatrix}, \quad R^{(i)}, Q_{11}^{(i)}, Q_{12}^{(i)}, Q_{21}^{(i)}, Q_{22}^{(i)} \in \mathbf{R}^{n \times n}.$$

- *Case $s_i = 1$ and $s_{i+1} = -1$. Compute the QR factorization of $\begin{bmatrix} Q_{11}^{(i-1)} \\ A_i^T Q_{21}^{(i-1)} \end{bmatrix}$:*

$$\begin{bmatrix} Q_{11}^{(i-1)} \\ A_i^T Q_{21}^{(i-1)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(i)} & Q_{12}^{(i)} \\ Q_{21}^{(i)} & Q_{22}^{(i)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(i)} \end{bmatrix}, \quad R^{(i)}, Q_{11}^{(i)}, Q_{12}^{(i)}, Q_{21}^{(i)}, Q_{22}^{(i)} \in \mathbf{R}^{n \times n}.$$

- *Case $s_i = -1$ and $s_{i+1} = 1$. Compute the QR factorization of $\begin{bmatrix} Q_{11}^{(i-1)} \\ A_i Q_{21}^{(i-1)} \end{bmatrix}$:*

$$\begin{bmatrix} Q_{11}^{(i-1)} \\ A_i Q_{21}^{(i-1)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(i)} & Q_{12}^{(i)} \\ Q_{21}^{(i)} & Q_{22}^{(i)} \end{bmatrix} \begin{bmatrix} 0 \\ R^{(i)} \end{bmatrix}, \quad R^{(i)}, Q_{11}^{(i)}, Q_{12}^{(i)}, Q_{21}^{(i)}, Q_{22}^{(i)} \in \mathbf{R}^{n \times n}.$$

- *Case $s_i = -1$ and $s_{i+1} = -1$. Compute the QR factorization of $\begin{bmatrix} Q_{11}^{(i-1)} \\ A_i Q_{21}^{(i-1)} \end{bmatrix}$:*

$$\begin{bmatrix} Q_{11}^{(i-1)} \\ A_i Q_{21}^{(i-1)} \end{bmatrix} = \begin{bmatrix} Q_{11}^{(i)} & Q_{12}^{(i)} \\ Q_{21}^{(i)} & Q_{22}^{(i)} \end{bmatrix} \begin{bmatrix} R^{(i)} \\ 0 \end{bmatrix}, \quad R^{(i)}, Q_{11}^{(i)}, Q_{12}^{(i)}, Q_{21}^{(i)}, Q_{22}^{(i)} \in \mathbf{R}^{n \times n}.$$

End loop.

In this algorithm, we first determine a value j such that $s_{j-1} = 1$ and $s_j = -1$. From there, we work further to the left and subsequently to the right, as explained above (note that in our implementation s_0 allows to take into account the type of operation required for $i = j + 2$). If $s_{j-1} = 1 = -s_j$ does not apply, but instead we have $s_j = 1$ and $s_{j-1} = -1$, then we can work with A^T instead of A . In these cases, we need only $m - 1$ QR-factorizations. Only if $s_1 = s_2 = \dots = s_m$, we have to plug in an artificial I and the method requires m QR-factorizations.

In Algorithm 1, the explicit computation of A_i^{-1} and explicit solution of the corresponding triangular linear system are avoided if $s_i = -1$. An example illustrating the importance of this point is given in the Appendix.

After reducing A to $Q_{11}^{(1)}(Q_{21}^{(1)})^{-1}$ by Algorithm 1, we can compute the SVD of A by computing the CSD of $Q_{11}^{(1)}$ and $Q_{21}^{(1)}$ by the Matlab command `gsvd`.

It is natural to ask in Algorithm 1 which j would be the best choice to start with, if there is more than one value for which $s_j = -s_{j+1}$. We just made an arbitrary choice here because it seems that there is no easy way to fix the order of the operations in an optimal way in advance.

So far, we have assumed that all matrices are square and that the matrices that are inverted, are nonsingular. Actually, for our method one can verify that there is no restriction on the size nor the rank of matrices of which $s_i = 1$. How to extend our theory to show what happens when some A_j of $s_j = -1$ is singular is an interesting topic for the further study.

2.4 Backward stability

In the following we explain that the computations involved in Algorithm 1 can be posed as left and right orthogonal transformations of a large matrix whose sub-blocks are the A_i or their transposes, several unit matrices, and the rest being zero matrices.

To have a good understanding of this reformulation, we first reconsider Examples 1 and 2.

- In Example 1, define

$$Q_i := \begin{bmatrix} Q_{11}^{(i)} & Q_{12}^{(i)} \\ Q_{21}^{(i)} & Q_{22}^{(i)} \end{bmatrix}, \quad i = 1, \dots, 4,$$

$$\mathcal{M}_4 := \begin{bmatrix} A_4 \\ A_5 \end{bmatrix}^T, \quad \mathcal{M}_3 := \begin{bmatrix} A_3 & 0 \\ 0 & I_n \end{bmatrix}, \quad \mathcal{M}_2 := \begin{bmatrix} A_2 & 0 \\ 0 & I_n \end{bmatrix}, \quad \mathcal{M}_1 := \begin{bmatrix} A_1 & 0 \\ 0 & I_n \end{bmatrix},$$

$$U := \begin{bmatrix} Q_4^T & 0 \\ 0 & Q_2^T \end{bmatrix}, \quad V := \begin{bmatrix} I_n & 0 & 0 \\ 0 & Q_3 & 0 \\ 0 & 0 & Q_1 \end{bmatrix}, \quad M := \begin{bmatrix} \mathcal{M}_4^T & \mathcal{M}_3 & 0 \\ 0 & \mathcal{M}_2^T & \mathcal{M}_1 \end{bmatrix}.$$

Then U, V are orthogonal and

$$UMV = R =: \begin{bmatrix} \mathcal{R}_4 & \mathcal{R}_3 & 0 \\ 0 & \mathcal{R}_2 & \mathcal{R}_1 \end{bmatrix},$$

where

$$\mathcal{R}_4 = \begin{bmatrix} 0 \\ R^{(4)} \end{bmatrix}, \mathcal{R}_3 = \begin{bmatrix} (R^{(3)})^T & 0 \\ \star & \star \end{bmatrix}, \mathcal{R}_2 = \begin{bmatrix} R^{(2)} & \star \\ 0 & \star \end{bmatrix}, \mathcal{R}_1 = \begin{bmatrix} 0 & (R^{(1)})^T \\ \star & \star \end{bmatrix}.$$

- In Example 2, define

$$\mathcal{Q}_i := \begin{bmatrix} \mathcal{Q}_{11}^{(i)} & \mathcal{Q}_{12}^{(i)} \\ \mathcal{Q}_{21}^{(i)} & \mathcal{Q}_{22}^{(i)} \end{bmatrix}, \quad i = 1, \dots, 5,$$

$$\mathcal{M}_5 := \begin{bmatrix} A_5 \\ A_6 \end{bmatrix}^T, \quad \mathcal{M}_4 := \begin{bmatrix} A_4 & 0 \\ 0 & I_n \end{bmatrix},$$

$$\mathcal{M}_3 := \begin{bmatrix} A_3 & 0 \\ 0 & I_n \end{bmatrix}, \quad \mathcal{M}_2 := \begin{bmatrix} A_2^T & 0 \\ 0 & I_n \end{bmatrix}, \quad \mathcal{M}_1 := \begin{bmatrix} A_1 & 0 \\ 0 & I_n \end{bmatrix},$$

$$U := \begin{bmatrix} \mathcal{Q}_5^T & 0 & 0 \\ 0 & \mathcal{Q}_3^T & 0 \\ 0 & 0 & \mathcal{Q}_1^T \end{bmatrix}, \quad V = \begin{bmatrix} I_n & 0 & 0 \\ 0 & \mathcal{Q}_4 & 0 \\ 0 & 0 & \mathcal{Q}_2 \end{bmatrix}, \quad M := \begin{bmatrix} \mathcal{M}_5^T & \mathcal{M}_4 & 0 \\ 0 & \mathcal{M}_3^T & \mathcal{M}_2 \\ 0 & 0 & \mathcal{M}_1^T \end{bmatrix}.$$

Then U, V are orthogonal and

$$UMV = R =: \begin{bmatrix} \mathcal{R}_5 & \mathcal{R}_4 & 0 \\ 0 & \mathcal{R}_3 & \mathcal{R}_2 \\ 0 & 0 & \mathcal{R}_1 \end{bmatrix},$$

where

$$\mathcal{R}_5 = \begin{bmatrix} 0 \\ R^{(5)} \end{bmatrix}, \quad \mathcal{R}_4 = \begin{bmatrix} (R^{(4)})^T & 0 \\ \star & \star \end{bmatrix}, \quad \mathcal{R}_3 = \begin{bmatrix} 0 & \star \\ R^{(3)} & \star \end{bmatrix},$$

$$\mathcal{R}_2 = \begin{bmatrix} 0 & (R^{(2)})^T \\ \star & \star \end{bmatrix}, \quad \mathcal{R}_1 = \begin{bmatrix} 0 & \star \\ R^{(1)} & \star \end{bmatrix}.$$

Now, we go back to Algorithm 1. For simplicity, we assume without loss of generality that $j = m - 1$ in Algorithm 1, i.e., $s_m = -1$ and $s_{m-1} = 1$.

Define

$$\mathcal{M}_{m-1} := \begin{bmatrix} A_{m-1} \\ A_m \end{bmatrix}^T, \quad \mathcal{Q}_i := \begin{bmatrix} \mathcal{Q}_{11}^{(i)} & \mathcal{Q}_{12}^{(i)} \\ \mathcal{Q}_{21}^{(i)} & \mathcal{Q}_{22}^{(i)} \end{bmatrix}, \quad i = 1, \dots, m - 1.$$

For $i = 1, \dots, m - 2$,

$$\mathcal{M}_i := \begin{bmatrix} A_i^T & 0 \\ 0 & I_n \end{bmatrix}, \text{ if } s_i = 1 \text{ and } s_{i-1} = 1, \text{ or } s_i = 1 \text{ and } s_{i-1} = -1,$$

$$\mathcal{M}_i := \begin{bmatrix} A_i & 0 \\ 0 & I_n \end{bmatrix}, \text{ if } s_i = -1 \text{ and } s_{i-1} = 1, \text{ or } s_i = -1 \text{ and } s_{i-1} = -1.$$

Set

$$U := \begin{bmatrix} Q_{m-1}^T & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & Q_2^T \end{bmatrix} \text{ if } m \text{ is odd, } U := \begin{bmatrix} Q_{m-1}^T & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & Q_1^T \end{bmatrix} \text{ if } m \text{ is even,}$$

$$V := \begin{bmatrix} I_n & 0 & 0 & 0 \\ 0 & Q_{m-2} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & Q_1 \end{bmatrix} \text{ if } m \text{ is odd, } V := \begin{bmatrix} I_n & 0 & 0 & 0 \\ 0 & Q_{m-2} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & Q_2 \end{bmatrix} \text{ if } m \text{ is even,}$$

$$M = \begin{bmatrix} \mathcal{M}_{m-1}^T & \mathcal{M}_{m-2} & 0 & 0 & 0 \\ 0 & \mathcal{M}_{m-3}^T & \mathcal{M}_{m-4} & 0 & 0 \\ 0 & 0 & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \mathcal{M}_2^T & \mathcal{M}_1 \end{bmatrix} \text{ if } m \text{ is odd,}$$

$$M = \begin{bmatrix} \mathcal{M}_{m-1}^T & \mathcal{M}_{m-2} & 0 & 0 & 0 \\ 0 & \mathcal{M}_{m-3}^T & \mathcal{M}_{m-4} & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \dots & \mathcal{M}_3^T & \mathcal{M}_2^T \\ 0 & 0 & 0 & 0 & \mathcal{M}_1^T \end{bmatrix} \text{ if } m \text{ is even.}$$

Then U and V are orthogonal matrices, and

$$(15) \quad U M V = R,$$

where

$$R = \begin{bmatrix} \mathcal{R}_{m-1} & \mathcal{R}_{m-2} & 0 & 0 & 0 \\ 0 & \mathcal{R}_{m-3} & \mathcal{R}_{m-4} & 0 & 0 \\ 0 & 0 & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \mathcal{R}_2 & \mathcal{R}_1 \end{bmatrix} \text{ if } m \text{ is odd,}$$

$$R = \begin{bmatrix} \mathcal{R}_{m-1} & \mathcal{R}_{m-2} & 0 & 0 & 0 \\ 0 & \mathcal{R}_{m-3} & \mathcal{R}_{m-4} & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \dots & \mathcal{R}_3 & \mathcal{R}_2 \\ 0 & 0 & 0 & 0 & \mathcal{R}_1 \end{bmatrix} \text{ if } m \text{ is even,}$$

$$\mathcal{R}_{m-1} = \begin{bmatrix} R^{(m-1)} \\ 0 \end{bmatrix} \text{ or } \mathcal{R}_{m-1} = \begin{bmatrix} 0 \\ R^{(m-1)} \end{bmatrix},$$

$\mathcal{R}_i \in \mathbf{R}^{n \times n}$, $i = 1, \dots, m - 2$, are of one of the following forms

$$\begin{bmatrix} R^{(i)} & \star \\ 0 & \star \end{bmatrix}, \begin{bmatrix} R^{(i)} & 0 \\ \star & \star \end{bmatrix}, \begin{bmatrix} \star & \star \\ 0 & R^{(i)} \end{bmatrix}, \begin{bmatrix} \star & 0 \\ \star & R^{(i)} \end{bmatrix},$$

$R^{(i)} \in \mathbf{R}^{n \times n}$ ($i = 1, \dots, m - 1$) are nonsingular.

Let \bar{X} denote the estimate of X computed with finite precision arithmetic, as opposed to exact arithmetic, and let ϵ denote the machine precision. From (15), we have [10]

$$(16) \quad \|\bar{U}^T \bar{U} - I_{2n}\| \approx \epsilon, \quad \|\bar{V}^T \bar{V} - I_{2n}\| \approx \epsilon, \quad \|\bar{U} M \bar{V} - \bar{R}\| \approx \epsilon \|M\|.$$

Hence, algorithm 1 is backward stable in the sense that (16) holds.

3 Numerical experiments

In this section we illustrate the performance of our method by means of some numerical examples. After reducing the matrix $A \in \mathbf{R}^{n \times n}$ in Eq.(2) to the form $Q_{11}^{(1)}(Q_{21}^{(1)})^{-1}$ by Algorithm 1, the SVD of A is obtained by computing the CSD of $Q_{11}^{(1)}$ and $Q_{21}^{(1)}$ using Van Loan's CSD algorithm [18] (i.e. Matlab command *gsvd*); here we set the parameter $\tau = \frac{1}{\sqrt{2}}$, which minimizes a backward error bound [3]. All our calculations were carried out in MATLAB 5 on a Sun Ultra 5 workstation with IEEE standard (machine accuracy $\epsilon \cong 10^{-16}$).

To quantify the accuracy of the results, we define the residual

$$(17) \quad \text{resSVD} = \frac{\|\hat{\Sigma} - \Sigma\|_2}{n \|\hat{\Sigma}\|_2},$$

in which

$$\begin{aligned} \hat{\Sigma} &= \text{diag}\{\hat{\sigma}_1, \hat{\sigma}_2, \dots, \hat{\sigma}_n\}, & \hat{\sigma}_1 &\geq \hat{\sigma}_2 \geq \dots \geq \hat{\sigma}_n > 0, \\ \Sigma &= \text{diag}\{\sigma_1, \sigma_2, \dots, \sigma_n\}, & \sigma_1 &\geq \sigma_2 \geq \dots \geq \sigma_n > 0, \end{aligned}$$

where $\hat{\sigma}_i$ and σ_i , $i = 1, 2, \dots, n$, are the computed and the exact singular values of A respectively.

We use the symbols η and $\kappa(X)$ to denote a value drawn from a uniform distribution over $[0, 1)$ and the 2-norm condition number of X , respectively.

Example 3 In this example, we test our method using some common-used matrix families including Lauchli matrices, Frank matrices, Cauchy matrices, Vandermonde matrices, Wilkinson matrices, Pascal matrices, Toeplitz matrices and Hankel matrices. Take

$$m = 6, s_1 = s_3 = s_4 = s_6 = -1, s_2 = s_5 = 1.$$

1) Matrices A_i ($i = 1, \dots, 6$) are generalized using the following Matlab commands:

```
X = gallery('lauchli', n, 0.1); A1 = X(1 : n, 1 : n);
A3 = gallery('frank', n, 1); A6 = vander(randn(n, 1));
A4 = gallery('cauchy', randn(n, 1), randn(n, 1));
A2 = A1 * A3; A5 = A4.
```

It is easy to see that $A = A_6^{-1}$ and hence we can get the singular values of A by Matlab command $svd(inv(A_6))$. The computed results are listed in Table 1.

Table 1.

n	$resSVD$	$\kappa(A_1)$	$\kappa(A_2)$	$\kappa(A_3)$	$\kappa(A_4)$	$\kappa(A_6)$
6	5.5×10^{-15}	60.1	9.7×10^4	4.2×10^3	1.7×10^3	1.4×10^3
7	8.2×10^{-14}	70.1	7.9×10^5	3.2×10^4	1.9×10^5	2.4×10^5
8	4.2×10^{-13}	80.1	7.3×10^6	2.8×10^5	3.2×10^5	1.9×10^3
9	8.6×10^{-11}	90.1	7.5×10^7	2.7×10^6	2.8×10^7	3.8×10^4
10	7.4×10^{-11}	1.0×10^2	8.4×10^8	2.9×10^7	1.3×10^4	3.6×10^5

2) Matrices A_i ($i = 1, \dots, 6$) are generalized using the following Matlab commands:

```
A1 = wilkinson(n); A4 = pascal(n);
c = randn(n, 1); r = randn(1, n); r(1, 1) = c(1, 1); A3 = toeplitz(c, r);
d = rand(n, 1); A6 = hankel(d);
A2 = A3; A5 = A4 * A6.
```

Obviously, $A = A_1^{-1}$ and we can get the singular values of A by Matlab command $svd(inv(A_1))$. The computed results are listed in the Table 2.

Table 2.

n	$resSVD$	$\kappa(A_1)$	$\kappa(A_3)$	$\kappa(A_4)$	$\kappa(A_5)$	$\kappa(A_6)$
6	1.7×10^{-14}	13.1	29.7	1.1×10^5	1.3×10^5	7.2
7	3.1×10^{-13}	14.1	29.3	1.5×10^6	2.3×10^6	1.8×10^3
8	9.4×10^{-11}	19.7	7.8	2.1×10^7	1.8×10^{11}	1.5×10^6
9	7.7×10^{-12}	18.6	81.8	2.9×10^8	1.4×10^{10}	5.3×10^2
10	6.3×10^{-11}	24.7	34.4	4.2×10^9	5.2×10^{11}	1.0×10^5

Example 4 We compare our Algorithm 1 with the method in [11] in this example. Let

$$A_1 = \text{pascal}(n), \quad A_2 = A_1, \quad s_1 = -1, \quad s_2 = 1.$$

Obviously, $A = I_n$. The computed $resSVD$ are listed in Table 3.

Table 3.

n	13	14	15	16	17	18
$resSVD_1$	2.6×10^{-7}	2.9×10^{-6}	3.1×10^{-5}	3.4×10^{-4}	0.002	0.02
$resSVD_2$	1.7×10^{-6}	4.5×10^{-5}	3.5×10^{-4}	8.4×10^{-4}	0.02	1.7
$resSVD_3$	2.0×10^{-6}	4.2×10^{-5}	2.6×10^{-4}	8.7×10^{-3}	0.07	1.14
$\kappa(A_1)$	1.3×10^{13}	1.9×10^{14}	2.8×10^{15}	4.2×10^{16}	6.4×10^{17}	9.4×10^{18}

In Table 3, $resSVD_1$, $resSVD_2$ and $resSVD_3$ denote the $resSVD$ computed by our Algorithm 1, the method in [11], and the command $svd(inv(A_1) * A_2)$, respectively.

In the next 6 examples, $m = 6$, $s_1 = s_3 = s_4 = s_6 = -1$ and $s_2 = s_5 = 1$. We have

$$\begin{aligned} A_1 &= U_1 \Sigma_1 V_1, & A_2 &= U_1 \Sigma_2 V_2, & A_3 &= \Sigma_3 V_2, \\ A_4 &= U_4 \Sigma_4, & A_5 &= U_4 \Sigma_5 V_5, & A_6 &= U_6 \Sigma_6 V_5, \end{aligned}$$

in which U_1, U_4, U_6, V_1, V_2 and V_5 are randomly chosen orthogonal matrices; the entries of $\Sigma_i = \text{diag}\{\sigma_{i1}, \dots, \sigma_{in}\}$, $i = 1, \dots, 6$, are specified below. For values of $n = 35, 36, \dots, 80$, the obtained residuals $resSVD$ are plotted in Figure 2.

Example 5 For $j = 1, \dots, n$,

$$\sigma_{ij} = (j + \eta_{ij}) * i, \quad i = 1, \dots, 4, 6,$$

and

$$\sigma_{5j} = (j + \eta_{5j}) * 5 * 10^{-\frac{7}{n}*j}.$$

Example 6 For $j = 1, \dots, n$,

$$\sigma_{ij} = (j + \eta_{ij}) * i, \quad i = 1, \dots, 4,$$

and

$$\sigma_{5j} = (j + \eta_{5j}) * 5 * 10^{-\frac{7}{n}*j}, \quad \sigma_{6j} = (j + \eta_{6j}) * 6 * 10^{-\frac{6}{n}*j}.$$

Example 7 For $j = 1, \dots, n$,

$$\sigma_{ij} = (j + \eta_{ij}) * i, \quad i = 1, \dots, 3,$$

and

$$\begin{aligned} \sigma_{ij} &= (j + \eta_{ij}) * i, \quad i = 1, \dots, 3, & \sigma_{4j} &= (j + \eta_{4j}) * 4 * 10^{-\frac{3}{n}*j}, \\ \sigma_{5j} &= (j + \eta_{5j}) * 5 * 10^{-\frac{8}{n}*j}, & \sigma_{6j} &= (j + \eta_{6j}) * 6 * 10^{-\frac{5}{n}*j}. \end{aligned}$$

Example 8 For $j = 1, \dots, n$,

$$\sigma_{ij} = (j + \eta_{ij}) * i, \quad i = 1, 2,$$

and

$$\begin{aligned} \sigma_{3j} &= (j + \eta_{3j}) * 3 * 10^{\frac{3}{n}*j}, & \sigma_{4j} &= (j + \eta_{4j}) * 4 * 10^{-\frac{3}{n}*j}, \\ \sigma_{5j} &= (j + \eta_{5j}) * 5 * 10^{-\frac{8}{n}*j}, & \sigma_{6j} &= (j + \eta_{6j}) * 6 * 10^{-\frac{5}{n}*j}. \end{aligned}$$

Example 9 For $j = 1, \dots, n$,

$$\begin{aligned} \sigma_{1j} &= (j + \eta_{1j}), & \sigma_{2j} &= (j + \eta_{2j}) * 2 * 10^{-\frac{4}{n}*j}, \\ \sigma_{3j} &= (j + \eta_{3j}) * 3 * 10^{\frac{3}{n}*j}, & \sigma_{4j} &= (j + \eta_{4j}) * 4 * 10^{-\frac{3}{n}*j}, \\ \sigma_{5j} &= (j + \eta_{5j}) * 5 * 10^{-\frac{7}{n}*j}, & \sigma_{6j} &= (j + \eta_{6j}) * 6 * 10^{-\frac{4}{n}*j}. \end{aligned}$$

Example 10

$$\begin{aligned} \sigma_{1j} &= (j + \eta_{1j}) * 10^{-\frac{3}{n}*j}, & \sigma_{2j} &= (j + \eta_{2j}) * 2 * 10^{-\frac{4}{n}*j}, \\ \sigma_{3j} &= (j + \eta_{3j}) * 3 * 10^{\frac{3}{n}*j}, & \sigma_{4j} &= (j + \eta_{4j}) * 4 * 10^{-\frac{3}{n}*j}, \\ \sigma_{5j} &= (j + \eta_{5j}) * 5 * 10^{-\frac{7}{n}*j}, & \sigma_{6j} &= (j + \eta_{6j}) * 6 * 10^{-\frac{4}{n}*j}. \end{aligned}$$

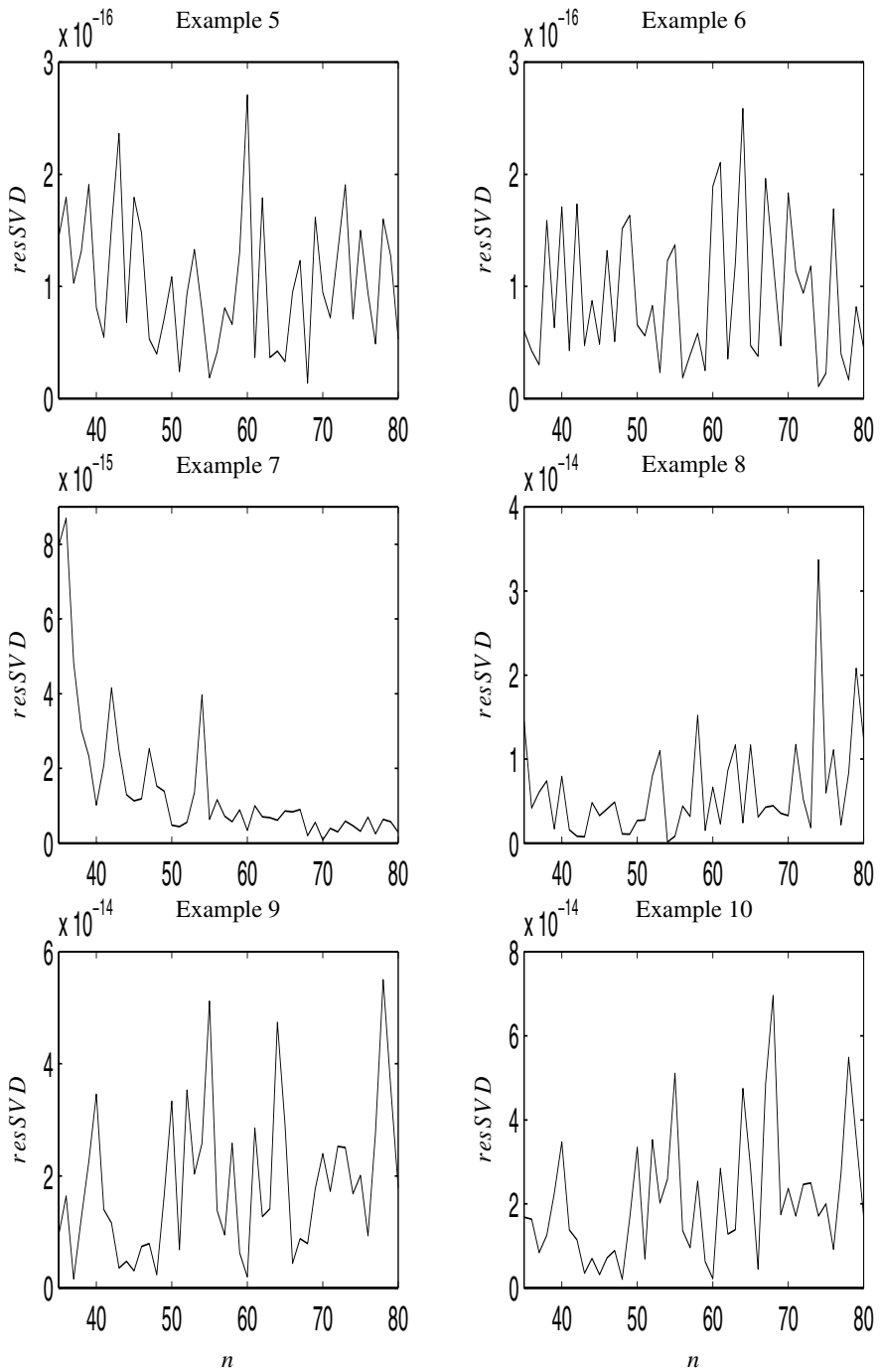


Fig. 1. Residuals $resSVD$ (see Eq. (17)) as a function of matrix size n , computed in Examples 5, ..., 10.

Obviously, the exact of SVDs of A in Examples 5–10 are

$$A = V_1 \Sigma U_6^T \text{ with } \Sigma = \Sigma_1^{-1} \Sigma_2 \Sigma_3^{-1} \Sigma_4^{-1} \Sigma_5 \Sigma_6^{-1}.$$

In examples 5–10, we choose the diagonal elements of Σ_i in such a way that different situations in terms of the condition number of A_i and A are to be dealt with. In detail,

- In Example 5, A_1, A_2, A_3, A_4 and A_6 are well-conditioned, A_5 and A are ill-conditioned with $\kappa(A_5) = (10^7)$ and $\kappa(A) = O(10^7)$.
- In Example 6, A_1, A_2, A_3, A_4 and A are well-conditioned, A_5 and A_6 are ill-conditioned with $\kappa(A_5) = O(10^7)$ and $\kappa(A_6) = O(10^6)$.
- In Example 7, A_1, A_2, A_3 and A are well-conditioned, A_4 has a moderate condition number, A_5 and A_6 are ill-conditioned with $\kappa(A_5) = O(10^8)$ and $\kappa(A_6) = (10^5)$.
- In Example 8, A_1 and A_2 are well-conditioned, A_3, A_4 and A have a moderate condition number, A_5 and A_6 are ill-conditioned with $\kappa(A_5) = O(10^8)$ and $\kappa(A_6) = O(10^5)$.
- In Example 9, A_1 is well-conditioned, A_2, A_3, A_4 and A_6 have a moderate condition number, A_5 and A are ill-conditioned with $\kappa(A_5) = O(10^7)$ and $\kappa(A) = O(10^7)$.
- In Example 10, A_1, A_2, A_3, A_4, A_6 and A have a moderate condition number, A_5 is ill-conditioned.

From Tables 1, 2 and 3, and Figure 1, we see that our results are satisfactory.

4 Conclusions

In this paper, we have studied the computation of the SVD of a general matrix product/quotient sequence. First we reduced the sequence by at most m QR-factorizations to the form $Q_{11}^{(1)}(Q_{21}^{(1)})^{-1}$, with $Q_{11}^{(1)}, Q_{21}^{(1)} \in \mathbf{R}^{n \times n}$ and $(Q_{11}^{(1)})^T Q_{11}^{(1)} + (Q_{21}^{(1)})^T Q_{21}^{(1)} = I$. Then we obtain the SVD of A by computing the CSD of $Q_{11}^{(1)}$ and $Q_{21}^{(1)}$ using the Matlab command *gsvd*. An advantage of our QR-type reduction is its flexibility for adding one more matrix from left or right to the matrix A of a matrix product/quotient, this feature is very useful for the applications like the estimation of Lyapunov exponents of dynamic systems. Some numerical examples were given to show the performance of the presented method.

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Appendix

Take

$$A_1 = \begin{bmatrix} 0.99999999987468 & 0.50000000236877 & 0.33333332305860 & 0.25000001557339 & 0.19999999236251 \\ 0.50000000236877 & 0.33333328856096 & 0.25000019420358 & 0.19999970564605 & 0.16666681102359 \\ 0.33333332305860 & 0.25000019420358 & 0.19999915762723 & 0.16666794344931 & 0.14285651669800 \\ 0.25000001557339 & 0.19999970564605 & 0.16666794344931 & 0.14285520764038 & 0.12500094906810 \\ 0.19999999236251 & 0.16666681102359 & 0.14285651669800 & 0.12500094906810 & 0.11111064566958 \end{bmatrix},$$

$$A_2 = [\sqrt{5} \ \sqrt{5} \ \sqrt{5} \ \sqrt{5} \ \sqrt{5}] A_1.$$

The exact value of the SVD of $A_2 A_1^{-1}$ is 5.

In the following we illustrate that the explicit computation of A_1^{-1} should be avoided.

We first compute the QR factorization of A_1 : $A_1 = QR$, and then compute the solution x of $xR = A_2$. Finally, the singular value of $A_2 A_1^{-1}$, estimated by means of the method in [11], is 5.00120891819209.

Now we use our Algorithm 1 to get a singular value estimate equal to 5.00000781367755.

The above performances are easy to understand. The exact value of x should satisfy

$$x Q^T = [\sqrt{5} \ \sqrt{5} \ \sqrt{5} \ \sqrt{5} \ \sqrt{5}].$$

However, the computed x only gives

$$x Q^T = [2.23668506012794 \ 2.22440444340721 \ 2.28665944307996 \ 2.15938659945574 \ 2.27367402298989].$$

Since

$$\begin{aligned} \|Q^T Q - I_5\|_2 &= 6.1061099 \times 10^{-16}, \\ \|A_1 - QR\|_2 &= 1.4262426 \times 10^{-16}, \\ \|A_1\|_2 &= 1.5670507. \end{aligned}$$

So, the computed Q and R are very accurate. But the computed x is not acceptable. Note that A_1 is ill-conditioned but well-balanced. However,

$$R = \begin{bmatrix} 1.20979796293064 & -0.68882024839475 & -0.49201446313907 & -0.38541132945901 & -0.31775934077732 \\ 0 & -0.13005981043404 & -0.14019190378167 & -0.13270023604854 & -0.12232288892133 \\ 0 & 0 & -0.00806537832143 & -0.01263254593415 & -0.01490828704240 \\ 0 & 0 & 0 & -0.00033807875859 & -0.00068936642389 \\ 0 & 0 & 0 & 0 & 0.00000000000001 \end{bmatrix}.$$

Thus, the computed R is not only ill-conditioned but also highly *non-balanced*, which leads to a catastrophic cancellation in the solution of the triangular linear system $xR = A_2$. Such a catastrophic cancellation seriously affects the computational accuracy. The situation is the same even when the QR factorization of A_1 is computed with *pivoting*. This example indicates that the explicit computation of the inverses of triangular matrices from the QR factorizations and the explicit solutions of corresponding triangular linear systems should be avoided in the computation of the SVD of matrix product/quotient, if this is possible.

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