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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 $A \in \mathbb{R}^{m\times n}$, $m \geq n$, 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 $\Sigma = \mathrm{diag}(\mathrm{s_1}, \ldots, \mathrm{s_n}) \in \mathbb{R}^{m\times n}$. 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

$$A(t) = U(t)\Sigma(t)V(t)^T, \tag{1}$$

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

In [2], it is shown that real analytic matrix 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 $\Sigma(t) = \mathrm{diag}(\mathrm{s_1(t)}, \ldots, \mathrm{s_n(t)}) \in \mathbb{R}^{m\times n}$ 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 by arbitrary.

II. Related Work

The generic scenario is that the branches $t \longmapsto s_i(t)$ 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 $H : \mathbb{R}\times\mathbb{R}^N \to \mathbb{R}^N$ 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].

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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

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

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

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

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 $\dim \mathrm{Ker}\, \mathcal{M}(s) \geq 1$.

Lemma 3.1: Let $s \neq 0$, $\mathcal{M}(s) \begin{pmatrix} u \\ v \end{pmatrix} = 0$. Then $u^T u = v^T v$.

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

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

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

$$u^T u = -\frac{1}{s} u^T A v\,, \quad v^T v = -\frac{1}{s} v^T A^T u\,.$$

Note that $v^T A^T u = (Av)^T u = u^T A v$. Therefore, $u^T u - v^T v = -\frac{1}{s}(u^T A v - u^T A v) = 0$. ■

Lemma 3.2: Let $s \neq 0$, $\mathcal{M}(s) \begin{pmatrix} u \\ v \end{pmatrix} = 0$, $\mathcal{M}(s) \begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix} = 0$. Then $u^T \tilde{u} = v^T \tilde{v}$.

Proof: We assume

$$-su + Av = 0\,, \quad A^T u - sv = 0\,,$$
$$-s\tilde{u} + A\tilde{v} = 0\,, \quad A^T \tilde{u} - s\tilde{v} = 0\,.$$

Therefore,

$$\tilde{u}^T(-su + Av) = 0\,, \quad \tilde{v}^T(A^T u - sv) = 0\,,$$
$$u^T(-s\tilde{u} + A\tilde{v}) = 0\,, \quad v^T(A^T \tilde{u} - s\tilde{v}) = 0\,.$$

Since $s \neq 0$,

$$\tilde{u}^T u = -\frac{1}{s}\tilde{u}^T A v\,, \quad \tilde{v}^T u = -\frac{1}{s}\tilde{v}^T A^T u = -\frac{1}{s}(A\tilde{v})^T u$$

and

$$u^T \tilde{u} = -\frac{1}{s} u^T A \tilde{v}\,, \quad v^T \tilde{v} = -\frac{1}{s} v^T A^T \tilde{u} = -\frac{1}{s}(Av)^T \tilde{u}\,.$$

We conclude that

$$\tilde{u}^T u - v^T \tilde{v} = -\frac{1}{s}\tilde{u}^T A v + \frac{1}{s}(Av)^T \tilde{u}\,.$$

Since $v^T \tilde{v} = \tilde{v}^T v$ and $(Av)^T \tilde{u} = \tilde{u}^T A v$,

$$\tilde{u}^T u - \tilde{v}^T v = 0\,.$$

■

Definition 3.3: We say that $s \in \mathbb{R}$ is a simple singular value of a matrix A if there exist $u \in \mathbb{R}^m$ and $v \in \mathbb{R}^n$ such that

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

are the only solutions to (2). A singular value s which is not a simple singular value is called nonsimple (multiple) singular value.

Lemma 3.3: A triplet $s \neq 0$, $u \in \mathbb{R}^m$ and $v \in \mathbb{R}^n$ satisfy (2) if and only if

$$A^T A v = s^2 v\,, \quad u = \frac{1}{s} A v\,, \quad \|v\| = 1\,, \quad s \neq 0\,. \qquad (3)$$

Proof: Let $s \neq 0$, u and v satisfy (2). From the first equation in (2), $Av - su = 0$, we conclude that $0 = A^T(Av - su) = A^T A v - sA^T u = A^T A v - s^2 v$ since $A^T u = sv$. Moreover, $su = Av$, i.e. $u = \frac{1}{s} Av$.

Let $s \neq 0$, u and v satisfy (3). Then $A^T u - sv = A^T(\frac{1}{s}Av) - sv = \frac{1}{s}A^T A v - sv = sv - sv = 0$ and $Av - su = Av - s(\frac{1}{s}Av) = Av - Av = 0$. Finally, $u^T u = u^T(\frac{1}{s}Av) = \frac{1}{s}u^T A v = \frac{1}{s}(A^T u)^T v = \frac{1}{s} s v^T v = 1$. ■

Note that a nonzero simple singular value s can be identified with a nonzero simple eigenvalue s^2 of the matrix $A^T A$, see Lemma 3.3.

Remark 3.2: Let $s \neq 0$. s is a simple singular value of A if and only if $\dim \mathrm{Ker}\, \mathcal{M}(s) = 1$.

Lemma 3.4: $s = 0$ is a simple singular value of A if and only if $m = n$ and $\dim \mathrm{Ker} A = 1$.

Proof: Let $m = n$, $\dim \mathrm{Ker} A = 1$. As a consequence, $\dim \mathrm{Ker} A^T = 1$. Then there exist $u \in \mathbb{R}^m$ and $v \in \mathbb{R}^n$ such that

$$Av = 0\,, \quad A^T u = 0\,, \quad \|u\| = \|v\| = 1\,, \qquad (4)$$

i.e. $(s = 0, u, v)$ satisfy (2). Clearly, $(s = 0, u, v)$ and $(s = 0, -u, -v)$ and $(s = 0, -u, v)$ and $(s = 0, u, -v)$ are the only possibilities to solve (2).

If $m > n$ then $\dim \mathrm{Ker} A^T \geq 2$ and hence (4) has infinitely many solutions. If $\dim \mathrm{Ker} A \geq 2$, 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 $s_i(t)$, $U_i(t) \in \mathbb{R}^m$, $V_i(t) \in \mathbb{R}^n$:

$$A(t)V_i(t) = s_i(t)U_i(t)\,, \quad A(t)^T U_i(t) = s_i(t)V_i(t)\,,$$
$$U_i(t)^T U_i(t) = V_i(t)^T V_i(t) = 1$$

for $t \in [a, b]$. We will add the natural orthogonality conditions $U_i(t)^T U_j(t) = V_i(t)^T V_j(t) = 0$, $i \neq j$, $t \in [a, b]$. 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

$$F : \mathbb{R} \times \mathbb{R}^p \times \mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p} \to \mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p} \times \mathbb{R}^{p\times p} \times \mathbb{R}^{p\times p} \tag{5}$$

be defined as

$$F(t, X) \equiv \left(A(t)V - U\Sigma, A^T(t)U - V\Sigma, U^TU - I, V^TV - I\right), \tag{6}$$

where $X \equiv (S, U, V) \in \mathbb{R}^p \times \mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p}$, $\Sigma = \mathrm{diag}(S)$ and $I \in \mathbb{R}^{p\times p}$ is the identity. Under certain assumptions, the set of *overdetermined nonlinear equations*

$$F(t, X) = 0 \tag{7}$$

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 $\mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p} \times \mathbb{R}^{p\times p} \times \mathbb{R}^{p\times p}$, and $\mathbb{R}^M$, $M = p(m + n + 2p)$, 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 $\delta\Sigma = \mathrm{diag}(\delta S) \in \mathbb{R}^{p\times p}$.

The differential DF in the direction $\delta X = (\delta S,\ \delta U,\ \delta V)$ is a linear operator

$$G : \mathbb{R}^p \times \mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p} \to \mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p} \times \mathbb{R}^{p\times p} \times \mathbb{R}^{p\times p} \tag{8}$$

The point $X = (S, U, V)$ is understood to be fixed and the dependence of G on the point is not explicitly marked. Let us describe the action of G:

$$\delta S \in \mathbb{R}^p,\ \delta U \in \mathbb{R}^{m\times p},\ \delta V \in \mathbb{R}^{n\times p} \longmapsto \tag{9}$$
$$\longmapsto G = (G_1, G_2, G_3, G_4),$$

where

$$G_1(\delta X) \equiv A\,\delta V - \delta U\,\Sigma - U\,\delta\Sigma, \tag{10}$$
$$G_2(\delta X) \equiv A^T\,\delta U - \delta V\,\Sigma - V\,\delta\Sigma, \tag{11}$$
$$G_3(\delta X) \equiv \delta U^T\,U + U^T\,\delta U, \tag{12}$$
$$G_4(\delta X) \equiv \delta V^T\,V + V^T\,\delta V, \tag{13}$$

$\Sigma = \mathrm{diag}(S)$, $\delta\Sigma = \mathrm{diag}(\delta S)$ and $A = A(t)$.

Let

$$G^* : \mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p} \times \mathbb{R}^{p\times p} \times \mathbb{R}^{p\times p} \to \mathbb{R}^p \times \mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p} \tag{14}$$

be the dual to G. The action of the dual is defined as

$$R \in \mathbb{R}^{m\times p},\ Y \in \mathbb{R}^{n\times p},\ W \in \mathbb{R}^{p\times p},\ Z \in \mathbb{R}^{p\times p} \longmapsto \tag{15}$$
$$G^* = (G_1^*, G_2^*, G_3^*),$$

where

$$G_1^*(R, Y, W, Z) \equiv \tag{16}$$
$$-\Big(\sum_{k=1}^{m} u_{k1}r_{k1} + \sum_{k=1}^{n} v_{k1}y_{k1}, \ldots, \sum_{k=1}^{m} u_{kp}r_{kp} + \sum_{k=1}^{n} v_{kp}y_{kp}\Big)^T, \tag{17}$$

$$G_2^*(R, Y, W, Z) \equiv -R\Sigma^T + AY + U(W^T + W), \tag{18}$$
$$G_3^*(R, Y, W, Z) \equiv -Y\Sigma^T + A^TR + V(Z^T + Z), \tag{19}$$

u_{kj}, r_{kj}, v_{kj} and y_{kj} are the relevant elements of matrices U, R, V and Y, and $\Sigma = \mathrm{diag}(S)$, $A = A(t)$.

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 $X \in \mathbb{R}^N$, $N = p(1+m+n)$. Therefore F, see (6), is interpreted as $F : \mathbb{R}^N \to \mathbb{R}^M$, $M = p(m + n + 2p)$. Similarly, differential G, see (8), and its dual G^*, see (14), are maps $G : \mathbb{R}^N \to \mathbb{R}^M$ and $G^* : \mathbb{R}^M \to \mathbb{R}^N$, respectively.

A solution (S, U, V) to (6) can be identified with a root $X^\star \in \mathbb{R}^N$ of $F : \mathbb{R}^N \to \mathbb{R}^M$. In order to find roots of F, we consider Gauss-Newton method for nonlinear least-squares problem namely, we define

$$X^\star = \arg \min_{X\in\mathbb{R}^N} \|F(X)\|_2^2, \tag{20}$$

see [3] p 92, as a local minimizer on $\mathbb{R}^N$; $\|\ \|_2$ is the Euclidean norm on $\mathbb{R}^M$. The method approximates $X^\star$ by a sequence $\{X^{(j)}\}_{j=0}^{\infty}$ of $X^{(j)} \in \mathbb{R}^N$, which is defined by the recurrence

$$G(X^{(j)})^T G(X^{(j)})\,\delta X = -G(X^{(j)})^T F(X^{(j)}), \tag{21}$$
$$X^{(j+1)} = X^{(j)} + \delta X. \tag{22}$$

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., $\mathrm{rank}(G(X)) = N$.

Theorem 4.1: Let $X = (S, U, V)$, $S = (s_1, \ldots, s_p)$, be a root of F. Then $\mathrm{rank}(G(X)) = N$ 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 $X^\star \in \mathbb{R}^N$ 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

$$G(X)^T G(X)\,\delta X = -G(X)^T F(X) \tag{23}$$

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

$$G(X) : \mathbb{R}^N \to \mathbb{R}^M\,, \quad G^*(X) \equiv G(X)^T : \mathbb{R}^M \to \mathbb{R}^N \quad (24)$$

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-function LSQR, 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 $\mathbb{R}^n$ 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 $\operatorname{Ker} G(X)$:

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 δU_i, δV_i, U_i and V_i denote the i-th column of δU, δV, U and V as $i = 1, \ldots, p$. Then $\delta X = (\delta S, \delta U, \delta V) \in \operatorname{Ker} G(X)$ if and only if $\delta S = 0$ and

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

$$\mathcal{M}(s_i) \begin{pmatrix} U_i \\ V_i \end{pmatrix} = 0\,, \quad \|U_i\| = \|V_i\| = 1\,, \quad (26)$$

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

$$U_i^T\,\delta U_j + U_j^T\,\delta U_i = 0\,, \quad V_i^T\,\delta V_j + V_j^T\,\delta V_i = 0 \quad (27)$$

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

Proof: Let $\delta X = (\delta S, \delta U, \delta V) \in \operatorname{Ker} G(X)$. Let us substitute $Z \equiv U^T\,\delta U$ and $W \equiv V^T\,\delta V$. Then

$$Z + Z^T = 0\,, \quad W + W^T = 0 \quad (28)$$

due to (12) and (13).

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

$$\delta\Sigma = \Sigma W - Z\Sigma\,. \quad (29)$$

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

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

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

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

If we adopt suggested notation for δU_i, δV_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 δU and δV satisfy (25)-(27) then it is easy to check that $\delta X \in \operatorname{Ker} G(X)$. ■

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

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 $\operatorname{rank}(G(X)) = N$.

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

Let $s_i \neq 0$ be a simple singular value. Referring to Remark 3.2, $\dim \operatorname{Ker} \mathcal{M}(s_i) = 1$. In particular, $\operatorname{Ker} \mathcal{M}(s_i) = \operatorname{span}\left\{ \begin{pmatrix} U_i \\ V_i \end{pmatrix} \right\}$, 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), $V_i \in \operatorname{Ker} A$ and $U_i \in \operatorname{Ker} A^T$. Following Lemma 3.4, $\operatorname{Ker} A = \operatorname{span}\{V_i\}$ and $\operatorname{Ker} A^T = \operatorname{span}\{U_i\}$. Due to (25), $\delta V_i \in \operatorname{Ker} A$, $V_i^T\delta V_i = 0$ and $\delta U_i \in \operatorname{Ker} A^T$, $U_i^T\delta U_i = 0$. 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 $\dim \operatorname{Ker} G(X) = 0$ and hence $\operatorname{rank}(G(X)) = N$. ■

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 $\dim \operatorname{Ker} G(X) \geq 1$. In particular

1) if $s_i \neq \pm s_j$ for all $j \neq i$, $j = 1, \ldots, p$, then $\dim \operatorname{Ker} G(X) \geq 1$,
2) if there exists $j \in \{1, \ldots, p\}$, $j \neq i$, such that either $s_i = s_j$ 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 $\dim \operatorname{Ker} G(X) \geq 1$.

Proof: We are going to construct particular vectors $\delta X = (\delta S, \delta U, \delta V)$ from $\operatorname{Ker} G(X)$. 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, $\dim \operatorname{Ker} \mathcal{M}(s_i) \geq 2$, 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 $\operatorname{Ker} \mathcal{M}(s_i)$ i.e.,

$$\left\{ \begin{pmatrix} U_i \\ V_i \end{pmatrix}, \begin{pmatrix} \delta U_i \\ \delta V_i \end{pmatrix} \right\} \subset \operatorname{Ker} \mathcal{M}(s_i)\,.$$

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

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

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 $\operatorname{Ker} G(X)$:

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

Recall that

$$AV_j = s_j U_j\,, \quad A^T U_j = s_j V_j\,, \quad V_j^T V_j = 1\,, \quad j \neq i\,, \tag{32}$$

$$A\,\delta V_i = s_i \delta U_i\,, \quad A^T \delta U_i = s_i \delta V_i\,, \quad \delta V_i^T \delta V_i = 1\,, \quad j \neq i\,. \tag{33}$$

Then multiplying (33) by U_j^T and V_j^T, and (32) by δU_j^T and δV_j^T yields

$$\begin{aligned} U_j^T A\,\delta V_i &= s_i U_j^T \delta U_i\,, \quad V_j^T A^T \delta U_i = s_i V_j^T \delta V_i \\ \delta U_i^T A V_j &= s_j \delta U_i^T U_j\,, \quad \delta V_i^T A^T U_j = s_j \delta V_i^T V_j \end{aligned}$$

Therefore

$$s_i U_j^T \delta U_i = s_j V_j^T \delta V_i\,, \quad s_j U_j^T \delta U_i = s_i V_j^T \delta V_i$$

i.e.,

$$\begin{pmatrix} s_i & -s_j \\ -s_j & s_i \end{pmatrix} \begin{pmatrix} U_j^T\,\delta U_i \\ V_j^T\,\delta V_i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \det(s_i^2 - s_j^2) \neq 0 \tag{34}$$

Hence $U_j^T\,\delta U_i = 0\,, \quad V_j^T\,\delta V_i = 0\,, \quad j \neq i$.

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

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

$$\delta V \equiv [0, \ldots, 0, c, 0, \ldots, 0, d, 0, \ldots 0]$$

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 $d \in \mathbb{R}^n$.

Let $s_i = -s_j$. Given real α and β, 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 $\delta X \in \operatorname{Ker} G(X)$: 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 $U_k^T\,\delta U_i = 0$, $V_k^T\,\delta V_i = 0$, 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

$$\begin{aligned} U_j^T\,\delta U_i + U_i^T\,\delta U_j &\equiv \alpha U_j^T U_j + \beta U_i^T U_i = 0 \\ V_j^T\,\delta V_i + V_i^T\,\delta V_j &\equiv -\alpha V_j^T V_j - \beta V_i^T V_i = 0\,. \end{aligned}$$

Setting $\alpha = 1$ and $\beta = -1$ the remaining condition is satisfied and hence we constructed a nontrivial $\delta X \in \operatorname{Ker} G(X)$.

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 $\dim \operatorname{Ker} G(X) \geq 1$. In particular

1) if $s_j \neq 0$ for all $j \neq i$, $j = 1, \ldots, p$, and $m = n$ then $\dim \operatorname{Ker} G(X) \geq 2$,
2) if $s_j \neq 0$ for all $j \neq i$, $j = 1, \ldots, p$, and $m > n$ then $\dim \operatorname{Ker} G(X) \geq m - n$,
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 $\dim \operatorname{Ker} G(X) \geq 1$.

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

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

Ad case 1: There exists $\delta V_i \in \operatorname{Ker} A$ such that $\|\delta V_i\| = 1$ and $V_i^T \delta V_i = 0$. Moreover, there exists $\delta U_i \in \operatorname{Ker} A^T$ such that $\|\delta U_i\| = 1$ and $U_i^T \delta U_i = 0$.

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

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

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

The claim is that $\delta X_1 \equiv (\delta S = 0, \delta U, \delta V)$ 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 $\operatorname{Ker} G(X)$. Obviously, δX_1 and δX_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 δU and δV. It remains to check (27): Recall (32). Then multiplying (32) by δU_i^T and δV_i^T yield

$$\delta U_i^T\,AV_j = s_j \delta U_i^T\,U_j\,, \quad \delta V_i^T\,A^T U_j = s_j \delta V_i^T\,V_j\,, \quad j \neq i\,.$$

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

Ad case 2: If $k = \dim \operatorname{Ker} A$ then $k \geq 1$ and $\dim \operatorname{Ker} A^T = m - n + k \geq m - n + 1 \geq 2$. Therefore, there exists $\delta U_i \in \mathbb{R}^m$ such that $\|\delta U_i\| = 1$ and $U_i^T \delta U_i = 0$. 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 $\operatorname{Ker} G(X)$. The proof of the claim follows from Lemma 4.1. It proves that $\dim \operatorname{Ker} G(X) \geq 1$. From the construction of δU_i, it is clear that δU_i is chosen from $(m-n)$-dimensional space of candidates. Therefore, $\dim \operatorname{Ker} G(X) \geq m - n$.

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

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

$$\delta V \equiv [0, \ldots, 0, c, 0, \ldots, 0, d, 0, \ldots 0]$$

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 $\operatorname{Ker} G(X)$.

The proof of the claim follows from Lemma 4.1 namely, we have to verify (25), (26) and (27) for the appropriate δX. 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 [3], 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

$$F_X(t, X)\,\delta X \;=\; -F_t(t, X)\,, \tag{35}$$

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 δX is defined via (9). Let us note that

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

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

$$G(X)^T G(X)\,\delta X \;=\; -G(X)^T\,F_t(t, X)\,, \quad G(X) \equiv F_X(t, X)\,, \tag{36}$$

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 δX to (35) and to (36) are the same.

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

$$X^0 \;=\; X \,+\, \delta t\,\delta X\,, \quad t := t \,+\, \delta t \tag{37}$$

to be the predictor.

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

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References

[1] E. Anderson, Z. Bay, J. Demmel, J. Dongara, J. D. Croz, A. Greenbaum, S. Hammarling, A. McKenney, S. Ostrouchov and D. Sorensen, *LAPACK User' Guide*, SIAM, Philadelphia, PA, USA, 1992

[2] A. Bunse-Gerstner, R. Byers, V. Mehrmann and N. K. Nichols, *Numerical Computation of an Analytic Singular Value Decomposition of a Matrix Valued Function*, Numer. Math. 60 (1991), pp. 1–39.

[3] P. Deuflhart and A. Hohmann, *Numerical Analysis in Modern Scientific Computing. An Introduction*, Springer Verlag, New York, 2003.

[4] G. H. Golub and C. F. van Loan, *Matrix Computations*, 3rd ed, The Johns Hopkins University Press, Baltimore, 1996.

[5] V. Janovský, D. Janovská, K. Tanabe, *Computing the Analytic Singular Value Decomposition via a pathfollowing*, submitted to: Proceedings of ENUMATH 2005

[6] T. Kato, *Perturbation Theory for Linear Operators, 2nd ed.*, Springer Verlag, New York, 1976.

[7] S. Krantz, H. Parks *A Primer of Real Analytic Functions*, Birkhauser, New York, 2002.

[8] V. Mehrmann and W. Rath, *Numerical Methods for the Computation of Analytic Singular Value Decompositions*, Electronic Transactions on Numerical Analysis, **1** (1993), pp. 72–88.

[9] K. Wright, *Differention equations for the analytic singular value decomposion of a matrix*, Numer. Math. 63 (1992), pp. 283–295.

[10] K. Wright, *Numerical solution of differential equations for the analytic singular value decomposion*, In: Bainov, D. and Covachev, V. (eds) Proceedings of the 1st International Colloquium on Numerical Analysis, Plovdiv, Bulgaria, 1992. VSP, Utrecht, pp. 131–140 (1993)

[11] K. Wright, *Recent developments in collocation methods for ordinary differential equations*, In: Bainov, D. and Covachev, V. (eds) Proceedings of the 5th International Colloquium on Differential Equations, Plovdiv, Bulgaria, 1994. VSP, Utrecht, pp. 353–362 (1995)