An algorithm for computing the Analytic Singular Value Decomposition

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Abstract—A proof of convergence of a new continuation algorithm for computing the Analytic SVD for a large sparse parameter-dependent matrix is given. The algorithm itself was developed and numerically tested in [5].

Keywords—Analytic Singular Value Decomposition, large sparse parameter–dependent matrices, continuation algorithm of a predictor-corrector type.

I. INTRODUCTION

A singular value decomposition (SVD) of a real matrix

\[ A \in \mathbb{R}^{m \times n}, \quad m \geq n, \]

is a factorization

\[ A = U \Sigma V^T, \]

where \( U \in \mathbb{R}^{m \times m} \) and \( V \in \mathbb{R}^{n \times n} \) are orthogonal matrices and

\[ \Sigma = \text{diag}(s_1, \ldots, s_n) \in \mathbb{R}^{n \times n}. \]

The values \( s_i, \ i = 1, \ldots, n, \) are called singular values. They may be defined to be nonnegative and nonincreasing, see [4]. For computational tools and reliable software, see [4] and [1], respectively.

Let \( A \) depend smoothly on a parameter \( t \in \mathbb{R}, \ t \in [a,b] \). The aim is to construct a path of SVD’s

\[ A(t) = U(t) \Sigma(t) V(t)^T, \]

where \( U(t), \Sigma(t) \) and \( V(t) \) depend smoothly on \( t \in [a,b] \).

In [2], it is shown that real analytic functions \( A = A(t) \in \mathbb{R}^{m \times n} \) on \( [a,b] \) is the right class to expect uniqueness of the decomposition. The notion of Analytic Singular Value Decomposition (ASVD) is introduced for the decomposition (1): There exists a factorization (1) that interpolates classical SVD defined at \( t = a \) i.e.,

- the factors \( U(t), V(t) \) and \( \Sigma(t) \) are real analytic on \( [a,b] \),
- for each \( t \in [a,b] \), both \( U(t) \in \mathbb{R}^{m \times m} \) and \( V(t) \in \mathbb{R}^{n \times n} \) are orthogonal matrices and \( \Sigma(t) = \text{diag}(s_1(t), \ldots, s_n(t)) \in \mathbb{R}^{n \times n} \) is a diagonal matrix
- at \( t = a \), the matrices \( U(a), \Sigma(a) \) and \( V(a) \) are the factors of the classical SVD of the matrix \( A(a) \).

Diagonal entries \( s_i(t) \in \mathbb{R} \) of \( \Sigma(t) \) are called singular values. Due to the requirement of smoothness, singular values may be negative and also their ordering may be arbitrary.

II. RELATED WORK

The generic scenario is that the branches \( t \mapsto s_i(t) \) of singular values, \( i = 1, \ldots, n \), may intersect at isolated points only namely, at the points where \( s_i(t) = s_j(t) \) or \( s_i(t) = -s_j(t) \) for \( i \neq j \), see [2], p. 8. Therefore, if ASVD interpolates classical SVD with positive and different singular values then ASVD is unique. In case that these initial singular values are multiple then the multiplicity of singular values is an invariant of ASVD. In other word, if there are clusters of multiple singular values then dimension of these clusters does not change with \( t \). Nevertheless, even in that case one can define ASVD uniquely, see the [2], the notion of minimum variation path.

As far as the computation is concerned, an incremental technique is proposed in [2]: Given a point on the path, one computes a classical SVD for a neighboring parameter value. Next, one computes permutation matrices which link the classical SVD to the next point on the path. The procedure is approximative with a local error of order \( O(h^2) \), where \( h \) is the step size.

An alternative technique for computing ASVD is presented in [9] and [10]: A non-autonomous vector field \( H : \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}^N \) of a huge dimension \( N = n + n^2 + m^2 \) can be constructed in such a way that the solution of the initial value problem for the system \( x' = H(t, x) \) is linked to the path of ASVD. Moreover, [9] contributes to the analysis of non-generic points, see [2], of the ASVD path. These points could be, in fact, interpreted as singularities of the vector field \( \mathbb{R}^N \).

In [8], two methods for computing ASVD are presented and compared. The first one modifies the technique of [2]. The difference is in the treatment of “clusters” of singular values. To that end, analytic polar decomposition (APD) is introduced. Both ASVD and APD are equivalent. Nevertheless, assuming “clusters”, the uniqueness of APD path is achieved very naturally (without solving an auxiliary ODE). The second method in [8] consists in solving ODE as in [9] but it uses an implicit integration technique. The comparison clearly prefers the former class of methods: The ODE integration, in spite of using an implicit scheme, lacks the precision.

A continuation algorithm for computing ASVD is presented in [5]. It follows a path of a few selected singular values and left/right singular vectors. It is aimed to treat large sparse matrices. The continuation algorithm is of a predictor-corrector type, see [3]. The relevant predictor is based on Euler method hence on an ODE solver. In this respect, there is a link to [9]. Nevertheless, the Newton-type corrector guarantees the solution with a prescribed precision. It defeats the objection of the study [8].

In this paper, we review the above mentioned continuation algorithm and supply details namely, the proof of Theorem 1 in [5].
III. FORMULATION OF THE PROBLEM

As a preliminary, let us recall the notion of singular value of a matrix $A \in \mathbb{R}^{m \times n}$, $m \geq n$:

**Definition 3.1:** We say that $s \in \mathbb{R}$ is a singular value of the matrix $A$ if there exist $u \in \mathbb{R}^m$ and $v \in \mathbb{R}^n$ such that

$$Av - su = 0, \quad A^Tu - sv = 0, \quad ||u|| = ||v|| = 1. \quad (2)$$

The vectors $v$ and $u$ are called the right and the left singular vectors of the matrix $A$.

Note that $s$ is defined up to its sign: if the triplet $(s, u, v)$ satisfies (2) then at least three more triplets

$$(s, -u, -v), \quad (-s, -u, v), \quad (-s, u, -v),$$

can be interpreted as singular values, left and right singular vectors of $A$.

**Definition 3.2:** For a given $s \in \mathbb{R}$, let us set

$$\mathcal{M}(s) \equiv \left( \begin{array}{cc} -sI_m & A \\ A^T & -sI_n \end{array} \right),$$

where $I_m \in \mathbb{R}^{m \times m}$ and $I_n \in \mathbb{R}^{n \times n}$ are identities.

**Remark 3.1:** $s$ is a singular value of $A$ if and only if $\dim \ker \mathcal{M}(s) \geq 1$.

**Lemma 3.1:** Let $s \neq 0$, $\mathcal{M}(s) \left( \begin{array}{c} u \\ v \end{array} \right) = 0$. Then $u^TAv = v^Tv$.

**Proof:** By the definition of $\mathcal{M}(s)$, we assume

$$-su + Av = 0, \quad A^Tu - sv = 0.$$

Multiplying the first equation by $u^T$ from the left and the second equation by $v^T$ from the left, we get

$$u^Tu = -\frac{1}{s}u^TAv, \quad v^Tv = -\frac{1}{s}v^TA^Tu.$$

Note that $v^TA^Tu = (Av)^Tv = u^TAv$. Therefore, $u^Tu - v^Tv = -\frac{1}{s}(u^TAv - v^TA^Tu) = 0$.

**Lemma 3.2:** Let $s \neq 0$, $\mathcal{M}(s) \left( \begin{array}{c} u \\ v \end{array} \right) = 0$.

**Proof:** We assume

$$-su + Av = 0, \quad A^Tu - sv = 0,$$

and hence (4) has infinitely many solutions. If $\dim \ker A \geq 2$, one can also find infinitely many solutions to (4).

**Remark 3.3:** Let $s_i, s_j, s_i \neq s_j$, be simple singular values of $A$. Then $s_i \neq s_j$.

We will consider branches of selected singular values and corresponding left/right singular vectors $s_i(t), U_i(t) \in \mathbb{R}^m$, $V_i(t) \in \mathbb{R}^n$:

$$A(t)V_i(t) = s_i(t)U_i(t), \quad A(t)^TU_i(t) = s_i(t)V_i(t),$$

for $t \in [a, b]$. We will add the natural orthogonality conditions $U_i(t)V_i(t) = V_i(t)^TU_i(t) = 0, \ i \neq j, \ t \in [a, b]$. We are interested in $p, \ p \leq n$, selected singular values $S(t) = (s_1(t), \ldots, s_p(t)) \in \mathbb{R}^p$, and in the corresponding left/right singular vectors $U(t) = [U_1(t), \ldots, U_p(t)] \in \mathbb{R}^{m \times p}$, $V(t) = [V_1(t), \ldots, V_p(t)] \in \mathbb{R}^{n \times p}$ as $t \in [a, b]$. 

In the operator setting, let
\begin{equation}
F : \mathbb{R} \times \mathbb{R}^p \times \mathbb{R}^{m \times p} \times \mathbb{R}^{n \times p} \rightarrow \mathbb{R}^{m \times p} \times \mathbb{R}^{p \times p} \times \mathbb{R}^{p \times p} \times \mathbb{R}^{p \times p}
\end{equation}
be defined as
\begin{equation}
F(t, X) \equiv (A(t)V - U\Sigma, A^T(t)U - V\Sigma, U^T(U - I), V^T V - I),
\end{equation}
where \( X \equiv (S, U, V) \in \mathbb{R}^p \times \mathbb{R}^{m \times p} \times \mathbb{R}^{n \times p} \), \( \Sigma = \text{diag}(S) \) and \( I \in \mathbb{R}^{p \times p} \) is the identity. Under certain assumptions, the set of overdetermined nonlinear equations
\begin{equation}
F(t, X) = 0
\end{equation}
implicitly defines a curve in \( \mathbb{R} \times \mathbb{R}^N \), where \( \mathbb{R}^N, N = p(1 + m + n) \), and \( \mathbb{R}^p \times \mathbb{R}^{m \times p} \times \mathbb{R}^{n \times p} \) are isomorphic. The image of \( F \), namely \( \mathbb{R}^{m \times p} \times \mathbb{R}^{p \times p} \times \mathbb{R}^{p \times p} \), and \( M, M = p(m + n + 2p) \), are isomorphic.

The curve (7) can be parameterized by \( t \) i.e., \( t \mapsto X(t) = (S(t), U(t), V(t)) \) so that \( F(t, X(t)) = 0 \) as \( t \in [a, b] \). Given a solution \( X(t) \) at \( t = a \), the curve is initialized. For this purpose, we may select \( p \) singular values and left/right singular vectors computed via the classical SVD of the matrix \( A(a) \).

We have in mind mainly the application when \( m \geq n \), \( n \) is large while \( p \) is comparatively small. We also want to exploit sparsity of \( A(t) \) as \( t \in [a, b] \).

We will apply tangent continuation, see [3], Algorithm 4.25, p. 107. It is a predictor-corrector algorithm with an adaptive stepsize control. As far as the implementation is concerned, the corrector is crucial. We will discuss it in next section.

IV. SOLVING DEFINING EQUATIONS

The role of our corrector is to find a root of \( F(t, X) = 0 \) for a fixed \( t \). The dependence on the parameter \( t \) is suppressed in this section.

A. Gauss-Newton method

The idea is to use Newton’s method to find the root. We consider the differential \( DF \) of \( F \) at \( X = (S, U, V) \) in the direction \( \delta X = (\delta S, \delta U, \delta V) \). \( \delta S \in \mathbb{R}^p, \delta U \in \mathbb{R}^{m \times p} \) and \( \delta V \in \mathbb{R}^{n \times p} \). The notation reflects calculus of variations i.e. the \( \delta \)'s are the increments. The increment \( \delta S \in \mathbb{R}^p \) can be identified with an increment of the diagonal matrix \( \delta \Sigma = \text{diag}(\delta S) \in \mathbb{R}^{p \times p} \).

The differential \( DF \) in the direction \( \delta X = (\delta S, \delta U, \delta V) \) is a linear operator
\begin{equation}
G : \mathbb{R}^p \times \mathbb{R}^{m \times p} \times \mathbb{R}^{n \times p} \rightarrow \mathbb{R}^{m \times p} \times \mathbb{R}^{p \times p} \times \mathbb{R}^{p \times p} \times \mathbb{R}^{p \times p}
\end{equation}
where
\begin{align}
G_1(\delta X) & \equiv A\delta V - \delta U \Sigma - U \delta \Sigma, \\
G_2(\delta X) & \equiv A^T \delta U - \delta V \Sigma - V \delta \Sigma, \\
G_3(\delta X) & \equiv \delta U^T U + \delta U^T \delta U, \\
G_4(\delta X) & \equiv \delta V^T V + \delta V^T \delta V,
\end{align}
and \( \Sigma = \text{diag}(S), \delta \Sigma = \text{diag}(\delta S) \) and \( A = A(t) \). Let \( G^* : \mathbb{R}^{m \times p} \times \mathbb{R}^{n \times p} \times \mathbb{R}^{p \times p} \times \mathbb{R}^{p \times p} \rightarrow \mathbb{R}^{p} \times \mathbb{R}^{m \times p} \times \mathbb{R}^{n \times p} \).

The action of the dual is defined as
\begin{equation}
R \in \mathbb{R}^{m \times p}, Y \in \mathbb{R}^{n \times p}, W \in \mathbb{R}^{p \times p}, Z \in \mathbb{R}^{p \times p} \mapsto
\end{equation}
where
\begin{equation}
G^*_1(R, Y, W, Z) \equiv \sum_{k=1}^{m} u_{k1}r_{k1} + \sum_{k=1}^{n} u_{k1}y_{k1} + \sum_{k=1}^{m} u_{kp}\bar{r}_{kp} + \sum_{k=1}^{n} u_{kp}\bar{y}_{kp},
\end{equation}
\begin{equation}
G^*_2(R, Y, W, Z) \equiv -R\Sigma^T + AY + U(W^T + W),
\end{equation}
\begin{equation}
G^*_3(R, Y, W, Z) \equiv -Y\Sigma^T + A^T R + V(Z^T + Z),
\end{equation}
\begin{equation}
u_{kj}, r_{kj}, v_{kj} \text{ and } y_{kj} \text{ are the relevant elements of matrices } U, R, V \text{ and } Y, \text{ and } \Sigma = \text{diag}(S), A = A(t).
\end{equation}

In order to simplify notation, we identify triplets \( (S, U, V) \) in \( \mathbb{R}^p \times \mathbb{R}^{m \times p} \times \mathbb{R}^{n \times p} \) with vectors \( X \in \mathbb{R}^N, N = p(1 + m + n + 2p) \). Therefore \( F \), if (6), is interpreted as \( F : \mathbb{R}^N \rightarrow \mathbb{M}, M = p(m + n + 2n) \). Similarly, differential \( G \), see (8), and its dual \( G^* \), see (14), are maps \( G : \mathbb{R}^N \rightarrow \mathbb{M} \) and \( G^* : \mathbb{M} \rightarrow \mathbb{R}^N \), respectively.

A solution \( (S, U, V) \) to (6) can be identified with a root \( X^* \in \mathbb{R}^N \) of \( F : \mathbb{R}^N \rightarrow \mathbb{M} \). In order to find roots of \( F \), we consider Gauss-Newton method for nonlinear least-squares problem namely, we define
\begin{equation}
X^* = \min_{X \in \mathbb{R}^N} \| F(X) \|_2^2,
\end{equation}
see [3] p 92, as a local minimizer on \( \mathbb{R}^N, \| \cdot \|_2 \) is the Euclidean norm on \( \mathbb{M} \). The method approximates \( X^* \) by a sequence \( \{ X(j) \}_{j=0}^{\infty} \) of \( X(j) \in \mathbb{R}^N \), which is defined by the recurrence
\begin{equation}
G(X(j))^{T}G(X(j))\delta X = -G(X(j))^{T}F(X(j)),
\end{equation}
\begin{equation}
X(j+1) = X(j) + \delta X.
\end{equation}
Solving the equation (21) for \( \delta X \in \mathbb{R}^N \) represents a linear least-squares problem.

We say that the root \( X = (S, U, V) \) of \( F \) is simple provided that the differential of \( F \) at \( X \) has full rank i.e., \( \text{rank}(G(X)) = N \).

**Theorem 4.1:** Let \( X = (S, U, V) \), \( S = (s_1, \ldots, s_p) \), be a root of \( F \). Then \( \text{rank}(G(X)) = N \) if and only if all singular values of \( A \) are simple (i.e., \( s_i \) is a simple singular value of \( A \) for each \( i = 1, \ldots, p \)).

We postpone the proof to subsection IV-B.

**Corollary 4.1:** If \( X^* \in \mathbb{R}^N \) is a simple root of \( F \) then the iterations \( X(j) \) in (21), (22) are locally convergent. The rate of convergence is quadratic.

**Proof:** The result follows from [3], Theorem 4.14, p 94.

The inner loop of our algorithm consists of solving the linear least-squares problem
\begin{equation}
G(X)^{T}G(X)\delta X = -G(X)^{T}F(X)
\end{equation}
for $\delta X \in \mathbb{R}^N$ as $X \equiv X^{(j)} \in \mathbb{R}^N$, see (21). Ready-made algorithms for solving linear least-squares problems are based on conjugate gradients, see section Normal equation approaches in [4], in particular the algorithms CGNR on p. 545 and CGNE on p. 546.

The complication is that the matrices $G(X)$ and $G(X)^T$ in (23) namely the linear operators

$$G(X): \mathbb{R}^N \rightarrow \mathbb{R}^M, \quad G^*(X) \equiv G(X)^T: \mathbb{R}^M \rightarrow \mathbb{R}^N$$

are not available in cartesian coordinates on $\mathbb{R}^N$ and $\mathbb{R}^M$. They are defined by actions as linear operators (8) and (14).

Observe that in the algorithms like CGNR or CGNE one needs to define just the action of $G(X)$ or $G(X)^T$ on a righthand side. In our code, we have used MATLAB functionLSQR, see MATLAB Function Reference, which is a modification of CGNE. One of the options is that you may define $G(X)$ and $G(X)^T$ by actions as linear operators in arbitrary coordinates e.g. in the format of (8) and (14).

Note that the actions of both $G = G(X)$ and $G^* = G^*(X)$ are composed from the actions of $A(t)$ and $A^T(t)$ on vectors from $\mathbb{R}^p$ and $\mathbb{R}^m$. Therefore, we may use the assumption that $A(t)$ and $A^T(t)$ are sparse when evaluating their actions.

B. Simplicity of the root

The aim is to prove Theorem 4.1. First, we analyze $\ker G(X)$:

**Lemma 4.1:** Let $X = (S, U, V)$, $S = (s_1, \ldots, s_p)$, be a root of $F$. Let $G(X)\delta X$ be the differential of $F$ at $X$ in a direction $\delta X = (\delta S, \delta U, \delta V)$. Let $\delta U_i$, $\delta V_i$, $U_i$ and $V_i$ denote the $i$-th column of $\delta U$, $\delta V$, $U$ and $V$ as $i = 1, \ldots, p$. Then $\delta X = (\delta S, \delta U, \delta V)$ is in $\ker G(X)$ if and only if $\delta S = 0$ and

$$\mathcal{M}(s_i) \begin{pmatrix} \delta U_i \\ \delta V_i \end{pmatrix} = 0, \quad U_i^T \delta U_i = 0, \quad V_i^T \delta V_i = 0 \quad (25)$$

for $i = 1, \ldots, p$ and

$$U_j^T \delta U_i + U_i^T \delta U_j = 0, \quad V_j^T \delta V_i + V_i^T \delta V_j = 0 \quad (26)$$

for $i, j = 1, \ldots, p$, $i \neq j$.

**Proof:** Let $\delta X = (\delta S, \delta U, \delta V)$ be in $\ker G(X)$. Let us substitute $Z \equiv U^T \delta U$ and $W \equiv V^T \delta V$. Then

$$Z + Z^T = 0, \quad W + W^T = 0 \quad (27)$$

due to (12) and (13).

By (11), $A^T \delta U - V \delta S - V \delta \Sigma = 0$. Therefore, $V^T A^T \delta U - V^T \delta V \Sigma - V^T \delta V \Sigma = V^T A^T \delta U - W \Sigma - \delta \Sigma = 0$. This equation being transposed yields $\delta U^T A V - W \Sigma - \delta \Sigma = 0$. Since we assume $AV = U \Sigma$, see (6)&(7), then $\delta U^T U \Sigma - \Sigma W^T - \delta \Sigma = Z^T Z - \Sigma W^T - \delta \Sigma = 0$. We conclude that $\delta \Sigma = \Sigma W - \Sigma Z$. (29)

Since $Z$ and $W$ are antisymmetric, see (28), diagonal entries vanish:

$$Z_{ii} = 0, \quad W_{ii} = 0, \quad i = 1, \ldots, p.$$ (30)

Therefore, the diagonal entries of $\delta \Sigma$ vanish i.e., $\delta S = 0 \in \mathbb{R}^p$. Due to (10) and (11), we may resume that

$$A^T \delta U - V \delta S - V \delta \Sigma = 0.$$ (31)

If we adopt suggested notation for $\delta U_i$, $\delta V_i$, $U_i$ and $V_i$ then (25) follows from (31) and (30), and (26) from (6)&(7). The conditions (27) follow from (12) and (13).

If $\delta X = (\delta S, \delta U, \delta V)$ so that $\delta S = 0$ and both $\delta U$ and $\delta V$ satisfy (25)-(27) then it is easy to check that $\delta X \in \ker G(X)$.

As a preliminary to the next lemma let us note that rank$(G(X)) = N$ if and only if dim$\ker(G(X)) = 0$.

**Lemma 4.2:** Let $X = (S, U, V)$, $S = (s_1, \ldots, s_p)$, be a root of $F$. If $s_i$ is a simple singular value of $A$ for all $i \in \{1, \ldots, p\}$ then rank$(G(X)) = N$.

**Proof:** Let $\delta X = (\delta S, \delta U, \delta V)$, $G(X)\delta X = 0$. Let $U_i$, $V_i$, $\delta U_i$ and $\delta V_i$ be the $i$-th columns of $U$, $V$, $\delta U$ and $\delta V$. Let $s_i = S_i$, $S_i$ and $\delta S_i$ be the $i$-th components of $S$ and $\delta S$. Due to Lemma 4.1, $\delta S_i = 0$ and the vectors $U_i$, $V_i$, $\delta U_i$ and $\delta V_i$ satisfy (25) & (26).

Let $s_i \neq 0$ be a simple singular value. Referring to Remark 3.2, dim$\ker M(s_i) = 1$. In particular, $\ker M(s_i) = \text{span} \begin{pmatrix} U_i \\ V_i \end{pmatrix}$, see (26). Obviously, (25) implies $\delta U_i = 0$ and $\delta V_i = 0$.

Let $s_i = 0$ be a simple singular value. As a consequence of (26), $V_i \in \ker A$ and $U_i \in \ker A^T$. Following Lemma 3.4, $A = \text{span} \{V_i\}$ and $A^T = \text{span} \{U_i\}$. Due to (25), $\delta V_i \in \ker A$, $V_i^T \delta V_i = 0$ and $\delta U_i \in \ker A^T$, $U_i^T \delta U_i = 0$. Therefore, $\delta V_i = 0$ and $\delta U_i = 0$.

We may resume that $\delta X = (\delta S, \delta U, \delta V) = 0$. It means that dim$\ker G(X) = 0$ and hence rank$(G(X)) = N$.

**Lemma 4.3:** Let $X = (S, U, V)$, $S = (s_1, \ldots, s_p)$, be a root of $F$. Let there exists $i \in \{1, \ldots, p\}$ such that $s_i \neq 0$ is a nonsimple singular value of $A$. Then dim$\ker G(X)$ is $\geq 1$.

1) if $s_i \neq \pm s_j$ for all $j \neq i$, $j = 1, \ldots, p$, then dim$\ker G(X)$ is $\geq 1$,

2) if there exists $j \in \{1, \ldots, p\}$, $j \neq i$, such that $s_i = s_j$ or $s_i = -s_j$ while $s_i \neq \pm s_k$ for all $k \neq i$, $k \neq j$, $k = 1, \ldots, p$, then dim$\ker G(X)$ is $\geq 1$.

**Proof:** We are going to construct particular vectors $\delta X = (\delta S, \delta U, \delta V)$ from $\ker G(X)$. Due to Lemma 4.1, $\delta S = 0$.

Ad case 1: Let $U_i$ and $V_i$ denote the $i$-th column of $U$ and $V$. Note that (26) is satisfied. By the assumption on $s_i$, dim$\ker M(s_i) \geq 2$, see Remark 3.1. Therefore, except of $(U_i; V_i)^T \in \mathbb{R}^{m+n}$ there exists an additional linearly independent vector $(\delta U_i; (\delta V_i)^T \in \mathbb{R}^{m+n}$ in $\ker M(s_i)$ i.e.,

$$\begin{pmatrix} U_i \\ V_i \end{pmatrix}, \begin{pmatrix} \delta U_i \\ \delta V_i \end{pmatrix} \subset \ker M(s_i).$$

We may assume that the eigenvectors are orthogonal i.e., $U_i^T \delta U_i + V_i^T \delta V_i = 0$. We may also assume that $\|\delta U_i\| = 1$, $\|\delta V_i\| = 1$ and $U_i^T \delta U_i = V_i^T \delta V_i$, see Lemma 3.1. Lemma 3.2. Therefore, $U_i^T \delta U_i = 0$ and $V_i^T \delta V_i = 0$.

Consider the matrices $\delta U \in \mathbb{R}^{m \times p}$ and $\delta V \in \mathbb{R}^{n \times p}$ of the form

$$\delta U \equiv [0, \ldots, 0, \delta U_i, 0, \ldots, 0], \quad \delta V \equiv [0, \ldots, 0, \delta V_i, 0, \ldots, 0]$$

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that consist of zero columns except of the $i$-th column with the prescribed entries. The claim is that $\delta X \equiv (\delta S = 0, \delta U, \delta V)$ belongs to $\ker G(X)$.

Due to Lemma 4.1, we have to verify (25), (26), (27). The conditions (25) and (26) follow from definition of $\delta U$, $\delta V$. Hence it remains to check (27) namely that $U^T \delta U_i = 0$, $V^T \delta V_i = 0$, $j \neq i$.

Recall that

$$AV_j = s_j U_j, \quad A^T U_j = s_j V_j, \quad V^T V_j = 1, \quad j \neq i, \quad (32)$$

$$A \delta V_i = s_i \delta U_i, \quad A^T \delta U_i = s_i \delta V_i, \quad \delta V_i^T \delta V_i = 1, \quad j \neq i. \quad (33)$$

Then multiplying (33) by $U^T_j$ and $V^T_i$, and (32) by $U^T_j$ and $\delta V^T_i$ yields

$$U^T_i A \delta V_i = s_i U^T_i \delta U_i, \quad V^T_i A^T \delta U_i = s_i V^T_j \delta V_i$$

$$\delta U^T_i A V_j = s_j \delta U^T_i U_j, \quad \delta V^T_i A^T U_j = s_j \delta V^T_i V_j$$

Therefore

$$s_i U^T_j \delta U_i = s_j V^T_j \delta V_i, \quad s_j U^T_j \delta U_i = s_i V^T_j \delta V_i$$

i.e.,

$$\begin{pmatrix} s_i - s_j \\ -s_j \\ s_i \end{pmatrix} \begin{pmatrix} U^T \delta U_i \\ V^T \delta V_i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \det(s_i^2 - s_j^2) \neq 0$$

(34)

Hence $U^T_i \delta U_i = 0$, $V^T_i \delta V_i = 0$, $j \neq i$.

Ad case 2: Let $U_i$ and $V_i$ denote the $i$-th column of $U$ and $V$. Let $U_j$ and $V_j$ denote the $j$-th column of $U$ and $V$. Assume $i < j$ without loss of generality.

Consider the matrices $\delta U \in \mathbb{R}^{m \times p}$ and $\delta V \in \mathbb{R}^{n \times p}$ of the form

$$\delta U \equiv [0, \ldots, 0, a, 0, \ldots, 0, b, 0, \ldots, 0], \quad \delta V \equiv [0, \ldots, 0, b, 0, \ldots, 0]$$

which consist of zero columns except of the $i$-th column which is equal to $a \in \mathbb{R}^m$ and $c \in \mathbb{R}^n$, and the $j$-th column which is equal to $b \in \mathbb{R}^m$ and $d \in \mathbb{R}^n$.

Let $s_i = -s_j$. Given real $\alpha$ and $\beta$, let $\delta X \equiv (\delta S = 0, \delta U, \delta V)$ for the setting $a = \alpha U_j$, $b = \beta U_i$, $c = -\alpha V_j$, $d = -\beta V_i$. Let us apply Lemma 4.1 in order to check that $\delta X \in \ker G(X)$: Verifying (25)\&(27) choose, say, $k$ and $l$ as the current indices since $i$ and $j$ are fixed already.

Obviously, (25)\&(26) are satisfied. Let us check (27).

In order to verify (27) for the fixed $i$ and arbitrary $k$, $k \neq i$, $k \neq j$, i.e., the claim that $U^T_k \delta U_i = 0$, $V^T_k \delta V_i = 0$, we use the same argument as on lines (32)-(34). It remains to verify (27) for the selected indices $i$ and $j$. In that case the condition reads

$$U^T \delta U_i + U^T \delta U_j = \alpha U^T U_j + \beta U^T U_i = 0$$

$$V^T \delta V_i + V^T \delta V_j = -\alpha V^T V_j - \beta V^T V_i = 0.$$ Setting $\alpha = 1$ and $\beta = -1$ the remaining condition is satisfied and hence we constructed a nontrivial $\delta X \in \ker G(X)$.

If $s_i = s_j$, the argument is similar.

Lemma 4.4: Let $X = (S, U, V)$, $S = (s_1, \ldots, s_p)$, be a root of $F$. Let there exists $i \in \{1, \ldots, p\}$ such that $s_i = 0$ is a nonsimple singular value of $A$. Then $\ker G(X) \geq 1$.

In particular

1) if $s_j \neq 0$ for all $j \neq i$, $j = 1, \ldots, p$, and $m = n$ then $\dim \ker G(X) \geq 2$.
2) if $s_j \neq 0$ for all $j \neq i$, $j = 1, \ldots, p$, and $m > n$ then $\dim \ker G(X) \geq m - n$.
3) if there exists $j \in \{1, \ldots, p\}$, $j \neq i$, such that $s_j = 0$ while $s_k \neq 0$ for all $k \neq i$, $k \neq j$, $k = 1, \ldots, p$, then $\dim \ker G(X) \geq 1$.

Proof: We construct particular vectors $\delta X = (\delta S, \delta U, \delta V)$ from $\ker G(X)$. Due to Lemma 4.1, $\delta S = 0$. Let $U_i$ and $V_i$ denote the $i$-th column of $U$ and $V$.

Assume $s_i \neq 0$ for all $j \neq i$, $j = 1, \ldots, p$, see case 1 and 2. From Lemma 3.4 it follows that either $m = n$, dim $\ker A \geq 2$ or $m > n$, dim $\ker A \geq 1$. This characterizes case 1 and case 2.

Ad case 1: There exists $\delta V_i \in \ker A$ such that $\|\delta S\| = 0$ and $\|\delta V\| = 0$. Moreover, there exists $\delta U_i \in \ker A^T$ such that $\|\delta U\| = 1$ and $U^T \delta U = 0$.

Consider the matrices $\delta U \in \mathbb{R}^{m \times p}$ and $\delta V \in \mathbb{R}^{n \times p}$ of the form

$$\delta U \equiv [0, \ldots, 0, 0, a, 0, \ldots, 0], \quad \delta V \equiv [0, \ldots, 0, b, 0, \ldots, 0]$$

which consist of zero columns except of the $i$-th column with the prescribed entries from $a \in \mathbb{R}^m$ and $b \in \mathbb{R}^n$.

The claim is that $\delta X_i \equiv (\delta S = 0, \delta U, \delta V)$ for the setting $a = \delta U_i$, $b = 0$ and $\delta X_2 \equiv (\delta S = 0, \delta U, \delta V)$ for the setting $a = 0$, $b = \delta V_i$ belong to $\ker G(X)$. Obviously, $\delta X_1$ and $\delta X_2$ are linearly independent. The proof of the claim follows from Lemma 4.1 namely, we have to verify (25), (26) and (27) for the appropriate $\delta X \equiv \delta X_1$ and $\delta X \equiv \delta X_2$.

The conditions (25)\&(26) are satisfied due to definition of $\delta U$ and $\delta V$. It remains to check (27): Recall (32). Then multiplying (32) by $U^T_i$ and $V^T_i$ yield

$$\delta U^T_i A V_j = s_j \delta U^T_i U_j, \quad \delta V^T_i A^T U_j = s_j \delta V^T_i V_j, \quad j \neq i.$$ By definition of $\delta U_i$ and $\delta V_i$, $\delta U^T_i A V_j = 0$ and $\delta V^T_i A^T U_j = 0$. Since $s_j \neq 0$ for $j \neq i$ then $\delta U^T_i U_j = 0$ and $\delta V^T_i V_j = 0$, which verifies (27).

Ad case 2: If $k = \dim \ker A$ then $k \geq 1$ and $\dim \ker A^T = m - n + k \geq m - n + 1 \geq 2$. Therefore, there exists $\delta U_i \in \mathbb{R}^m$ such that $\|\delta U\| = 1$ and $U^T \delta U = 0$. Let $\delta U \equiv [0, \ldots, 0, \delta U_i, 0, \ldots, 0] \in \mathbb{R}^{m \times p}$ be composed from zero columns except of the $i$-th column with the prescribed entries. Let $\delta V \in \mathbb{R}^{n \times p}$ be the zero matrix. The claim is that $\delta X \equiv (\delta S = 0, \delta U, \delta V)$ belongs to $\ker G(X)$. The proof of the claim follows from Lemma 4.1. It proves that $\dim \ker G(X) \geq 1$. From the construction of $\delta U_i$, it is clear that $\delta U_i$ is chosen from $(m - n)$-dimensional space of candidates. Therefore, $\dim \ker G(X) \geq m - n$.

Ad case 3: Assume $i < j$ without loss of generality. Consider the matrices $\delta U \in \mathbb{R}^{m \times p}$ and $\delta V \in \mathbb{R}^{n \times p}$ of the form

$$\delta U \equiv [0, \ldots, 0, a, 0, \ldots, 0, b, 0, \ldots, 0], \quad \delta V \equiv [0, \ldots, 0, c, 0, \ldots, 0, d, 0, \ldots, 0]$$
which consist of zero columns except of the $i$-th column which is equal to $a \in \mathbb{R}^m$ and $c \in \mathbb{R}^n$, and the $j$-th column which is equal to $b \in \mathbb{R}^m$ and $d \in \mathbb{R}^n$.

The claim is that $\delta X \equiv (\delta S = 0, \delta U, \delta V)$ for the setting $a = U_j, b = -U_i, c = V_j, d = -V_i$ belongs to $\text{Ker } G(X)$.

The proof of the claim follows from Lemma 4.1 namely, we have to verify (25), (26) and (27) for the appropriate $\delta X$. The argument is similar to the proof of Lemma 4.3, Ad case 2.

**Proof of Theorem 4.1**

- Due to Lemma 4.2, the simplicity of all singular values yield full rank of $G(X)$.
- Lemma 4.3 and 4.4 imply that the simplicity of all singular values is the necessary condition for $G(X)$ to have full rank.

### V. Continuation Algorithm

We will briefly sketch the implementation of tangent continuation, see [2], Algorithm 4.25, p. 107. Let $(t, X)$ satisfy (6) & (7).

**Predictor step:** Find $\delta X \in \mathbb{R}^p \times \mathbb{R}^{m \times p} \times \mathbb{R}^{n \times p}$ such that

$$F_X(t, X) \delta X = -F_t(t, X),$$

where $F_X$ and $F_t$ are partial differentials of $F$ with respect to state $X$ and time $t$ at the point $(t, X)$. In the notation of Section IV, $F_X(t, X) = G(X)$ and the action of $F_X(t, X)$ on $\delta X$ is defined via (9). Let us note that

$$F_t(t, X) = (A'(t)V, (A'(t))^T U) \in \mathbb{R}^{p \times p}, 0 \in \mathbb{R}^{p \times p}$$

$$X = (S, U, V).$$

This particular $\delta X$ can be interpreted as the tangent to the curve implicitly defined by (6) & (7) at $(t, X)$. We will consider $\delta X$ to be least-squares solution to (35),

$$G(X)^T G(X) \delta X = -G(X)^T F_t(t, X), \quad G(X) \equiv F_X(t, X),$$

compare with (23). Let us assume that $X = (S, U, V), S = (s_1, \ldots, s_p), s_i$ be simple singular values of $A(t)$ for each $i = 1, \ldots, p$. Due to Theorem 4.1, the solution $\delta X$ to (35) and to (36) are the same.

Given a small time increment $\delta t > 0$, we set

$$X^0 = X + \delta t \delta X, \quad t := t + \delta t$$

(37)
to be the predictor.

**Corrector step:** Generate the sequence $\{X^{(i)}\}_{i=0}^\infty$ of $X^{(i)} \in \mathbb{R}^n$, see (21) & (22), up to the required convergence. In (21) & (22), it is understood that $F(X^{(i)}) \equiv F(t, X^{(i)}), G(X^{(i)}) \equiv F_X(t, X^{(i)})$ for just updated $t$ in (37).

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