Numer. Math. 60, 1–39 (1991)

Numerische Mathematik

Numerical computation of an analytic singular value decomposition of a matrix valued function

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Received September 6, 1990/Revised version received June 10, 1991

Summary. This paper extends the singular value decomposition to a path of matrices $E(t)$. An analytic singular value decomposition of a path of matrices $E(t)$ is an analytic path of factorizations $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ where $X(t)$ and $Y(t)$ are orthogonal and $S(t)$ is diagonal. To maintain differentiability the diagonal entries of $S(t)$ are allowed to be either positive or negative and to appear in any order. This paper investigates existence and uniqueness of analytic SVD's and develops an algorithm for computing them. We show that a real analytic path $E(t)$ always admits a real analytic SVD, a full-rank, smooth path $E(t)$ with distinct singular values admits a smooth SVD. We derive a differential equation for the left factor, develop Euler-like and extrapolated Euler-like numerical methods for approximating an analytic SVD and prove that the Euler-like method converges.

Mathematics Subject Classification (1991): 65F20, 65F25, 65L05

1 Introduction

A singular value decomposition (SVD) of a constant matrix $E \in \mathbb{R}^{m\times n}$, $m \geqq n$, is a factorization $E = U\Sigma V^{\mathrm{T}}$ where $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ are orthogonal and $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \sigma_3, \ldots, \sigma_n)$. The singular values $\sigma_1, \sigma_2, \sigma_3, \ldots, \sigma_n$ may

* Partial support received from SFB 343, Diskrete Strukturen in der Mathematik, Universität Bielefeld

** Partial support received from FSP Mathematisierung, Universität Bielefeld

*** Partial support received from National Science Foundation grant CCR-8820882. Some support was also received from the University of Kansas through International Travel Fund 560478 and General Research Allocations #3758-20-0038 and #3692-20-0038.

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Offprint requests to: A. Bunse-Gerstner be chosen to be nonnegative and nonincreasing. An important tool in numerous applications, the SVD is well-studied and good numerical methods are available [4, 5, 6, 7, 16].

For a real analytic matrix valued function $E(t) : [a, b] \to \mathbb{R}^{m\times n}$, an analytic *SVD* (ASVD) is a path of factorizations

$$E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$$

where $X(t) : [a, b] \to \mathbb{R}^{m\times m}$ is orthogonal, $S(t) : [a, b] \to \mathbb{R}^{m\times n}$ is diagonal, $Y(t) : [a, b] \to \mathbb{R}^{m\times n}$ is orthogonal and $X(t)$, $S(t)$ and $Y(t)$ are analytic.

This paper presents conditions under which ASVD's exist, investigates the degrees of freedom in the choice of an ASVD, and derives a numerical method for tracking a particular ASVD.

The ASVD has applications in time dependent linear quadratic optimal control problems for descriptor systems [2, 9] and in differential algebraic equations [15]. A numerical method for the continuous time Riccati equation proposed in [9] need all three factors of an explicit smoothly varying SVD *and* the derivative of the right-hand factor.

In [15], Reinholdt uses the smoothly varying left nullspace of a matrix function $E(t)$ to construct a smoothly varying system of local charts on a manifold. He studies the problem of constructing a smooth QR-factorization $E(t) = Q(t)R(t)$ where $Q(t)$ is orthogonal and $R(t)$ is upper triangular. The columns of $Q(t)$ that span the left nullspace of $E(t)$ give the required local charts. A smoothly varying basis of the nullspace can also be obtained from a smooth SVD. Although the SVD is more expensive, it is considered to be more reliable for determining rank in the presence of rounding errors. In particular, a smooth SVD is more likely to detect that $E(t)$ "nearly" changes rank. Rank changes signal singularities in the underlying problem and near rank changes are associated with ill-conditioning [3, 17, 18].

The numerical method proposed in [15] uses a reference decomposition, $E(t_0) = Q(t_0)R(t_0)$. For other values of t, $Q(t)$ is chosen to minimize the Frobenius norm $\|Q(t) - Q(t_0)\| = \sqrt{\sum |q_{ij}(t) - q_{ij}(t_0)|^2}$ over all orthogonal factors $Q(t)$. Reinholdt gives explicit formulae for the minimizer and shows that under mild assumptions this choice follows a smooth path in a neighborhood of $t = t_0$. The method can easily be adapted to find a smooth SVD in a region around $t = t_0$. Unfortunately, even when a globally smooth SVD exists, the path generated by this method may not be smooth outside a neighborhood of $t = t_0$.

Example 1. For $t \in [0, \pi]$, define

$$E(t) = \begin{bmatrix} 3\cos(2t) + 1 & 3\sin(2t) \\ -3\sin(2t) & 3\cos(2t) - 1 \end{bmatrix}.$$

At $t_0 = 0$ select the reference SVD

$$E(0) = X(0)S(0)Y(0)^{\mathrm{T}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

The following path results from choosing $X(t)$ to minimize the Frobenius norm distance $\|X(t) - X(0)\|$.

$$E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$$
$$= \begin{cases} \begin{bmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{bmatrix} & t \in [0, \frac{\pi}{2}) \\ \begin{bmatrix} -\cos(t) & -\sin(t) \\ \sin(t) & -\cos(t) \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} -\cos(t) & -\sin(t) \\ \sin(t) & -\cos(t) \end{bmatrix} & t \in [\frac{\pi}{2}, \pi] \end{cases}.$$

The path of SVD's is smooth in $[0, \frac{\pi}{2})$, but using the single reference matrix $X(0) = I$ forces $X(t)$ and $Y(t)$ to have discontinuities. Note that there exist paths of SVD's that are smooth for all t. For example,

(1) $$E(t) = \begin{bmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} \cos(t) & \sin(t)(\\ -\sin(t) & \cos(t) \end{bmatrix}.$$

The discontinuities in this example are caused by using a *fixed* reference SVD to define the smooth path.

In this paper, we establish the existence and uniqueness of an ASVD $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ that minimizes the total variation (or arc length)

(2) $$Vrn(X(t)) = \int_a^b \|dX(t)/dt\| \, dt$$

over all feasible choices of $X(t)$ and minimizes $Vrn(Y(t))$ over the feasible choices of $Y(t)$ subject to (2) being minimum. The signs and order of the singular values are selected to be consistent with $X(t)$ and $Y(t)$. The left singular factor $X(t)$ of minimal variation is shown to satisfy a set of differential equations, and a numerical method for calculating the minimum variation ASVD is derived. This technique retains the flavor of Rheinboldt's "least change possible" approach without using a fixed reference SVD.

The two orthogonal factors $X(t)$ and $Y(t)$ are treated asymmetrically, but often, as in [9, 15], one factor is of more interest than another. A procedure that treats the two orthogonal factors symmetrically is a special case of our asymmetric basic procedure.

Other authors have also investigated properties of the singular values and singular vectors of a real analytic matrix. In [17, 18] SVD's of real analytic functions of *several* variables are examined, and first and second order perturbation theorems are given. In a recent, as yet unpublished report [1], Boyd and DeMoor use explicit derivatives of $E(t)$ to derive first order Taylor series approximations to the singular values and singular vectors in the case that the singular values are distinct (as analytic functions). They do not provide a method for constructing smooth left and right singular factors in the case of multiple singular values. In particular, they do not treat the problem of finding a smooth basis for the nullspace. (These authors refer to analytic SVD's by the acronym "USVD". We prefer the acronym ASVD.)

This paper is organized as follows. In Sect. 2 we investigate the existence and uniqueness of both smooth and analytic SVD's. We derive an initial value problem (IVP) that determines a minimum variation, globally smooth choice of the factors $X(t)$ and $Y(t)$ in the case that $E(t)$ is analytic. The minimal variation SVD is uniquely determined by its IVP. Section 3 derives a numerical method to track a minimum variation SVD based on its defining IVP. The method is shown to converge to the minimum variation path as the step size tends to zero. This section also presents a few numerical examples and extensions to related problems.

2 Existence and uniqueness of smooth SVD's

This section develops some basic results on the existence and uniqueness of smooth singular value decompositions.

2.1 Notation

Throughout the remainder of this paper, we make the simplifying assumption that $m \geqq n$. The case $m < n$ is similar.

We denote by

- $\mathbb{R}^{m \times n}$ the real m-by-n matrices;
- $\mathscr{U}_{m,n}$ the set of real m-by-n matrices with orthonormal columns;
- $C^1_{m,n}([a, b])$ the set of continuously differentiable functions on $[a, b]$ with values in $\mathbb{R}^{m \times n}$;
- $\mathscr{A}_{m,n}([a, b])$ the set of real analytic functions on $[a, b]$ with values in $\mathbb{R}^{m \times n}$; (Real analytic functions are those functions with Taylor series that, in a neighborhood of each point, converge to the original function.)
- $\mathscr{D}_{m,n}$ the set of diagonal matrices in $\mathbb{R}^{m \times n}$; ($A \in \mathscr{D}_{m,n}$ if and only if $i \neq j$ implies $a_{ij} = 0$.)
- I_n then n-by-n identity matrix;
- $\langle A, B \rangle = \mathrm{Trace}(A^T B)$ the Frobenius inner product for $A, B \in \mathbb{R}^{m \times n}$;
- $\|A\|$ the Frobenius norm, i.e., $\|A\| =_{\mathrm{def}} \sqrt{\langle A, A \rangle}$ for $A \in \mathbb{R}^{m \times n}$;
- $\Omega(A)$ the orthogonal matrix nearest (in the Frobenius norm) to the nonsingular, n-by-n matrix A [7, Chap. 12.4].

Occasionally, where there is no ambiguity, we drop subscripts and omit the explicit interval $[a, b]$. If $A(t) \in C^1_{m,n}$, then we sometimes denote the derivative of $A(t)$ by $\dot{A}(t)$.

2.2 Existence

The next example demonstrates that on analytic SVD must allow "negative singular values" and (sometimes) an ordering different from the usual nonincreasing one. (In the context of spectral decompositions, this point is also discussed in [12].) It also shows that nonuniqueness in the choice of singular vectors must be resolved in a smooth way – especially in the case of multiple and/or zero singular values.

Example 2. Define $E(t) : \mathbb{R} \to \mathbb{R}^{2\times 2}$ by

$$E(t) = \begin{bmatrix} 1-t & 0 \\ 0 & 1+t \end{bmatrix} .$$

Selecting singular values to be nonnegative and in nonincreasing order along the diagonal of $S(t)$ and resolving other nonuniqueness arbitrarily, an SVD path of $E(t)$ is

$$E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$$
$$= \begin{cases} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1-t & 0 \\ 0 & -1-t \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & t \in (-\infty, -1] \\ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1-t & 0 \\ 0 & 1+t \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & t \in (-1, 0) \\ \begin{bmatrix} 3/5 & 4/5 \\ -4/5 & 3/5 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 3/5 & -4/5 \\ 4/5 & 3/5 \end{bmatrix} & t = 0 \\ \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1+t & 0 \\ 0 & 1-t \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & t \in (0, 1] \\ \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1+t & 0 \\ 0 & -1+t \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & t \in (1, \infty) \end{cases}$$

Although $E(t)$ is linear in t, $X(t)$, $S(t)$ and $Y(t)$ have jump discontinuities and/or discontinuous derivatives. Discontinuities can occur if the order and signs of the singular values are chosen without considering their choices at nearby values of t. In the example, at every value of t, the singular values are chosen to be positive and in nonincreasing order along the diagonal of $S(t)$. This forces a discontinuity where the singular value paths intersect.

The choice of the orthogonal matrices $X(0)$ and $Y(0)$ is arbitrary. Even if $S(t)$ were smooth, resolving the nonuniqueness in $X(t)$, $Y(t)$ arbitrarily can cause discontinuities.

Note that in this example $E(t)$ admits real analytic singular value decompositions, for example,

$$E(t) = U(t)\Sigma(t)V(t)^{\mathrm{T}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1-t & 0 \\ 0 & 1+t \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} . \tag{3}$$

Example 2 motivates the following definition. A *smooth singular value decomposition* of $E(t) \in C^1_{m,n}([a, b])$ is a path of factorizations

$$E(t) = X(t)S(t)Y(t)^{\mathrm{T}} ,$$

where

$$X(t) \in \mathcal{U}_{m,m} \cap C^1_{m,m}([a, b]),$$
$$Y(t) \in \mathcal{U}_{n,n} \cap C^1_{n,n}([a, b])$$

and

$$S(t) \in \mathcal{D}_{m,n} \cap C^1_{m,n}([a, b]).$$

A path of SVD's is an *analytic SVD* (ASVD) if

$$X(t) \in \mathcal{U}_{m,m} \cap \mathcal{A}_{m,m}([a, b]),$$
$$Y(t) \in \mathcal{U}_{n,n} \cap \mathcal{A}_{n,n}([a, b])$$

and

$$S(t) \in \mathcal{D}_{m,n} \cap \mathcal{A}_{m,n}([a, b]).$$

In both the smooth and analytic cases, the diagonal entries of $S(t)$ may appear in any order and may be negative for some values of t.

The existence of smooth SVD's is obtained implicitly as the existence of smooth eigenvalue-eigenvector decompositions of symmetric matrices [8, pp. 70–71, 120–122]. The following theorem makes this explicit.

Theorem 1. *If* $E(t) \in \mathcal{A}_{m,n}([a, b])$, *then there exists an ASVD on* $[a, b]$.

Proof. Kato [8, pp. 120–122] shows that there exists an orthogonal matrix $Q(t) \in \mathcal{A}_{m+n,\,m+n}([a, b])$ and a diagonal matrix $\Lambda(t) \in \mathcal{A}_{m+n,m+n}([a, b])$ such that

$$M(t) = \begin{bmatrix} 0 & E(t) \\ E(t)^{\mathrm{T}} & 0 \end{bmatrix} = Q(t)\Lambda(t)Q(t)^{\mathrm{T}}. \tag{4}$$

Eigenvalues and their corresponding eigenvectors appear in $\pm$ pairs. It is easy to verify that if $x(t) = \left[\begin{smallmatrix} u(t) \\ v(t) \end{smallmatrix}\right] \in \mathbb{R}^{(m+n)}$ (partitioned conformally with (4)) is an eigenvector of M corresponding to the eigenvalue $\lambda(t)$, then $\hat{x}(t) = \left[\begin{smallmatrix} u(t) \\ -v(t) \end{smallmatrix}\right]$ is an eigenvector corresponding to the eigenvalue $-\lambda(t)$.

The corresponding eigenvector pairs may be chosen to be orthonormal. Hence, corresponding to the r nonzero (as analytic functions) eigenvalues we may construct a matrix with orthonormal columns

$$Q_1(t) = \frac{1}{\sqrt{2}} \begin{bmatrix} X_1(t) & X_1(t) \\ Y_1(t) & -Y_1(t) \end{bmatrix} \in \mathcal{U}_{m+n,2r} \cap \mathcal{A}_{m+n,2r}$$

and a diagonal matrix

$$\Lambda_1(t) = \begin{bmatrix} S_1(t) & 0 \\ 0 & -S_1(t) \end{bmatrix} \in \mathcal{D}_{2r,2r} \cap \mathcal{A}_{2r,2r}$$

such that

$$M(t)Q_1(t) = Q_1(t)\Lambda_1(t)$$

or equivalently

$$(5) \qquad \begin{aligned} E(t)Y_1(t) &= X_1(t)S_1(t) \\ E(t)^{\mathrm{T}}X_1(t) &= Y_1(t)S_1(t). \end{aligned}$$

Here, the diagonal entries of $\Lambda_1(t)$ include all nonzero (as analytic functions) eigenvalues of $M(t)$ and the diagonal entries of $S_1(t)$ include exactly one member from each $\pm$ pair of nonzero eigenvalues.

An easy calculation based on the orthonormality of the columns of Q_1 shows that

$$X_1(t)^{\mathrm{T}}X_1(t) = Y_1(t)^{\mathrm{T}}Y_1(t) = I_r.$$

If $r = m$, then we may take $X(t) = X_1(t)$ and $Y(t) = Y_1(t)$.

If $r < m$, then we must construct an analytic basis of the left nullspace of $E(t)$, and if $r < n$, then we must construct an analytic basis of the right nullspace of $E(t)$. The projection onto Range $(X_1(t))$, $P_1(t) = X_1(t)X_1(t)^{\mathrm{T}}$, is an analytic, symmetric matrix, because $X_1(t)$ is analytic. Applying the results of [8, pp. 120–122] to $P_1(t)$ gives $X_2(t) \in \mathscr{U}_{m,m-r} \cap \mathscr{A}_{m,m-r}$ whose columns form an analytic, orthonormal set of eigenvectors corresponding to the zero eigenvalues of $P_1(t)$. The columns of $X_2(t)$ form an orthonormal basis of the orthogonal complement of Range $(X_1(t))$, so $[X_1(t), X_2(t)]$ is orthogonal and analytic. By construction, Range $(E(t)) \subset$ Range$(X_1(t))$ and hence

$$(6) \qquad X_2(t)^{\mathrm{T}}E(t) = 0.$$

Set $X(t) = [X_1(t), X_2(t)]$.

If $r = n$, then we may use $Y(t) = Y_1(t)$, so suppose that $r < n$. Applying the same argument used to construct $X_2(t)$, we may construct a matrix $Y_2(t) \in \mathscr{U}_{n,n-r} \cap \mathscr{A}_{n,n-r}$ such that $[Y_1(t), Y_2(t)] \in \mathscr{U}_{n,n} \cap \mathscr{A}_{n,n}$ and

$$(7) \qquad E(t)Y_2(t) = 0.$$

Set $Y(t) = [Y_1(t), Y_2(t)]$.

It follows from (5), (6) and (7) that $S(t) = X(t)^{\mathrm{T}}E(t)Y(t)$ is of the form

$$(8) \qquad S(t) = \begin{bmatrix} S_1(t) & 0 \\ 0 & 0 \end{bmatrix} \in \mathscr{D}_{m,n} \cap \mathscr{A}_{m,n}$$

and $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ is an ASVD. (If $r = n$, then the last column of (8) is vacuous and does not appear. If $r = n = m$, then all the zero blocks in (8) are vacuous and do not appear.) □

Theorem 1 is stated without proof in [1]. A related result about individual singular values and singular vectors of real analytic functions of *several variables* appears in [17, 18].

If the hypothesis that $E(t)$ is analytic is dropped, then many pathologies can arise. The next example shows that even for $E(t) \in C^{\infty}$, a smooth SVD may not exist. It is similar to examples in [8, p. 111], [12] and [14].

Example 3. Let $E(t) : \mathbb{R} \to \mathbb{R}^{2\times 1}$ be the C^∞ function

$$E(t) = \begin{cases} e^{(-1/t^2)} \begin{bmatrix} \cos(1/t) \\ \sin(1/t) \end{bmatrix} & t \neq 0 \\ \begin{bmatrix} 0 \\ 0 \end{bmatrix} & t = 0 \end{cases}$$

For $t \neq 0$, $E(t)$ has full column rank, so the matrix

$$Q(t) = E(t)(E(t)^{\mathrm{T}} E(t))^{-\frac{1}{2}} = \begin{bmatrix} \cos(1/t) \\ \sin(1/t) \end{bmatrix}$$

is well defined. If $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ is any SVD path, and $X_{*1}(t)$ is the first column of $X(t)$, then $Q(t) = \pm X_{*1}(t)Y(t)^{\mathrm{T}}$ with the sign depending on the sign of the one singular value of $E(t)$. The limit $\lim_{t\to 0} \pm Q(t)$ does not exist. This implies that there is no SVD for which both $X(t)$ and $Y(t)$ are continuous at $t = 0$.

Although there is no smooth SVD at $t = 0$, $E(t)$ does have C^∞ smooth SVD's at other values of t. For example,

$$(9) \qquad E(t) = X(t)S(t)Y(t)^{\mathrm{T}} = \begin{bmatrix} \cos(1/t) & -\sin(1/t) \\ \sin(1/t) & \cos(1/t) \end{bmatrix} \begin{bmatrix} e^{(-1/t^2)} \\ 0 \end{bmatrix} [\ 1\ ].$$

It is no coincidence that at the point that does not admit a smooth SVD, $E(t)$ neither has full rank nor is analytic. The next theorem shows that if $E(t) \in C^1_{m,n}$ has full rank and distinct singular values, then there is a smooth SVD.

Theorem 2. *If $E(t) \in C^1_{m,n}([a, b])$ has full column rank and distinct singular values for all $t \in [a, b]$, then there exists a smooth SVD.*

Proof. If $E(t)$ is full rank and has distinct singular values, then the nonzero eigenvalues of

$$M(t) = \begin{bmatrix} 0 & E(t) \\ E(t)^{\mathrm{T}} & 0 \end{bmatrix}$$

are distinct. Remark 5.10 in [8, p. 115] shows that each nonzero eigenvalue is a continuously differentiable function of t, and the projection onto its invariant subspace is also continuously differentiable. The invariant subspaces are of dimension one. It is easy to construct a smooth eigenvector from a smooth projection onto a one dimensional space. Hence, there are matrices $X_1(t) \in \mathscr{U}_{m,n} \cap C^1_{m,n}([a, b])$, $Y_1(t) \in \mathscr{U}_{m,n} \cap C^1_{m,n}([a, b])$ and$S_1(t) \in \mathscr{D}_{m,n} \cap C^1_{m,n}([a, b])$ that satisfy (5). The result now follows from an argument similar to the proof of Theorem 1. □

2.3 Uniqueness

The freedom of choice on constructing an SVD of a matrix is well known. This section reviews this theory in order to lay down notation and to establish rigorously and precisely what parts of the SVD are uniquely determined by

$E(t)$ and what parts may be chosen freely. *To calculate an ASVD, it is essential that this freedom be resolved in an analytic way.*

A crucial point in the resolution is the correct identification of the multiplicity of the singular values of $E(t)$ considered as analytic functions and the identification of the dimensions of the corresponding singular subspaces. Note that if an ASVD has two singular values of opposite sings, $s_i(t) = -s_j(t)$, there is no natural way to distinguish the singular subspaces of $s_i(t)$ from the singular subspaces of $s_j(t)$. For example let

$$D = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

and suppose $E(t) = tD$. If $X(t) \in \mathscr{A}_{2,2} \cap \mathscr{U}_{2,2}$ is *any* analytic, orthogonal matrix, then $E(t) = X(t)(tD)(DX(t)D)^{\mathrm{T}}$ is an ASVD.

If $s_1(t), s_2(t), s_3(t), \ldots, s_n(t)$ are the singular values of $E(t)$ and if, for any i and j, $s_i(t)$ is identical as an analytic function to neither $+s_j(t)$ nor $-s_j(t)$, then $s_i(t)$ and $\pm s_j(t)$ may intersect only at isolated points. Likewise, a nonzero $s_i(t)$ may have only isolated roots. The value of an ASVD of $E(t)$ at such an isolated point does not give enough information to identify the dimensions of the singular subspaces, the multiplicities of the singular values and/or the signs of the singular values of the ASVD.

We refer to these isolated, exceptional values of t as *nongeneric* and to the others as *generic*. Formally, generic points are defined as follows. Let $E(t) \in \mathscr{A}_{m,n}([a, b])$. By [8, pp. 120–122], there are real analytic functions $\lambda_1(t)$, $\lambda_2(t), \lambda_3(t), \ldots, \lambda_K(t)$ which are the *distinct* (as analytic functions) eigenvalues of

$$M(t) = \begin{bmatrix} 0 & E(t) \\ E(t)^{\mathrm{T}} & 0 \end{bmatrix}. \tag{10}$$

The $\lambda_j(t)$'s are just the singular values of $E(t)$, their negatives and (possibly) and additional zero function. A point $t_1 \in [a, b]$ is a *generic* point of $E(t)$, if for $i, j = 1, 2, 3, \ldots, K$, $i \neq j$ implies $\lambda_i(t_1) \neq \lambda_j(t_1)$. If $E(t)$ is identically zero, then all points t are generic. If t is not a generic point of $E(t)$, then we say it is *nongeneric*. The nongeneric points are isolated, because the $\lambda_j(t)$'s are analytic functions.

We now look in detail at the freedom of choice in the construction of an ASVD.

If $E(t)$ has two ASVD's

$$E(t) = X(t)S(t)Y(t)^{\mathrm{T}} = \widehat{X}(t)\widehat{S}(t)\widehat{Y}(t)^{\mathrm{T}},$$

then the two paths are said to be *equivalent*. If in addition $S(t) = \widehat{S}(t)$, then the paths are called *parallel*. The two ASVD's are equivalent, if and only if there exists $Q_{\mathrm{L}}(t) \in \mathscr{U}_{m,m} \cap \mathscr{A}_{m,m}$ and $Q(t) \in \mathscr{U}_{n,n} \cap \mathscr{A}_{n,n}$ such that

$$\widehat{X}(t) = X(t)Q_{\mathrm{L}}(t),$$
$$Q_{\mathrm{L}}(t)^{\mathrm{T}}S(t)Q(t) = \widehat{S}(t)$$

and

$$\widehat{Y}(t) = Y(t)Q(t).$$

Both $S(t)$ and $\widehat{S}(t)$ must be diagonal, so $Q_L(t)$ have a special structure. The main theorem of this section clarifies the structure of such Q_L and Q. We build appropriate choices of $Q_L(t)$ and $Q(t)$ as products of three elementary equivalences: one that reorders the singular values along the diagonal of $S(t)$, one that changes the signs of the diagonal entries of $S(t)$ and one that selects bases of the left and right singular subspaces. The numerical methods in Sec. 3 are constructed from these elementary equivalences.

2.3.1 Permutation equivalence and diagonal equivalence

The first two equivalences that we discuss are permutation equivalence and diagonal equivalence, which are used to fix the order and the signs of the singular values.

Let $\mathscr{P}_n \subset \mathbb{R}^{n\times n}$ denote the set of permutation matrices in $\mathbb{R}^{n\times n}$. For each $P \in \mathscr{P}_n$ call $P_L \in \mathscr{P}_m$ a *permutation collaborator* of P, if P_L is of the form

$$P_L = \begin{bmatrix} P & 0 \\ 0 & I_{m-n} \end{bmatrix}.$$

(If $m = n$, then $P_L = P$.) If $P \in \mathscr{P}_n$ and $P_L \in \mathscr{P}_m$ are permutation collaborators and $S \in \mathscr{D}_{m,n}$, then $P_L^T S P \in \mathscr{D}_{m,n}$.

The first elementary equivalence is permutation equivalence. Two ASVD paths $X(t)S(t)Y(t)^T$ and $\widehat{X}(t)\widehat{S}(t)\widehat{Y}(t)^T$ are *P-equivalent* if there exists $P \in \mathscr{P}_n$ and a permutation collaborator $P_L \in \mathscr{P}_m$ such that

$$\widehat{X}(t) = X(t)P_L,$$
$$\widehat{Y}(t) = Y(t)P$$

and

$$\widehat{S}(t) = P_L^T S(t)P.$$

P-equivalence is an equivalence relation on ASVD's. Trivially, if two ASVD's are P-equivalent, then they are equivalent. Replacing $S(t)$ by $P_L^T S(t)P$ simply reorders the singular values along the diagonal of $S(t)$. Moreover, by choosing $P \in \mathscr{P}_n$ appropriately, any order of the diagonal entries can be achieved.

The second elementary equivalence is sign equivalence. Two ASVD paths $X(t)S(t)Y(t)^T$ and $\widehat{X}(t)\widehat{S}(t)\widehat{Y}(t)^T$ are D-equivalent, if there exists $D \in \mathscr{D}_{n,n} \cap \mathscr{U}_{n,n}$ such that

$$\widehat{Y}(t) = Y(t)D$$

and

$$\widehat{S}(t) = S(t)D.$$

The matrix D is just a diagonal matrix of ± 1's, so $D^2 = I$. D-equivalence is an equivalence relation on ASVD's. Trivially, if two ASVD's are D-equivalent, then they are equivalent. Replacing $S(t)$ by $S(t)D$ changes the sign of some of the diagonal entries of $S(t)$. Moreover, by choosing $D \in \mathscr{D}_{n,n} \cap \mathscr{U}_{n,n}$ appropriately, at any one distinguished time $t = t_0$ all the diagonal entries of $S(t_0)D$ may be made nonnegative.

2.3.2 Block orthogonal equivalence

The nonuniqueness of the bases of the left and right singular subspaces is the most complex part of the uniqueness theory, and resolving this nonuniqueness in a smooth way is the most difficult part of numerical methods.

In the following, to simplify notation, we consider ASVD's in which multiple singular values appear in clusters along the diagonal of $S(t)$. Define a diagonal factor $S(t) \in \mathscr{D}_{m,n} \cap \mathscr{A}_{m,n}$ to be *gregarious*, if $S(t)$ has the form

$$(11) \qquad S(t) = \begin{bmatrix} s_1(t)I_{m_1} & 0 & 0 & \cdots & 0 \\ 0 & s_2(t)I_{m_2} & 0 & \cdots & 0 \\ 0 & 0 & s_2(t)I_{m_3} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & s_k(t)I_{m_k} \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

where $s_1(t), s_2(t), s_3(t), \ldots, s_{k-1}(t)$ are distinct, nonzero, analytic functions; for $i \neq j$, $s_i(t) \neq \pm s_j(t)$ (except possibly at isolated points); and $s_k(t) \equiv 0$ is identically zero. If $E(t)$ has no identically zero singular values, then $m_k = 0$, and the last column and penultimate row of (11) do not appear. If $m = n$, then the last row does not appear. We say that an ASVD $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ is gregarious, if its diagonal factor $S(t)$ is gregarious. Note that the multiplicities of the singular values in any open subinterval of the domain of $S(t) \in \mathscr{A}_{m,n}([a, b])$ are identical to their multiplicities over the entire domain $[a, b]$. In this sense, the multiplicities are independent of t.

Gregarious ASVD's have no remarkable special properties. We use gregarious ASVD's to simplify the details of the proofs and algorithms.

We frequently need the following properties which follow directly from the definition of generic points.

Lemma 3. 1. *If $E(t) = X(t)S(t)Y(t)^{\mathrm{T}} = \widehat{X}(t)\widehat{S}(t)\widehat{Y}(t)^{\mathrm{T}}$ are two equivalent ASVD's and $S(t_1) = \widehat{S}(t_1)$ at some generic point $t = t_1$, then $S(t)$ and $\widehat{S}(t)$ are identical functions, i.e., the two ASVD's are parallel.*

2. If $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ is an ASVD and t_1 is a generic point of $E(t)$ such that the constant SVD $E(t_1) = X(t_1)S(t_1)Y(t_1)^{\mathrm{T}}$ is gregarious, then the (possibly) nonconstant ASVD is gregarious.

3. Every ASVD can be transformed a gregarious ASVD by a sequence of constant P-equivalences and D-equivalences. The ordering and the sings of the singular values are not unique, but any ordering and choice of sings can be obtained.

Suppose now that $S(t)$ is a gregarious path with the structure (11). Let $\mathscr{B}_S \subset \mathscr{A}_{n,n}$ be the subspace of matrices that commute with $S(t)$. Thus, $\mathscr{B}_S$ is the set of n-by-n block diagonal matrices with block sizes $m_1, m_2, m_3, \ldots, m_k$ i.e., $Z \in \mathscr{B}_S$ if and only if it is of the form

$$Z = \begin{bmatrix} Z_1 & 0 & 0 & \ldots & 0 & 0 \\ 0 & Z_2 & 0 & \ldots & 0 & 0 \\ 0 & 0 & Z_3 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & Z_{k-1} & 0 \\ 0 & 0 & 0 & \ldots & 0 & T_k \end{bmatrix} \tag{12}$$

where for $j = 1, 2, 3, \ldots, k-1$, $Z_j \in \mathbb{R}^{m_j \times m_j}$ and $T_k \in \mathbb{R}^{m_k \times m_k}$. If $S(t)$ has no identically zero singular value, then $m_k = 0$ and the last row and column of (12) do not appear.

For each orthogonal matrix $Z \in \mathscr{B}_S \cap \mathscr{U}_{n,n}$ we call $Z_L \in \mathscr{U}_{m,m} \cap \mathscr{A}_{m,m}$ a *collaborator* of Z, if Z_L is of the form

$$Z = \begin{bmatrix} Z_1 & 0 & 0 & \ldots & 0 & 0 \\ 0 & Z_2 & 0 & \ldots & 0 & 0 \\ 0 & 0 & Z_3 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & Z_{k-1} & 0 \\ 0 & 0 & 0 & \ldots & 0 & Z_k \end{bmatrix} \tag{13}$$

where the blocks $Z_1, Z_2, Z_3, \ldots Z_{k-1}$ are as in (12), $Z_k \in \mathbb{R}^{\widetilde{m}_k \times \widetilde{m}_k}$ and $\widetilde{m}_k = m - \sum_{j=1}^{k-1} m_j$. If $\widetilde{m}_k = 0$, then the last row and column of (13) do not appear. The set of block diagonal matrices in $\mathscr{A}_{m,m}$ with the block structure of (13) will be denoted $\mathscr{B}_{L,S}$.

Note that *by construction*, if $E(t) = X(t)S(t)Y(t)^T$ is a gregarious ASVD, i.e., $S(t)$ in the form of (11), then for any pair of collaborators $Z(t) \in \mathscr{B}_S \cap \mathscr{U}_{n,n}$ and $Z_L(t) \in \mathscr{B}_{L,S} \cap U_{m,m}$, we have

$$Z_L(t)^T S(t) Z(t) = S(t) \tag{14}$$

and

$$\begin{aligned} E(t) &= X(t)S(t)Y(t)^T \\ &= (X(t)Z_L(t))(Z_L(t)^T S(t) Z(t))(Z(t)^T Y(t))^T \\ &= (X(t)Z_L(t))S(t)(Z(t)^T Y(t))^T . \end{aligned} \tag{15}$$

Each choice of $Z(t)$ and $Z_L(t)$ in (15) corresponds to a different choice of the orthogonal bases of the left and right singular subspaces of $E(t)$.

We say that two parallel ASVD's $X(t)S(t)Y(t)^T$ and $\widehat{X}(t)\widehat{S}(t)\widehat{Y}(t)^T$ are *Z-equivalent*, if $S(t)$ is gregarious and for some $Z(t) \in \mathscr{B}_S \cap \mathscr{U}_{n,n}$ and some collaborator $Z_L(t) \in \mathscr{B}_{L,S} \cap \mathscr{U}_{m,m}$,

$$\widehat{X}(t) = X(t)Z_L(t)$$

and

$$\widehat{Y}(t) = Y(t)Z(t).$$

The crux of the problem of computing an ASVD is the problem of selecting an appropriate Z-equivalence. As Example 1 shows, a poor choice leads to an ASVD that does not extend to the entire domain of $E(t)$.

Lemma 4. *The matrix $E(t) \in \mathscr{A}_{m,n}$ has two parallel, gregarious ASVD's,*

$$E(t) = X(t)S(t)Y(t)^T = \widehat{X}(t)S(t)\widehat{Y}(t)^T, \tag{16}$$

if and only if the two paths are Z-equivalent.

Proof. If the two paths are Z-equivalent, then it follows from (14) and (15) that $\widehat{X}(t)S(t)\widehat{Y}(t)^T = X(t)S(t)Y(t)^T$.

Conversely, suppose (16) holds for some gregarious matrix $S(t)$. Define $Z(t) \in \mathscr{U}_{n,n} \cap \mathscr{A}_{n,n}$ and $Z_L(t) \in \mathscr{U}_{m,m} \cap \mathscr{A}_{m,m}$ by

$$Z(t) = Y(t)^T\widehat{Y}(t)$$

and

$$Z_L(t) = X(t)^T\widehat{X}(t).$$

We now show that Z and Z_L are collaborators.

Observe that

$$\begin{aligned} Y(t)^TE(t)^TE(t)Y(t) &= S(t)^TS(t) \\ &= \left(Y(t)^T\widehat{Y}(t)\right)\left(S(t)^TS(t)\right)\left(Y(t)^T\widehat{Y}(t)\right)^T \end{aligned}$$

or equivalently

$$\left(S(t)^TS(t)\right)Z(t) = Z(t)\left(S(t)^TS(t)\right). \tag{17}$$

Let $S(t)$ be as in (11), and partition $Z = [Z_{ij}]$ conformally with (12). Equation (17) implies that for $i, j = 1, 2, 3, \ldots, k$

$$s_i^2(t)Z_{ij}(t) = Z_{ij}(t)s_j^2(t).$$

If $i \neq j$, then the squares of the singular values $s_i(t)$ and $s_j(t)$ are distinct *analytic* functions. Thus, for $i \neq j$, $s_i^2(t) \neq s_j^2(t)$ except, possibly, for isolated values of t. Therefore, for $i \neq j$, $Z_{ij}(t) = 0$ and $Z \in \mathscr{B}_S$. Similarly,using $E(t)E(t)^T$ we can show that $Z_L(t) \in \mathscr{B}_{L,S}$.

Equation (16) implies that

$$\left(\widehat{X}(t)^TX(t)\right)S(t)\left(Y(t)^T\widehat{Y}(t)\right) = Z_L^TS(t)Z = S(t).$$

It follows that

$$s_i(t)Z_{\mathrm{L},i}^{\mathrm{T}}Z_i = s_i(t)I_{m_i}$$

where $Z_{\mathrm{L},i}$ is the i-th diagonal block of $Z_{\mathrm{L}} \in \mathscr{B}_{\mathrm{L},S}$ and Z_i is as in (12). By construction, for $i = 1, 2, 3, \ldots, k-1$, $s_i(t) \neq 0$ (except possibly for isolated values of t), so $Z_{\mathrm{L},i} = Z_i$. Therefore, Z and Z_{L} are the collaborators of a Z-equivalence. □

This brings us to the main theorem of this section.

Theorem 5. *Suppose*

$$E(t) = \widehat{X}(t)\widehat{S}(t)\widehat{Y}(t)^{\mathrm{T}} \tag{18}$$

is a gregarious ASVD. The matrix $E(t)$ has an equivalent ASVD

$$E(t) = X(t)S(t)Y(t)^{\mathrm{T}} = \widehat{X}(t)\widehat{S}(t)\widehat{Y}(t)^{\mathrm{T}}, \tag{19}$$

if and only if there exist $Q_{\mathrm{L}}(t) \in \mathscr{U}_{m,m}$ and $Q(t) \in \mathscr{U}_{n,n}$ such that

$$Y(t)^{\mathrm{T}}\widehat{Y}(t) = Q(t) = DPZ(t), \tag{20}$$

$$X(t)^{\mathrm{T}}\widehat{X}(t) = Q_{\mathrm{L}}(t) = P_{\mathrm{L}}Z_{\mathrm{L}}(t) \tag{21}$$

and

$$\widehat{S}(t) = P_{\mathrm{L}}^{\mathrm{T}}S(t)DP, \tag{22}$$

where $P \in \mathbb{R}^{n\times n}$ is a constant permutation matrix, P_{L} is the corresponding collaborator of a P-equivalence, $D \in \mathscr{D}_{n,n}$ is a constant diagonal matrix of ± 1's, and $Z(t) \in \mathscr{B}_{P_{\mathrm{L}}^{\mathrm{T}}SDP} = \mathscr{B}_{\widehat{S}}$ and $Z_{\mathrm{L}}(t) \in \mathscr{B}_{\mathrm{L},P_{\mathrm{L}}^{\mathrm{T}}SDP} = \mathscr{B}_{\mathrm{L},\widehat{S}}$ are the collaborators of a Z-equivalence.

Proof. Clearly, if (20), (21) and (22) are satisfied, then (19) holds and the two ASVD's are equivalent.

Conversely, suppose that (19) holds. The two ASVD's give the following two spectral decompositions of $E(t)^{\mathrm{T}}E(t)$.

$$E(t)^{\mathrm{T}}E(t) = Y(t)\left(S(t)^{\mathrm{T}}S(t)\right)Y(t)^{\mathrm{T}} = \widehat{Y}(t)\left(\widehat{S}(t)^{\mathrm{T}}\widehat{S}(t)\right)\widehat{Y}(t)^{\mathrm{T}}.$$

The diagonal entries of $S(t)$ and $\widehat{S}(t)$ may differ only in the order and signs of the diagonal entries. Thus, there are constant D- and P-equivalences such that

$$P_{\mathrm{L}}^{\mathrm{T}}S(t)DP = \widehat{S}(t). \tag{23}$$

Lemma 4 applied to the two parallel, gregarious ASVD paths

$$E(t) = (X(t)P_{\mathrm{L}})\widehat{S}(t)(Y(t)DP)^{\mathrm{T}} = \widehat{X}(t)\widehat{S}(t)\widehat{Y}(t)^{\mathrm{T}}$$

shows that there exist $Z(t) \in \mathscr{B}_{\widehat{S}}$ and a collaborator $Z_{\mathrm{L}}(t) \in \mathscr{B}_{\mathrm{L},\widehat{S}}$ such that

$$\widehat{X}(t) = X(t)P_{\mathrm{L}}Z_{\mathrm{L}}(t)$$

and

$$\widehat{Y}(t) = Y(t)DPZ(t).$$

These last two equations are equivalent to (20) and (21). □

For completeness we summarize the discussion of the previous two sections in a theorem, which displays exactly what is determined by the underlying path $E(t)$ and what can be freely chosen.

Theorem 6. *The matrix $E(t) \in \mathscr{A}_{m,n}$ has two equivalent ASVD's,*

$$E(t) = X(t)S(t)Y(t)^{\mathrm{T}} = \widehat{X}(t)\widehat{S}(t)\widehat{Y}(t)^{\mathrm{T}}, \tag{24}$$

if and only if there exist $Q_{\mathrm{L}}(t) \in \mathscr{U}_{m,m}$ and $Q(t) \in \mathscr{U}_{n,n}$ such that

$$Y(t)^{\mathrm{T}}\widehat{Y}(t) = Q(t) = \left(DPZ(t)\widehat{P}^{\mathrm{T}}\widehat{D}\right), \tag{25}$$

$$X(t)^{\mathrm{T}}\widehat{X}(t) = Q_{\mathrm{L}}(t) = \left(P_{\mathrm{L}}Z_{\mathrm{L}}(t)\widehat{P}_{\mathrm{L}}^{\mathrm{T}}\right) \tag{26}$$

and

$$\widehat{S}(t) = \widehat{P}_{\mathrm{L}}P_{\mathrm{L}}^{\mathrm{T}}S(t)DP\widehat{P}^{\mathrm{T}}\widehat{D}, \tag{27}$$

where $P \in \mathbb{R}^{n\times n}$ and $\widehat{P} \in \mathbb{R}^{n\times n}$ are constant permutation matrices, P_{L} and $\widehat{P}_{\mathrm{L}}$ are the corresponding collaborators of a P-equivalence, $D \in \mathscr{D}_{n,n}$ and $\widehat{D} \in \mathscr{D}_{n,n}$ are constant diagonal matrices of ± 1's, $P_{\mathrm{L}}^{\mathrm{T}}SDP = \widehat{P}_{\mathrm{L}}^{\mathrm{T}}\widehat{S}\widehat{D}\widehat{P}$ is gregarious, and $Z(t) \in \mathscr{B}_{P_{\mathrm{L}}^{\mathrm{T}}SDP} = \mathscr{B}_{\widehat{P}_{\mathrm{L}}^{\mathrm{T}}\widehat{S}\widehat{D}\widehat{P}}$ and $Z_{\mathrm{L}}(t) \in \mathscr{B}_{\mathrm{L},P_{\mathrm{L}}^{\mathrm{T}}SDP} = \mathscr{B}_{\mathrm{L},\widehat{P}_{\mathrm{L}}^{\mathrm{T}}\widehat{S}\widehat{D}\widehat{P}}$ are the collaborators of a Z-equivalence.

Proof. The proof is similar to the proof of Theorem 5. □

2.4 ASVD interpolation

In the following interpolation theorem, we show that ASVD's are flexible enough to interpolate any initial condition at a generic point and "almost" interpolate a final condition. The derivation of the Euler-like numerical method in Sec. 3 depends on this property.

We say that an ASVD $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ interpolates the SVD initial condition $E(t_0) = U\Sigma V^{\mathrm{T}}$ at $t = t_0$ if $X(t_0) = U$, $S(t_0) = \Sigma$ and $Y(t_0) = V$.

Theorem 7. *Suppose that t_0 and t_1, $t_0 \neq t_1$, are generic points of $E(t) \in \mathscr{A}_{m,n}$. If $E(t_0) = U_0\Sigma_0V_0^{\mathrm{T}}$ and $E(t_1) = U_1\Sigma_1V_1^{\mathrm{T}}$ are gregarious, constant SVD's, then there exists an ASVD $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$, diagonal orthogonal matrices $D_{\mathrm{L}} \in \mathscr{D}_{m,m} \cap \mathscr{U}_{m,m}$, $D_{\mathrm{R}} \in \mathscr{D}_{n,n} \cap \mathscr{U}_{n,n}$, and $D_1 \in \mathscr{D}_{n,n} \cap \mathscr{U}_{n,n}$ and a pair of permutation collaborators $P_1 \in \mathscr{P}_n$ and $P_{\mathrm{L}1} \in \mathscr{P}_m$ such that*

$$X(t_0) = U_0, \quad S(t_0) = \Sigma_0, \quad Y(t_0) = V_0 \tag{28}$$

and

$$X(t_1) = U_1P_{\mathrm{L}1}D_{\mathrm{L}}, \quad S(t_1) = P_{\mathrm{L}1}^{\mathrm{T}}\Sigma_1D_1P_1, \quad Y(t_1) = V_1D_1P_1D_{\mathrm{R}}. \tag{29}$$

Proof. By Theorem 1, there exists an ASVD $E(t) = \widetilde{X}(t)\widetilde{S}(t)\widetilde{Y}(t)^{\mathrm{T}}$. Theorem 6 applied to the constant SVD's $E(t_0) = \widetilde{X}(t_0)\widetilde{S}(t_0)\widetilde{Y}(t_0)^{\mathrm{T}}$ and $E(t_0) = U_0\Sigma_0V_0^{\mathrm{T}}$ shows that there exist constant permutation collaborators $P_0 \in \mathscr{P}_n$ and $P_{\mathrm{L}0} \in \mathscr{P}_m$, a constant diagonal orthogonal matrix $D_0 \in \mathscr{D}_{n,n} \cap \mathscr{U}_{n,n}$ and constant orthogonal collaborators $Z_0 \in \mathscr{B}_{\Sigma_0} \cap \mathscr{U}_{n,n}$ and $Z_{\mathrm{L}0} \in \mathscr{B}_{\mathrm{L},\Sigma_0} \cap \mathscr{U}_{n,n}$ such that

$$\Sigma_0 = P_{\mathrm{L}0}^{\mathrm{T}}\widetilde{S}(t_0)D_0P_0,$$
$$U_0 = \widetilde{X}(t_0)P_{\mathrm{L}0}Z_{\mathrm{L}0}$$

and

$$V_0 = \widetilde{Y}(t_0)D_0P_0Z_0.$$

Note that because t_0 is generic,

$$\mathscr{B}_{\Sigma_0} = \mathscr{B}_{P_{\mathrm{L}0}^{\mathrm{T}}\widetilde{S}D_0P_0}$$

and

$$\mathscr{B}_{\mathrm{L},\Sigma_0} = \mathscr{B}_{\mathrm{L},P_{\mathrm{L}0}^{\mathrm{T}}\widetilde{S}D_0P_0}.$$

Hence,

$$Z_{\mathrm{L}0}^{\mathrm{T}}P_{\mathrm{L}0}^{\mathrm{T}}\widetilde{S}(t)D_0P_0Z_0 = P_{\mathrm{L}0}^{\mathrm{T}}\widetilde{S}(t)D_0P_0$$

is diagonal for all t. Because P_0, $P_{\mathrm{L}0}$, D_0, Z_0 and $Z_{\mathrm{L}0}$ are constant, $E(t) = \check{X}(t)\check{S}(t)\check{Y}(t)^{\mathrm{T}}$ is an ASVD that interpolates (28) where

$$\check{X}(t) = \widetilde{X}(t)P_{\mathrm{L}0}Z_{\mathrm{L}0},$$
$$\check{S}(t) = P_{\mathrm{L}0}^{\mathrm{T}}\widetilde{S}(t)D_0P_0$$

and

$$\check{Y}(t) = \widetilde{Y}(t)D_0P_0Z_0.$$

Repeating the above construction on the constant SVD's $E(t_1) = U_1\Sigma_1V_1^{\mathrm{T}}$ and $\check{E}(t_1) = \check{X}(t_1)\check{S}(t_1)\check{Y}(t_1)^{\mathrm{T}}$ at the generic point t_1, we conclude that for appropriately chosen $D_1 \in \mathscr{D}_{n,n} \cap \mathscr{U}_{n,n}$, permutation collaborators $P_1 \in \mathscr{P}_n$ and $P_{\mathrm{L}1} \in \mathscr{P}_m$ and constant orthogonal collaborators $Z_1 \in \mathscr{B}_{\check{S}}$ and $Z_{\mathrm{L}1} \in \mathscr{B}_{\mathrm{L},\check{S}}$,

$$\check{S}(t_1) = P_{\mathrm{L}1}^{\mathrm{T}}\Sigma_1D_1P_1,$$
$$\check{X}(t_1) = U_1P_{\mathrm{L}1}Z_{\mathrm{L}1}$$

and

$$\check{Y}(t_1) = V_1D_1P_1Z_1.$$

Choose $D_{\mathrm{L}} = \mathrm{diag}(\pm 1) \in \mathscr{D}_{m,m}$, so that, with

$$W_{\mathrm{L}1} =_{\mathrm{def}} D_{\mathrm{L}}Z_{\mathrm{L}1} \in \mathscr{B}_{\mathrm{L},\check{S}} \cap \mathscr{U}_{m,m}$$

partitioned as in (13), each diagonal block of $W_{\mathrm{L}1}$ has determinant equal to 1.

Note that $D_{\mathrm{L}} \in \mathscr{B}_{\mathrm{L}\check{S}} \cap \mathscr{U}_{m,m}$. So, D_{L} has a collaborator D_{R}. Define $W_1 \in \mathscr{B}_{\check{S}} \cap \mathscr{U}_{m,m}$ by

$$W_1 =_{\mathrm{def}} D_{\mathrm{R}} Z_1 \in \mathscr{B}_{\check{S}} .$$

It is easy to check that $W_1 \in \mathscr{B}_{\check{S}} \cap \mathscr{U}_{n,n}$ is a collaborator of $W_{\mathrm{L}1}$. The collaborators W_1 and $W_{\mathrm{L}1}$ have the block structure of (12) and (13). It follows that if $\check{S}$ has no singular value that is identically zero, then the diagonal blocks of W_1 have determinant 1. If $\check{S}$ has some identically zero singular values, then there is some freedom in the last few diagonal positions of D_{R} that can be used to make the final diagonal block of $W_1 = D_{\mathrm{R}} Z_1$ have determinant 1.

By construction, the diagonal blocks of $W_{\mathrm{L}1}$ and W_1 have determinant 1. Hence, there are real skew-symmetric matrices $K_{\mathrm{L}} = \ln(W_{\mathrm{L}1})$ and $K = \ln(W_1)$ such that $K_{\mathrm{L}} \in \mathscr{B}_{\mathrm{L},\check{S}}$ and $K \in \mathscr{B}_{\check{S}}$, $\exp(K_{\mathrm{L}}) = W_{\mathrm{L}1}$ and $\exp(K) = W_1$. Define $Z(t) \in \mathscr{U}_{n,n} \cap \mathscr{A}_{n,n}$ and $Z_{\mathrm{L}}(t) \in \mathscr{U}_{m,m} \cap \mathscr{A}_{m,m}$ by

$$Z_{\mathrm{L}}(t) = \exp\left(\left(\frac{t - t_0}{t_1 - t_0}\right) K_{\mathrm{L}}\right)$$

and

$$Z(t) = \exp\left(\left(\frac{t - t_0}{t_1 - t_0}\right) K\right).$$

The block structure, $K_{\mathrm{L}} \in \mathscr{B}_{\mathrm{L},\check{S}}$ and $K \in \mathscr{B}_{\check{S}}$, implies that $Z_{\mathrm{L}}(t) \in \mathscr{B}_{\mathrm{L},\check{S}}$ and $Z(t) \in \mathscr{B}_{\check{S}}$. Because t_1 is generic,

$$\mathscr{B}_{\check{S}} = \mathscr{B}_{P_{\mathrm{L}1}^{\mathrm{T}} \Sigma_1 D_1 P_1},$$

$$\mathscr{B}_{\mathrm{L},\check{S}} = \mathscr{B}_{\mathrm{L},\, P_{\mathrm{L}1}^{\mathrm{T}} \Sigma_1 D_1 P_1}$$

and

$$Z_{\mathrm{L}}(t) \check{S}(t) Z(t)^{\mathrm{T}} = \check{S}(t)$$

is diagonal for all t. Moreover,

$$Z(t_0) = I_n, \quad Z(t_1) = W_1, \quad Z_{\mathrm{L}}(t_0) = I_m, \quad Z_{\mathrm{L}}(t_1) = W_{\mathrm{L}1}.$$

With

$$X(t) = \check{X}(t) Z_{\mathrm{L}}(t)^{\mathrm{T}},$$
$$S(t) = \check{S}(t)$$

and

$$Y(t) = \check{Y}(t) Z(t)^{\mathrm{T}}$$

the ASVD $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ satisfies both (28) and (29), because $D_{\mathrm{L}} \check{S}(t) D_{\mathrm{R}} = \check{S}(t)$. □

The hypothesis that the t_j's are generic points is needed in Theorem 7 to guarantee the existence of an ASVD that interpolates an arbitrary SVD (28) and essentially a permutation of a second arbitrary SVD (29). If the assumption is dropped, then there may be no such ASVD. For example, there is no ASVD of

(30) $$E(t) = \begin{bmatrix} 2t & 0 \\ 0 & t \end{bmatrix}$$

that interpolates the SVD

(31) $$E(0) = \begin{bmatrix} 4/5 & 3/5 \\ -3/5 & 4/5 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} .$$

If (28) and (29) lie on ASVD's, then the conclusion of Theorem 7 holds regardless of whether t_0 and t_1 are generic or not.

2.5 *Minimum variation paths*

Theorem 6 displays the degrees of freedom in the choice of an ASVD. This section resolves the freedom of choice to give a particular ASVD that is well suited to numerical computation.

Define the total variation (or arc length) of $X(t) \in \mathscr{U}_{m,m} \cap C^1_{m,m}$ over the interval $[a, b]$ by

$$Vrn(X(t)) = \int_a^b \|dX/dt\| \, dt .$$

We establish here the existence and uniqueness of ASVD's in which $Vrn(X(t))$ is minimal. The numerical methods of Sec. 3 track such minimal variation paths. The approach retains the flavor of Rheinboldt's [15] "least change possible" approach without using a fixed reference SVD.

The following lemma shows the existence of a unique gregarious ASVD which satisfies an initial condition and whose orthogonal factors have a minimal variation property.

In order to construct this ASVD we need the projections onto the spaces of block diagonal matrices $\mathscr{B}_S \subset \mathscr{A}_{n,n}$ and $\mathscr{B}_{L,S} \subset \mathscr{A}_{m,m}$ defined in Section 2.3.2. We use $\Phi_S(\cdot)$ to denote the projection in the Frobenius inner product $\langle \cdot, \cdot \rangle$ from $\mathscr{A}_{n,n}$ onto $\mathscr{B}_S$. The projection from $\mathscr{A}_{m,m}$ onto $\mathscr{B}_{L,S}$ is denoted by $\Phi_{L,S}(\cdot)$. The projections $\Phi_S(\cdot)$ and $\Phi_{L,S}(\cdot)$ operate by simply setting the entries outside the relevant block diagonal to zero. The orthogonal complements are given by $\Phi_S^\perp(X) =_{\text{def}} X - \Phi_S(X)$ and $\Phi_{L,S}^\perp(X) =_{\text{def}} X - \Phi_{L,S}(X)$.

If $Z_L(t), W_L(t) \in \mathscr{B}_{L,S}$ and $X(t) \in \mathbb{R}^{m \times m}$, then the projections onto $\mathscr{B}_{L,S}$ and orthogonal to $\mathscr{B}_{L,S}$ obey

(32) $$\Phi_{L,S}(W_L(t)X(t)Z_L(t)) = W_L(t)\Phi_{L,S}(X(t))Z_L(t)$$

and

(33) $$\Phi_{L,S}^\perp(W_L(t)X(t)Z_L(t)) = W_L(t)(\Phi_{L,S}^\perp(X(t)))Z_L(t) .$$

Lemma 8. *If*

$$E(t) = X(t)S(t)Y(t)^{\mathrm{T}} \tag{34}$$

is a gregarious ASVD on $[a, b]$, *then there is a unique, parallel, equivalent ASVD* $E(t) = \widehat{X}(t)S(t)\widehat{Y}(t)^{\mathrm{T}}$ *such that* $\widehat{X}(t_0) = X(t_0) = Y(t_0)$,

$$Vrn(\widehat{X}(t)) = \min\left\{ Vrn(\widetilde{X}(t)) \,\middle|\, \begin{array}{l} E(t) = \widetilde{X}(t)S(t)\widetilde{Y}(t)^{\mathrm{T}} \text{ is an ASVD} \\ \text{parallel to (34)} \end{array} \right\} \tag{35}$$

and

$$Vrn(\widehat{Y}(t)) = \min\left\{ Vrn(\widetilde{Y}(t)) \,\middle|\, \begin{array}{l} E(t) = \widehat{X}(t)S(t)\widetilde{Y}(t)^{\mathrm{T}} \text{ is an ASVD} \\ \text{parallel to (34) subjet to (35)} \end{array} \right\}. \tag{36}$$

Proof. As shown in Lemma 4, all parallel, gregarious ASVD's are of the form

$$E(t) = (X(t)Z_{\mathrm{L}}(t))S(t)(Y(t)Z(t))^{\mathrm{T}} \tag{37}$$

for some $Z_{\mathrm{L}}(t) \in \mathscr{B}_{\mathrm{L},S}$. The total variation of the left-hand factor of (37) is

$$\begin{aligned} Vrn(X(t)Z_{\mathrm{L}}(t)) &= \int_a^b \left\| \dot{X}Z_{\mathrm{L}}(t) + X(t)\dot{Z}_{\mathrm{L}}(t) \right\| dt \\ &= \int_a^b \left\| X(t)^{\mathrm{T}}\dot{X}(t)Z_{\mathrm{L}}(t) + \dot{Z}_{\mathrm{L}}(t) \right\| dt. \end{aligned}$$

We have,

$$\begin{aligned} &\|X(t)^{\mathrm{T}}\dot{X}(t)Z_{\mathrm{L}}(t) + \dot{Z}_{\mathrm{L}}(t)\|^2 \\ &\quad = \|\Phi_{\mathrm{L},S}(X(t)^{\mathrm{T}}\dot{X}(t)Z_{\mathrm{L}}(t) + \dot{Z}_{\mathrm{L}}(t))\|^2 + \|\Phi^{\perp}_{\mathrm{L},S}(X(t)^{\mathrm{T}}\dot{X}(t)Z_{\mathrm{L}}(t) + \dot{Z}_{\mathrm{L}}(t))\|^2 \\ &\quad = \|\Phi_{\mathrm{L},S}(X(t)^{\mathrm{T}}\dot{X}(t))Z_{\mathrm{L}}(t) + \dot{Z}_{\mathrm{L}}(t)\|^2 + \|\Phi^{\perp}_{\mathrm{L},S}(X(t)^{\mathrm{T}}\dot{X}(t))\|^2 \end{aligned}$$

Therefore,

$$Vrn(X(t)Z_{\mathrm{L}}(t))$$

$$= \int_a^b \sqrt{\left\|\Phi_{\mathrm{L},S}\left(X(t)^{\mathrm{T}}\dot{X}(t)\right)Z_{\mathrm{L}}(t) + \dot{Z}_{\mathrm{L}}(t)\right\|^2 + \left\|\Phi^{\perp}_{\mathrm{L},S}\left(X(t)^{\mathrm{T}}\dot{X}(t)\right)\right\|^2}\, dt \tag{38}$$

$$\geqq \int_a^b \left\|\Phi^{\perp}_{\mathrm{L},S}\left(X(t)^{\mathrm{T}}\dot{X}(t)\right)\right\| dt. \tag{39}$$

We now show that there exists a choice of $Z_L(t) \in \mathscr{B}_{L,S} \cap \mathscr{U}_{m,m} \cap \mathscr{A}_{m,m}$ which achieves the minimum by annihilating the first term under the square root in (38). Observe first that, because $X(t)$ is orthogonal,

$$0 = \frac{d(X^T X)}{dt} = \dot{X}(t)^T X(t) + X(t)^T \dot{X}(t).$$

Thus, $X(t)^T \dot{X}(t)$ is skew symmetric.

Consider the initial value problem

$$\begin{aligned} \dot{Z}_L(t) &= -\Phi_{L,S}\left(X(t)^T \dot{X}(t)\right) Z_L(t) \\ &= \Phi_{L,S}\left(\dot{X}(t)^T X(t)\right) Z_L(t); \\ Z_L(t_0) &= I_m. \end{aligned} \tag{40}$$

The matrix $\Phi_{L,S}\left(\dot{X}(t)^T X(t)\right)$ is analytic and so, *a fortiori*, (40) satisfies a Lipschitz condition. Therefore, a unique, analytic solution $\hat{Z}_L(t)$ exists, at least in a neighborhood of the initial condition [11, p. 2]. The solution $\hat{Z}_L(t)$ is orthogonal, because

$$\begin{aligned} \frac{d(\hat{Z}_L(t)^T \hat{Z}_L(t))}{dt} &= \hat{Z}_L(t)^T \dot{\hat{Z}}_L(t) + \dot{\hat{Z}}_L(t)^T \hat{Z}_L(t) \\ &= \hat{Z}_L(t)^T \Phi_{L,S}\left(\dot{X}(t)^T X(t)\right) \hat{Z}_L(t) + \hat{Z}_L(t)^T \left(\Phi_{L,S}\left(\dot{X}(t)^T X(t)\right)\right)^T \hat{Z}_L(t) \\ &= \hat{Z}_L(t)^T \Phi_{L,S}\left(\dot{X}(t)^T X(t) + \left(\dot{X}(t)^T X(t)\right)^T\right) \hat{Z}_L(t) \\ &= 0, \end{aligned}$$

where the last equation follows from the skew symmetry of $X(t)^T \dot{X}(t)$. The orthogonality of $\hat{Z}_L(t)$ now follows from the initial condition $\hat{Z}_L(t_0)^T \hat{Z}_L(t_0) = I_m$. This implies that the right-hand-side of (40) is analytic and bounded, so the solution $\hat{Z}_L(t)$ extends to the entire interval $[a, b]$.

Note also that the solution $\hat{Z}_L(t)$ lies in $\mathscr{B}_{L,S}$ for all $t \in [a, b]$, because the initial condition $\hat{Z}_L(t_0) = I_m$ and the derivatives lie in $\mathscr{B}_{L,S}$.

Choosing $\hat{X}(t) = X(t)\hat{Z}_L(t)$ annihilates the first term in (38). Therefore, $\hat{X}(t) = X(t)\hat{Z}_L(t)$ minimizes $Vrn(X(t))$ over all ASVD's by achieving the lower bound (39). The uniqueness of $\hat{X}(t)$ is guaranteed by the uniqueness of the solution $\hat{Z}_L$ of the initial value problem (40).

Having chosen $\hat{Z}_L \in \mathscr{B}_{S,L}$, we must now choose $\hat{Z} \in \mathscr{B}_S$ to collaborate with $\hat{Z}_L$ and thus choose $Y(t)$. From (12) and (13) it is clear that the choice of $\hat{Z}_L(t)$ determines $\hat{Z}(t)$ except for the trailing m_k-by-m_k block. (If there is no identically zero singular value, then $m_k = 0$ and $\hat{Z}(t)$ is entirely determined by $\widehat{Z}_{\mathrm{L}}(t)$.) Using a construction similar to that for $\widehat{Z}_{\mathrm{L}}(t)$ we can determine a unique choice of $\widehat{Z}(t)$ and $\widehat{Y}(t) = Y(t)\widehat{Z}(t)$ that minimizes (36). □

The following corollaries are used in Sect. 3.

Corollary 9. *If $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ is a gregarious ASVD on $[a, b]$ and $E(t) = \widehat{X}(t)S(t)\widehat{Y}(t)^{\mathrm{T}}$ is the unique, parallel, minimum variation path that satisfies the initial condition $E(t_0) = X(t_0)S(t_0)Y(t_0)^{\mathrm{T}}$ at the generic point t_0, then $\widehat{X}(t) = X(t)Z_{\mathrm{L}}(t)$ where $Z_{\mathrm{L}}(t) \in \mathscr{B}_{\mathrm{L},S}$ solves the initial value problem*

$$\dot{Z}_{\mathrm{L}}(t) = \Phi_{\mathrm{L},S}\left(\dot{X}(t)^{\mathrm{T}}X(t)\right)Z_{\mathrm{L}}(t), \quad Z_{\mathrm{L}}(t_0) = I_m. \tag{41}$$

Proof. The result follows directly from the proof of Lemma 8. □

Corollary 10. *If $E(t) \in \mathscr{A}_{m,n}([a, b])$ has two parallel, gregarious, minimum variation paths, $E(t) = \widehat{X}(t)S(t)\widehat{Y}(t)^{\mathrm{T}} = \widetilde{X}(t)S(t)\widetilde{Y}(t)^{\mathrm{T}}$, then there are constant collaborators $Z_{\mathrm{L}} \in \mathscr{B}_{\mathrm{L},S}$ and $Z \in \mathscr{B}_S$ such that $\widehat{X}(t) = \widetilde{X}(t)Z_{\mathrm{L}}$ and $\widehat{Y}(t) = \widetilde{Y}(t)Z$.*

Proof. Let t_0 be a generic point in $[a, b]$. By Lemma 4 applied to the two *constant* SVD's

$$E(t_0) = \widehat{X}(t_0)S(t_0)\widehat{Y}(t_0)^{\mathrm{T}} = \widetilde{X}(t_0)S(t_0)\widetilde{Y}(t_0)^{\mathrm{T}},$$

there are a pair of orthogonal collaborators $Z_{\mathrm{L}} \in \mathscr{B}_{\mathrm{L},S(t_0)}$ and $Z \in \mathscr{B}_{S(t_0)}$ such that $\widehat{X}(t_0) = \widetilde{X}(t_0)Z_{\mathrm{L}}$ and $\widehat{Y}(t_0) = \widetilde{Y}(t_0)Z_{\mathrm{L}}$. Obviously, Z_{L} and Z can be chosen to be constant. Because t_0 is generic, $\mathscr{B}_{\mathrm{L},S(t_0)} = \mathscr{B}_{\mathrm{L},S}$ and $\mathscr{B}_{S(t_0)} = \mathscr{B}_S$. Hence, $Z_{\mathrm{L}}^{\mathrm{T}}S(t)Z = S(t)$ for all $t \in [a, b]$. For constant orthogonal matrices Z_{L} and Z, $Vrn(\widetilde{X}Z) = Vrn(\widetilde{X})$ and $Vrn(\widetilde{Y}Z) = Vrn(\widetilde{Y})$. Hence,

$$E(t) = \left(\widetilde{X}(t)Z_{\mathrm{L}}\right)S(t)\left(\widetilde{Y}(t)Z\right)^{\mathrm{T}}$$

is a minimum variation ASVD that agrees with $E(t) = \widehat{X}(t)S(t)\widehat{Y}(t)$ at the generic point t_0. The uniqueness part of Lemma 8 implies that $\widehat{X}(t) = \widetilde{X}Z_{\mathrm{L}}$ and $\widehat{Y}(t) = \widetilde{Y}Z$. □

The following theorem is the main result of this section. It shows that there is a uniquely defined minimal variation ASVD that interpolates any initial constant SVD at a generic point. The numerical methods of Sect. 3 are designed to compute this ASVD.

Theorem 11. *Suppose that $E(t) \in \mathscr{A}_{m,n}([a, b])$ and $t_0 \in [a, b]$ is generic. If $E(t_0) = U\Sigma V^{\mathrm{T}}$ is a given, constant SVD, then there exists a unique ASVD on $t \in [a, b]$, $E(t) = \widehat{X}(t)\widehat{S}(t)\widehat{Y}(t)^{\mathrm{T}}$ such that $\widehat{X}(t_0) = U$, $\widehat{S}(t_0) = \Sigma$, $\widehat{Y}(t_0) = V$,*

$$Vrn(\widehat{X}(t)) = \min\{Vrn(X(t)) | E(t) = X(t)S(t)Y(t)^{\mathrm{T}} \quad \textit{is an ASVD}\} \tag{42}$$

and

$$\text{(43)} \qquad Vrn(\widehat{Y}(t)) = \min\left\{ Vrn(Y(t)) \,\middle|\, \begin{array}{c} E(t) = \widehat{X}(t)S(t)Y(t)^{\mathrm{T}} \\ \textit{is an ASVD} \\ \textit{subject to } (42) \end{array} \right\}$$

Proof. Let $P \in \mathscr{P}_n$ and $P_{\mathrm{L}} \in \mathscr{P}_m$ be constant permutation collaborators and $D \in \mathscr{D}_{n,n} \cap \mathscr{U}_{n,n}$ be chosen such that $(UP_{\mathrm{L}})(P_{\mathrm{L}}^{\mathrm{T}}\Sigma DP)(VDP)^{\mathrm{T}} = \widetilde{U}\widetilde{\Sigma}\widetilde{V}^{\mathrm{T}}$ is a constant, gregarious SVD. By hypothesis, t_0 is generic, so by Theorem 7 there is a gregarious ASVD $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ such that $X(t_0) = UP_{\mathrm{L}}$, $S(t_0) = P_{\mathrm{L}}^{\mathrm{T}}\Sigma DP$ and $Y(t_0) = VDP$. By Lemma 8, this ASVD may be chosen to satisfy (42) and (43) and this choice is unique. If $\widehat{X} = XP_{\mathrm{L}}^{\mathrm{T}}$, $\widehat{S}(t) = P_{\mathrm{L}}S(t)P^{\mathrm{T}}D$ and $\widehat{Y}(t) = YP^{\mathrm{T}}D$, then $E(t) = \widehat{X}(t)\widehat{S}(t)\widehat{Y}(t)^{\mathrm{T}}$ is an ASVD such that $\widehat{X}(t_0) = U$, $\widehat{S}(t_0) = \Sigma$ and $\widehat{Y}(t_0) = V$. Because P_{L}, P and D are constant, orthogonal matrices, $Vrn(\widehat{X}(t)) = Vrn(X(t))$ and $Vrn(\widehat{Y}(t)) = Vrn(Y(t))$, so (42) and (43) are satisfied.

Uniqueness follows from Lemma 8. □

3 Numerical methods

We now develop a numerical procedure for tracing the minimal variation ASVD that interpolates a given initial condition. It is impossible to use a general initial value problem solver directly on Corollary 9, because the term $\Phi_{\mathrm{L},\mathrm{S}}(\dot{X}(t)^{\mathrm{T}}X(t))$ in (41) involves the left-hand factor of an unknown *a priori* ASVD. Moreover, a general numerical integration procedure cannot guarantee the orthogonality of the numerical solution approximating $X(t)$ in (41).

In this section we derive a method which uses Corollary 9 to approximate a minimal variation path without an *a priori* ASVD. In essence, the method operates as follows. Given an SVD at $t = t_0$, $E(t_0) = X_0S_0Y_0^{\mathrm{T}}$, the method approximates the minimal variation ASVD at $t = t_1 = t_0 + h$, by the SVD $E(t_1) = \widehat{X}_1\widehat{S}_1\widehat{Y}_1^{\mathrm{T}}$, in which $\widehat{X}_1$ minimizes the distance $\|\widehat{X}_1 - X_0\|$ over all possible left-hand factors X_1. *Any* (constant) SVD of $E(t_1)$ gives a "basis" for the possible factors. Using such a "basis", the computation of $\widehat{X}_1$ can be reduced to solving several small orthogonal Procrustes' problems.

This approach is similar to Euler's method for approximating the solution to (41). Like Euler's method, the global discretization error is $O(h)$, but extrapolation can be used to increase the order of accuracy.

In principle the same approach could be used in conjunction with a higher-order difference approximation to (41). (The construction of such approximations is currently under investigation. Some preliminary work has appeared in [10].)

A detailed derivation of this Euler-like approximation to (41) and its local truncation error appears in the next subsection, and computational algorithms appear in the following subsection. The convergence as the step size h tends to zero is established in Sect. 3.3. The procedures are then extended to the computation of an analytic spectral decomposition of a symmetric matrix in Subsect. 3.4. The final subsection lists the results of a few numerical tests.

3.1 An Euler-like method at generic points

Suppose t_0 is generic and

$$E(t_0) = U_0 \Sigma_0 V_0^{\mathrm{T}} \tag{44}$$

is some gregarious, constant SVD. Let $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ be any gregarious ASVD that interpolates the initial condition (44). Corollary 9 shows that if $Z_{\mathrm{L}}(t) \in \mathscr{B}_{\mathrm{L},S}$, solves the initial value problem

$$\dot{Z}_{\mathrm{L}}(t) = \Phi_{\mathrm{L},S}(\dot{X}(t)^{\mathrm{T}} X(t)) Z_{\mathrm{L}}(t), \quad Z_{\mathrm{L}}(t_0) = I_m, \tag{45}$$

then the left-hand, orthogonal factor, $\widehat{X}(t)$, of the minimal variation ASVD $E(t) = \widehat{X}(t)S(t)\widehat{Y}(t)^{\mathrm{T}}$ that interpolates (44) is given by

$$\widehat{X}(t) = X(t) Z_{\mathrm{L}}(t). \tag{46}$$

Expanding $Z_{\mathrm{L}}(t)$ in a Taylor series about t_0 gives

$$\begin{aligned} Z_{\mathrm{L}}&(t_0 + h) \\ &= Z_{\mathrm{L}}(t_0) + h\dot{Z}_{\mathrm{L}}(t_0) + O(h^2) \\ &= Z_{\mathrm{L}}(t_0) + h\Phi_{\mathrm{L},S}\left(\dot{X}(t_0)^{\mathrm{T}} X(t_0)\right) Z_{\mathrm{L}}(t_0) + O(h^2) \\ &= I_m + h\Phi_{\mathrm{L},S}\left(\left(\frac{X(t_0+h)^{\mathrm{T}} - X(t_0)^{\mathrm{T}}}{h}\right) X(t_0) + O(h)\right) + O(h^2) \\ &= \Phi_{\mathrm{L},S}(X(t_0+h)^{\mathrm{T}} X(t_0)) + O(h^2). \end{aligned} \tag{47}$$

In the penultimate equation, we have used the initial condition $Z_{\mathrm{L}}(t_0) = I_m$. Thus,

$$\widehat{X}(t_0 + h) = X(t_0 + h) Z_{\mathrm{L}}(t_0 + h) \approx X(t_0 + h)\Phi_{\mathrm{L},S}(X(t_0 + h)^{\mathrm{T}} X(t_0)) \tag{48}$$

is an $O(h^2)$ accurate Euler-like approximation to $\widehat{X}(t_0 + h)$.

Equation (46) implies

$$\begin{aligned} X&(t_0 + h)\Phi_{\mathrm{L},S}(X(t_0 + h)^{\mathrm{T}} X(t_0)) \\ &= \widehat{X}(t_0 + h) Z_{\mathrm{L}}(t_0 + h)^{\mathrm{T}} \Phi_{\mathrm{L},S}\left(Z_{\mathrm{L}}(t_0 + h)\widehat{X}(t_0 + h)^{\mathrm{T}} \widehat{X}(t_0) Z_{\mathrm{L}}(t_0)^{\mathrm{T}}\right) \\ &= \widehat{X}(t_0 + h)\Phi_{\mathrm{L},S}\left(\widehat{X}(t_0 + h)^{\mathrm{T}} \widehat{X}(t_0)\right). \end{aligned}$$

The last equality follows from (32), the initial condition in (45) and the orthogonality of $Z_{\mathrm{L}}(t)$. Thus, the approximation (48) is independent of the particular choice of the *a priori* ASVD. Therefore, we may use (48) with *any*

ASVD that interpolates the initial condition (44) – even an ASVD that depends on h – to obtain an $O(h^2)$ accurate approximation of $\widehat{X}(t_0+h)$.

To evaluate the right-hand-side of (48), we need $X(t_0)$ and $X(t_0+h)$. The a priori ASVD interpolates (44), i.e., $X(t_0) = U_0$. Thus, only $X(t_0+h)$ needs to be chosen. Suppose that t_0+h is generic and

$$E(t_0+h) = U_h \Sigma_h V_h^{\mathrm{T}} \tag{50}$$

is a constant gregarious SVD. (For practical purposes, (50) may be obtained from any good numerical method, e.g., [4, 5, 6, 7, 16].) By Theorem 7, there exists an "almost" interpolating ASVD

$$E(t) = X_h(t) S(t) Y_h(t)^{\mathrm{T}} \tag{51}$$

such that

$$\begin{aligned} X_h(t_0) &= U_0, \\ S(t_0) &= \Sigma_0, \\ Y_h(t_0) &= V_0, \end{aligned} \tag{52}$$

and

$$\begin{aligned} X_h(t_0+h) &= U_h P_{\mathrm{L}h} D_{\mathrm{L}h}, \\ S(t_0+h) &= P_{Lh}^{\mathrm{T}} \Sigma_h D_h P_h, \\ Y_h(t_0+h) &= V_h D_h P_h D_{\mathrm{R}h}, \end{aligned} \tag{53}$$

where $D_h, D_{\mathrm{R}h} \in \mathscr{D}_{n,n}, D_{\mathrm{L}h} \in \mathscr{D}_{m,m}$ are diagonal matrices of ± 1's and $P_h \in \mathscr{P}_n$ and $P_{\mathrm{L}h} \in \mathscr{P}_m$ are permutation collaborators. (All ASVD's that interpolate the initial condition (52) are parallel, because t_0 is generic. Hence, the diagonal factor in (51) does not depend on h.) If a suitable permutation matrix $P_{\mathrm{L}h}$ and an orthogonal, diagonal matrix $D_{\mathrm{L}h}$ can be found, then $X(t_0+h) = X_h(t_0+h) = U_h P_{\mathrm{L}h} D_{\mathrm{L}h}$ may be used in (48).

For small enough h, suitable permutation matrices $P_{\mathrm{L}h}$ are identified by the property $\Phi_{\mathrm{L},S}^{\perp}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0) = O(h)$. This can be seen as follows. Lemma 4 implies that there exists an orthogonal matrix $Z_{\mathrm{L}h}(t) \in \mathscr{B}_{\mathrm{L},S}$ such that $X_h(t) = \widehat{X}(t) Z_{\mathrm{L}h}(t)$. Thus,

$$\Phi_{\mathrm{L},S}^{\perp}(D_{\mathrm{L}h}^{\mathrm{T}} P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0) = \Phi_{\mathrm{L},S}^{\perp}\left(Z_{\mathrm{L}h}(t_0+h)^{\mathrm{T}} \widehat{X}(t_0+h)^{\mathrm{T}} \widehat{X}(t_0)\right).$$

It follows from the orthogonality of $Z_{\mathrm{L}h}(t)$, $D_{\mathrm{L}h} \in \mathscr{B}_{\mathrm{L},S}$ and (32) that

$$\|\Phi_{\mathrm{L},S}^{\perp}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0)\| = \left\|\Phi_{\mathrm{L},S}^{\perp}\left(\widehat{X}(t_0+h)^{\mathrm{T}} \widehat{X}(t_0)\right)\right\| = O(h). \tag{54}$$

Equation (54) may not identify $P_{\mathrm{L}h}$ uniquely. However, if $P_{\mathrm{L}h}$ and $\widetilde{P}_{\mathrm{L}h}$ are permutation matrices that each satisfy (54), then $\widetilde{P}_{\mathrm{L}h} = P_{\mathrm{L}h} W$ for some $W \in \mathscr{B}_{\mathrm{L},S} \cap \mathscr{P}_m$. Substituting $\widetilde{P}_{\mathrm{L}h}$ in place of $P_{\mathrm{L}h}$ is equivalent to substituting the left-hand, orthogonal factor, $X(t)$ in (48) by one from a parallel ASVD. As noted above, both choices yield the same approximation to $\widehat{X}(t_0+h)$.

Because t_0 is generic, $\Phi^{\perp}_{\mathrm{L},S} = \Phi^{\perp}_{\mathrm{L},\Sigma_0}$, so the information needed to choose $P_{\mathrm{L}h}$ is available from the initial condition (44) and the constant SVD (50).

Determining a suitable choice $P_{\mathrm{L}h}$ from (54) is easy. Partition $U_h^{\mathrm{T}}U_0$ as $U_h^{\mathrm{T}}U_0 = [U_1, U_2, U_3, \ldots, U_k]$ where $U_j \in \mathbb{R}^{m\times m_j}$ and m_j is the multiplicity of the j-th group of multiple singular values of $S(t)$. Equation (54) shows that exactly m_j rows of U_j contain entries of magnitude greater than $O(h)$. The permutation matrix $P_{\mathrm{L}h}$ may be any permutation matrix that interchanges these largest rows with rows $\left(1+\sum_{l=1}^{j-1} m_l\right)$ through $\left(\sum_{l=1}^{j} m_l\right)$.

With the above choice of $P_{\mathrm{L}h}$, the approximation (48) becomes

$$
\begin{aligned}
\widehat{X}(t_0+h) &\approx U_h P_{\mathrm{L}h} D_{\mathrm{L}h} \Phi_{\mathrm{L},S}(D_{\mathrm{L}h}^{\mathrm{T}} P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0) \\
&= U_h P_{\mathrm{L}h} \Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0)
\end{aligned}
\tag{55}
$$

with local error

$$
\widehat{X}(t_0+h) - U_h P_{\mathrm{L}h} \Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0) = O(h^2)\,.
$$

We do not need to make an explicit choice of $D_{\mathrm{L}h}$, because, as shown by (55), $D_{\mathrm{L}h}$ cancels out of the final approximation of $\widehat{X}(t_0+h)$.

Although $\widehat{X}(t_0+h)$ is an orthogonal matrix, the approximation (55) is not in general orthogonal. Thus, it may be improved (at least qualitatively) by replacing it by the nearest orthogonal matrix. Recall the following special case of the orthogonal Procrustes problem.

Lemma 12. *If $A \in \mathbb{R}^{n\times n}$ and $A = U\Sigma V^{\mathrm{T}}$ is a conventional, constant SVD with nonnegative singular values, then UV^{T} is an orthogonal matrix nearest to A in the Frobenius norm, i.e., $Q = UV^{\mathrm{T}}$ is a solution to the orthogonal Procrustes problem*

$$
\|A - Q\| = \min_{W\in\mathcal{U}_{n,n}} \|A - W\|\,.
$$

If A is nonsingular, then the nearest orthogonal matrix is unique.

Proof. [7, Chap. 12.4] □

We use $\Omega(A)$ to denote the orthogonal matrix nearest to the nonsingular matrix A.

An Euler-like approximation to $\widehat{X}(t_0+h)$ that is also an orthogonal matrix is

$$
\begin{aligned}
\widehat{X}(t_0+h) \approx \widehat{X}_1 &=_{\mathrm{def}} \Omega(U_h P_{\mathrm{L}h} \Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0)) \\
&= U_h P_{\mathrm{L}h} \Omega(\Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0))\,.
\end{aligned}
\tag{56}
$$

If h is small enough, then (54) implies that $\Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0)$ is nonsingular and (56) is uniquely defined.

The local error of (56) is also $O(h^2)$. To see this, recall that $\widehat{X}(t_0+h)$ is itself orthogonal, so

$$\begin{aligned}
&\|\widehat{X}(t_0+h) - \Omega(U_h P_{\mathrm{L}h} \Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0)\| \\
&\leqq \|\widehat{X}(t_0+h) - U_h P_{\mathrm{L}h} \Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0)\| \\
&\quad + \|U_h P_{\mathrm{L}h} \Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0) - \Omega(U_h P_{\mathrm{L}h} \Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0))\| \\
&\leqq 2\|\widehat{X}(t_0+h) - U_h P_{\mathrm{L}h} \Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0)\| \\
&= O(h^2)\,.
\end{aligned}$$

The following lemma summarizes the above discussion.

Lemma 13. *Suppose $E(t) = \widehat{X}(t)S(t)\widehat{Y}(t)^{\mathrm{T}}$ is the minimal variation ASVD that interpolates the gregarious initial condition*

$$E(t_0) = \widehat{X}(t_0)S(t_0)\widehat{Y}(t_0)^{\mathrm{T}} = U_0 \Sigma_0 V_0^{\mathrm{T}}$$

at the generic point t_0. Suppose t_0+h is generic and

$$E(t_0+h) = U_h \Sigma_h V_h^{\mathrm{T}}$$

is a constant, gregarious SVD. Let $P_{\mathrm{L}h} \in \mathscr{P}_m$ be such that

$$\|\Phi_{\mathrm{L},S}^{\perp}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0)\| = O(h)\,.$$

Define $\widehat{X}_1$ by

$$\widehat{X}_1 = U_h P_{\mathrm{L}h} \Omega(\Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0))\,. \tag{57}$$

If h is small enough, then

$$\|\widehat{X}(t_0+h) - \widehat{X}_1\| = O(h^2)\,. \tag{58}$$

•

Given the approximation $\widehat{X}_1$, consider the problem of finding the approximation $\widehat{Y}_1 \approx \widehat{Y}(t_0+h)$. Let $E(t_0+h) = U_h \Sigma_h V_h^{\mathrm{T}}$ and $P_{\mathrm{L}h}$ be as in Lemma 13, and let $Z_{\mathrm{L}h} \in \mathscr{B}_{\mathrm{L},S}$ be the matrix

$$Z_{\mathrm{L}h} = \Omega(\Phi_{\mathrm{L},S}(P_{\mathrm{L}h}^{\mathrm{T}} U_h^{\mathrm{T}} U_0))\,.$$

Thus, $\widehat{X}_1 = U_h P_{\mathrm{L}h} Z_{\mathrm{L}h}$ and, from (53) $\widehat{Y}_1$ must be of the form

$$\widehat{Y}_1 = V_h D_h P_h D_{\mathrm{R}h} Z_h \tag{59}$$

where Z_h is a collaborator of $Z_{\mathrm{L}h}$, P_h is a permutation collaborator of $P_{\mathrm{L}h}$ and D_h, $D_{\mathrm{R}h} = \mathrm{diag}(\pm 1) \in \mathscr{D}_{n,n} \cap \mathscr{U}_{n,n}$.

The permutation P_h is determined by $P_{\mathrm{L}h}$, but D_h and possibly the final diagonal block of Z_h remain to be chosen. Reasoning as above, D_h and Z_h should be chosen to minimize $\|V_h D_h P_h D_{\mathrm{R}h} Z_h - V_0\|$. This is equivalent to choosing Z_h and $\widetilde{D}_h = P_h^T D_h P_h D_{Rh}$ to minimize $\| Z_h(V_0^T V_h P_h)\widetilde{D}_h - 1 I_n \|$. Note that $\widetilde{D}_h$ is also a diagonal matrix of ± 1's.

If $E(t_0 + h)$ has no identically zero singular values, then Z_h is determined by Z_{Lh}. Therefore, the sign of the diagonal entries of $\widetilde{D}_h$ should be chosen to be the same as the signs of the corresponding diagonal entries of $Z_h V_0^T V_h P_h$. (If some diagonal entry of $Z_h V_0^T V_h P_h$ is zero, then the approximations produced by Euler's method are not likely to be very accurate. In this case, the step size h should be reduced.)

Suppose now that $E(t_0 + h)$ has $m_k > 0$ identically zero singular values. The trailing m_k-by-m_k diagonal block of Z_h must be chosen as well as $\widetilde{D}_h$. The trailing m_k-by-m_k block of Z_h affects only the final m_k diagonal entries of $Z_h V_0^T V_h P_h \widetilde{D}_h$, so the initial $n - m_k$ diagonal entries of $\widetilde{D}_h$ should be chosen, as above, to agree with the signs of the corresponding diagonal entries of $Z_h V_0^T V_h P_h$. It is easy to check that ultimately, the signs of the final m_k diagonal entries of $\widetilde{D}_h$ cancel out of the final approximation $\widehat{Y}_1$, so they may be set arbitrarily to 1. If $W_k \in \mathscr{U}_{m_k, m_k}$ is the trailing m_k-by-m_k principal submatrix of $V_0^T V_h P_h$, then the final m_k-by-m_k block of Z_h, T_k should be chosen such that

$$(60) \qquad \| T_k^T - W_k \| = \min\{ \| Q - W_k \| \;\; | Q \in \mathscr{U}_{m_k, m_k} \} .$$

Lemma 12 may be used to determine T_k.

It can be shown using Theorem 6 and Lemma 12 that (57) minimizes the Frobenius norm distance to U_0 over all left-hand, orthogonal factors of SVD's of $E(t_0 + h)$, i.e.,

$$(61) \quad \| \widehat{X}_1 - U_0 \| = \min \left\{ \| X - U_0 \| \;\middle|\; \begin{array}{l} E(t_0 + h) = X S Y^T , \\ (X, S, Y) \in \mathscr{U}_{m,m} \times \mathscr{D}_{m,n} \times \mathscr{U}_{n,n} \end{array} \right\} .$$

Similarly, it can be shown that for the above choices of P_h, Z_h and $D_h = P_h \widetilde{D}_h P_h^T$ in (59),

$$\| \widehat{Y}_1 - V_0 \| = \min \left\{ \| Y - V_0 \| \big| E(t_0 + h) = \widehat{X}_1 S Y^T , (S, Y) \in \mathscr{D}_{m,n} \times \mathscr{U}_{n,n} \right\} .$$

3.2 Computational considerations

Lemma 13 uses $\Phi_{L,S} = \Phi_{L,\Sigma_0}$ and $\Phi_{L,S}^{\perp} = \Phi_{L,\Sigma_0}^{\perp}$ to determine $\widehat{X}_1 \approx \widehat{X}(t_0 + h)$. To aid convergence at nongeneric points, it is better to use Φ_{L,Σ_h} and $\Phi_{L,\Sigma_h}^{\perp}$ instead (see Sect. 3.3). This is done as follows. From (53), we obtain

$$(62) \qquad P_{Lh} S(t_0 + h) P_h^T D_h = \Sigma_h .$$

Both Σ_0 and $S(t)$ are gregarious, so (62) is essentially just a reordering of the groups of multiple singular values. This corresponds to reordering the diagonal blocks of $\mathscr{B}_{\mathrm{L},S}$, because

$$P_{\mathrm{L}h}\mathscr{B}_{\mathrm{L},S}P_{\mathrm{L}h}^{\mathrm{T}} =_{\mathrm{def}} \{P_{\mathrm{L}h}Z_{\mathrm{L}}P_{\mathrm{L}h}^{\mathrm{T}} | Z_{\mathrm{L}} \in \mathscr{B}_{\mathrm{L},S}\} = \mathscr{B}_{\mathrm{L},P_{\mathrm{L}h}SP_h^{\mathrm{T}}D_h} = \mathscr{B}_{\Sigma_h}.$$

Therefore, for any $W \in \mathbb{R}^{m\times m}$, we have

$$P_{\mathrm{L}h}\Phi_{\mathrm{L},S}(W)P_{\mathrm{L}h}^{\mathrm{T}} = \Phi_{\mathrm{L},\Sigma_h}(P_{\mathrm{L}h}WP_{\mathrm{L}h}^{\mathrm{T}}),$$

and

$$P_{\mathrm{L}h}\Phi_{\mathrm{L},S}^{\perp}(W)P_{\mathrm{L}h}^{\mathrm{T}} = \Phi_{\mathrm{L},\Sigma_h}^{\perp}(P_{\mathrm{L}h}WP_{\mathrm{L}h}^{\mathrm{T}}).$$

In particular (54) becomes

$$\|\Phi_{\mathrm{L},\Sigma_h}^{\perp}(U_h^{\mathrm{T}}U_0P_{\mathrm{L}h}^{\mathrm{T}})\| = O(h) \tag{63}$$

and (57) becomes

$$\begin{aligned}\widehat{X}(t_0+h) \approx \widehat{X}_1 &= \Omega(U_h\Phi_{\mathrm{L},\Sigma_h}(U_h^{\mathrm{T}}U_0P_{\mathrm{L}h}^{\mathrm{T}})P_{\mathrm{L}h}) \\ &= U_h\Omega(\Phi_{\mathrm{L},\Sigma_h}(U_h^{\mathrm{T}}U_0P_{\mathrm{L}h}^{\mathrm{T}}))P_{\mathrm{L}h}.\end{aligned} \tag{64}$$

The advantage of (63) and (64) over (54) and (57) is that the best approximation property (61) holds even if t_0 and/or t_0+h are not generic.

For computational convenience the algorithms below calculate the constant SVD (50) through the "preprocessed" SVD

$$U_0^{\mathrm{T}}E(t_0+h)V_0 = U\Sigma_hV^{\mathrm{T}}.$$

Thus, $U_h = U_0U$ and (63) and (64) become

$$\Phi_{\mathrm{L},\Sigma_h}^{\perp}(U^{\mathrm{T}}P_{\mathrm{L}h}^{\mathrm{T}}) = \Phi_{\mathrm{L},\Sigma_h}^{\perp}(P_{\mathrm{L}h}U)^{\mathrm{T}} = O(h)$$

and

$$\widehat{X}(t_0+h) \approx \widehat{X}_1 = U_0U\Omega(\Phi_{\mathrm{L},\Sigma_h}(P_{\mathrm{L}h}U))^{\mathrm{T}}P_{\mathrm{L}h}.$$

The following algorithm calculates on step of the Euler-like method described above.

Algorithm 1

Input: a constant, gregarious SVD $E_0 = U_0\Sigma_0V_0^{\mathrm{T}}$, and a constant matrix $E_1 \in \mathbb{R}^{m\times n}$

Output: a constant gregarious SVD $E_1 = \widehat{X}_1S_1\widehat{Y}_1^{\mathrm{T}}$ that approximates one point on the minimal variation SVD through $E_0 = U_0\Sigma_0V_0^{\mathrm{T}}$

1. Obtain any gregarious, constant SVD $U_0^T E_1 V_0 = U\Sigma_1 V^T$ from any good method, e.g., [4, 5, 6, 7, 16].
2. Determine the multiplicities of the singular values of Σ_1.
3. Select a permutation matrix P_L that minimizes $\|\Phi^{\perp}_{L,\Sigma_1}(P_L U)\|$. Let $P \in \mathscr{P}_n$ be its permutation collaborator.
4. Use Lemma 12 to evaluate $Z_L = \Omega(\Phi_{L,\Sigma_1}(P_L U))^T$.
5. Find a collaborator $Z \in \mathscr{B}_{L,\Sigma_1}$ of Z_L. If E_1 is full rank, then Z is determined by Z_L. Otherwise, the final block T_k of Z is given by (60), where W_k is now the trailing m_k-by-m_k principal submatrix of $P^T V$.
6. Set $D \leftarrow \text{diag}(\pm 1)$ chosen to make the diagonal entries of $V Z P D$ nonnegative.
7. Set $\widehat{X}_1 \leftarrow U_0 U Z_L P_L$; $\quad S_1 \leftarrow P_L^T \Sigma_1 P D$; $\quad \widehat{Y}_1 \leftarrow V_0 V Z P D$.

Computational details:

Step 2: Rounding errors can make this step difficult and delicate. To allow for rounding errors, it is reasonable to consider "small" singular values to be zero and to consider singular values whose relative difference is "small" to be equal. An ad-hoc, interpretation of "small" is "less than $c\|E_1\|\varepsilon$" where c is an empirically determined $O(1)$ constant and ε is the precision of the arithmetic.

Step 4: It is more efficient to assemble the SVD of $\Phi_{L,\Sigma_1}(P_L U)$ from the SVD's of the diagonal blocks (which may be as small as 1-by-1) than to treat it as a general m-by-m orthogonal Procrustes problem.)

The following algorithm is a simple Euler-like method for tracking a minimal variation SVD.

Algorithm 2

Input: An initial gregarious SVD $E(t_0) = \widehat{X}_0 S_0 \widehat{Y}_0^T$ of $E(t) \in \mathscr{A}_{m,n}$ at a generic point t_0, a step size h, and the number of steps desired, N.

Output: SVD's $E(t_0 + jh) = \widehat{X}_j S_j \widehat{Y}_j^T$ that approximate values of the minimal variation SVD through initial condition $E(t_0) = \widehat{X}_0 S_0 \widehat{Y}_0^T$ at points $t = t_0 + jh$.

– For $j = 1, 2, 3, \ldots, N$ apply Algorithm 1 with inputs $E_1 = E(t_0 + jh)$ and $E_0 = E(t_0 + (j-1)h)$, $U_0 = \widehat{X}_{j-1}$, $\Sigma_0 = S_{j-1}$ and $V_0 = \widehat{Y}_{j-1}$ to obtain the output SVD $E(t_0 + jh) = \widehat{X}_j S_j \widehat{Y}_j^T$.

We show in Sec. 3.3 that as h tends to zero, the approximations of Algorithm 2 converge to the minimum variation ASVD through the initial condition $E(t_0) = \widehat{X}_0 S_0 \widehat{Y}_0^T$. However, like Euler's method, the global error is only $O(h)$, so it converges too slowly to be an attractive numerical procedure.

A more rapidly converging procedure is obtained by applying extrapolation [11, Chapter 6]. The following algorithm is an example of an $O(h^3)$ extrapolated Euler-like method. We use it combined with a simple halving/doubling variable step size strategy to compute the numerical examples in Sect. 3.5.

Algorithm 3

Input: An analytic function $E(t) \in \mathscr{A}_{m,n}$ a step size h, an initial gregarious SVD $E(t_0) = \widehat{X}_0 S_0 \widehat{Y}_0^{\mathrm{T}}$ at a generic point t_0.

Output: An SVD $E(t_0 + h) = \widehat{X}_1 S_1 \widehat{Y}_1^{\mathrm{T}}$ that approximates a value of the minimal variation ASVD, $E(t) = \widehat{X}(t_0 + h) S(t_0 + h) \widehat{Y}(t_0 + h)^{\mathrm{T}}$, through initial condition $E(t_0) = \widehat{X}_0 S_0 \widehat{Y}_0^{\mathrm{T}}$, and an error estimate

$$\delta \approx \|\widehat{X}(t_0 + h) - \widehat{X}_1\| + \|\widehat{Y}(t_0 + h) - \widehat{Y}_1\|$$

1. For $l = 1, 2, 4$, apply Algorithm 2 with input $E_0 = \widehat{X}_0 S_0 \widehat{Y}_0^{\mathrm{T}}$ step size h/l and number of steps l to get output SVD $E_1 = X_{h/l} S_1 Y_{h/l}^{\mathrm{T}}$.
2. $\widehat{X}_1 \leftarrow \Omega\left(\frac{8X_{h/4} - 6X_{h/2} + X_h}{3}\right)$; $\quad \widehat{Y}_1 \leftarrow \Omega\left(\frac{8Y_{h/4} - 6Y_{h/2} + Y_h}{3}\right)$
3. $\delta \leftarrow \frac{1}{3}\left(\|3X_{h/2} - 2X_{h/4} - X_h\| + \|3Y_{h/2} - 2Y_{h/4} - Y_h\|\right)$

Computational Details:

Step 1: In exact arithmetic, if h is small enough, then each call to Algorithm 2 produces the same diagonal factor S_1. Rounding errors may cause the computed diagonal factors to differ by a modest multiple of the machine precision times $\|E(t_0 + h)\|$.
Step 2: The orthogonal Procrustes function Ω is used in Step 2 to insure that $\widehat{X}_1$ and $\widehat{Y}_1$ are orthogonal. Its use in Algorithm 1, Step 4 is now redundant and may be safely omitted.

Provided higher order approximations to $\Phi_{\mathrm{L},S}(\dot{X}_0(t)^{\mathrm{T}} X(t_0))$ in (47) can be obtained, it is likely that one-step numerical methods for integrating ordinary differential equations including Runge-Kutta methods, can replace Euler's method in (47) to give higher order one step methods for tracking minimum variation ASVD's. A direct formula for $\dot{X}(t)$ in terms of $E(t)$ would be the best of all such approximations. Recently, [10] provided such a formula for bases of the kernel and cokernel of $E(t)$ in the special case that $E(t)$ has constant rank. This formula could in principle be extended to compute $\dot{X}(t)$ at generic points. At this writing, we do not know how to extend the formula to nongeneric points.

3.3 Convergence

The following theorem shows that the approximations obtained from Algorithm 2 converge to $\widehat{X}(t)$ as the step size h tends to zero. This is the same kind of convergence required of numerical methods for the solution of ordinary differential equation [11].

Theorem 14. *Suppose that $E(t) \in \mathscr{A}_{m,n}[a, b]$ and $E(t) = \widehat{X}(t) S(t) \widehat{Y}(t)^{\mathrm{T}}$ is the minimum variation path through the initial condition*

$$E(t_0) = \widehat{X}_0 S_0 \widehat{Y}_0^{\mathrm{T}} \tag{65}$$

at the generic point t_0. For any $t_f \in [a, b]$, if $\widehat{X}_j(h)$ and $\widehat{Y}_j(h)$ are approximations produced by Algorithm 2 at generic points $t_j = t_0 + jh$, $j = 1, 2, 3, \ldots, N$, with initial condition (65), then

$$\lim_{N \to \infty} \widehat{X}_N((t_f - t_0)/N) = \widehat{X}(t_f)$$

and

$$\lim_{N \to \infty} \widehat{Y}_N((t_f - t_0)/N) = \widehat{Y}(t_f).$$

Proof. Let $h = h_N = (t_f - t_0)/N$, and let the error at step j be denoted by

$$\delta_j =_{\text{def}} \|\widehat{X}(t_j) - \widehat{X}_j(h)\| .$$

Observe that for all integers $N > 0$, $t_f = t_N$. We must, therefore, show that $\lim_{N \to \infty} \delta_N = 0$.

By Theorem 11, for each $j = 1, 2, 3, \ldots, N$, there exists a minimum variation ASVD $E(t) = \widehat{W}_j(t)S(t)\widehat{Q}_j(t)^{\mathrm{T}}$ which interpolates the initial condition $E(t_j) = \widehat{X}_j(h)S(t_j)\widehat{Y}_j(h)^{\mathrm{T}}$. Corollary 10 implies that there are *constant*, orthogonal, block diagonal matrices $Z_{\mathrm{L},j} \in \mathscr{B}_{\mathrm{L},S}$ and $Z_j \in \mathscr{B}_S$ such that

$$\widehat{X}(t) = \widehat{W}_j(t)Z_{\mathrm{L},j} \tag{66}$$

and

$$\widehat{Y}(t) = \widehat{Q}_j(t)Z_j .$$

The matrix $Z_{\mathrm{L},j} - I_m$ is a measure of the error made by following the minimal variation path $\widehat{W}_j(t)$ which passes through the "incorrect" initial condition $\widehat{W}_j(t_j) = \widehat{X}_j(h)$.

In terms of this notation, we can bound δ_{j+1} in terms of δ_j by

$$\begin{aligned}\delta_{j+1} &= \|\widehat{X}(t_{j+1}) - \widehat{X}_{j+1}(h)\| \\ &\leqq \|\widehat{X}(t_{j+1}) - \widehat{W}_j(t_{j+1})\| + \|\widehat{W}_j(t_{j+1}) - \widehat{X}_{j+1}(h)\| \\ &= \|Z_{\mathrm{L},j} - I_m\| + \|\widehat{W}_j(t_{j+1}) - \widehat{X}_{j+1}(h)\| \\ &= \|\widehat{X}(t_j) - \widehat{W}_j(t_j)\| + \|\widehat{W}_j(t_{j+1}) - \widehat{X}_{j+1}(h)\|\end{aligned}$$

The last step is a consequence of (66). The initial condition of $\widehat{W}_j(t)$, was $\widehat{W}_j(t_j) = \widehat{X}_j(h)$. Consequently,

$$\delta_{j+1} \leqq \delta_j + \|\widehat{W}_j(t_{j+1}) - \widehat{X}_{j+1}(h)\| . \tag{67}$$

The matrix $\widehat{X}_{j+1}(h)$ is the Euler-like approximation to $\widehat{W}_j(t_{j+1})$ given by (57) with $\widehat{W}(t)$ in place of $\widehat{X}(t)$ and t_j in place of t_0. Equation (58) gives

$$\|\widehat{W}(t_{j+1}) - \widehat{X}_{j+1}(h)\| = O(h^2).$$

With (67), this implies

$$\delta_{j+1} \leqq \delta_j + O(h^2)\,.$$

An easy induction shows

$$\delta_N \leqq \delta_0 + NO(h^2) = \delta_0 + (t_f - t_0)O(h)\,.$$

It follows that $\lim_{N\to\infty}\delta_N = \delta_0$. Then initial condition $\hat{X}(t_0)$ is known exactly from (65), so $\delta_0 = 0$. The convergence for $\hat{Y}_N((t_f - t_0)/N)$ is proved analogously. □

If t_0 is not generic and the initial condition $E(t_0) = E_0 = X_0 S_0 Y_0^T$ does not lie on an ASVD, then the methods converge to the minimum variation SVD path $E(t) = \hat{X}(t)S(t)\hat{Y}(t)^T$ such that $\|\hat{X}(t_0) - X_0\|$ is minimal. For example, if $t_0 = 0$, $E(t)$ is given by (30) with initial condition (31), then Algorithms 1,2 and 3 track the ASVD

$$E(t) = \begin{bmatrix} 2t & 0 \\ 0 & t \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 2t & 0 \\ 0 & t \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\,.$$

Suppose that $E(t) = \hat{X}(t)S(t)\hat{Y}(t)^T$ is a gregarious, minimum variation path through $E(t_0) = \hat{X}_0 S_0 \hat{Y}_0^T$ where t_0 is generic and $S(t)$ is as in (11). Suppose further that $t_1 = t_0 + h$ is nongeneric and for some $i \neq j$, $s_i(t_1) = s_j(t_1)$. Algorithm 1 applied to $E_1 = E(t_1)$ will "over cluster" by treating the two singular subspaces corresponding to $s_i(t_1)$ and $s_j(t_1)$ as one singular subspace of higher dimension. Algorithm 1 uses (64), so $\hat{X}_1$ is a minimizer of (61). Thus,

$$O(h) = \|\hat{X}(t_0 + h) - \hat{X}_0\| \geqq \|\hat{X}_1 - \hat{X}_0\|\,.$$

This implies that

$$\begin{aligned} \|\hat{X}(t_0 + h) - \hat{X}_1\| &\leqq \|\hat{X}(t_0 + h) - \hat{X}_0\| + \|\hat{X}_0 - \hat{X}_1\| \\ &= O(h) \end{aligned}$$

Although $\hat{X}_1$ may not be part of any ASVD of $E(t)$, it does lie distance $O(h)$ from its desired value of $\hat{X}(t_0 + h)$. It follows that a numerical method based on Algorithm 1 that converges to $\hat{X}(t)$ at generic points, also converges at nongeneric points.

The point $t_1 = t_0 + h$ would also be nongeneric if some singular values of $S(t)$ had a root at t_1. This case is similar to the case of intersecting singular values.

It is probably impossible to overcome this confusion of singular subspaces entirely using finite precision arithmetic. The theorem of the gap [13, p. 225] shows that an arbitrarily small perturbation of $E(t)$ in a neighborhood of the nongeneric point t_1 can make large changes in the two singular subspaces.

3.4 Extensions

With minor modifications, the numerical procedure described in Sect. 3.2 extends to calculating an analytic spectral decomposition of a symmetric matrix. If $A(t) \in \mathbb{R}^{n \times n}$ is an analytic symmetric matrix then [8, pp. 70–71, 120–122] shows that there exist an analytic matrix $X(t) \in \mathscr{U}_{n,n}$ and an analytic diagonal matrix of eigenvalues $S(t) \in \mathscr{D}_{n,n}$ such that $A(t) = X(t)S(t)X(t)^{\mathrm{T}}$. By our definitions $A(t) = X(t)S(t)X(t)^{\mathrm{T}} = X(t)S(t)Y(t)^{\mathrm{T}}$ is also an ASVD, but the symmetric eigenvalue problem requires $Y(t) = X(t)$. Even if the initial condition $A(t_0) = \hat{X}_0 S_0 \hat{Y}_0^{\mathrm{T}}$ meets the restriction $\hat{Y}_0 = \hat{X}_0$, Algorithm 1 does not necessarily set $\hat{Y}_1 = \hat{X}_1$.

Fortunately, this difficulty is easily repaired by the following modified version of Algorithm 1. Define a gregarious symmetric spectral decomposition $A(t) = X(t)S(t)X(t)^{\mathrm{T}}$, $X(t) \in \mathscr{U}_{n,n} \cap \mathscr{A}_{n,n}$, $S(t) \in \mathscr{D}_{n,n} \cap \mathscr{A}_{n,n}$ to be one such that $S(t)$ is in the form of (11) except that two diagonal entries of $S(t)$ may be negatives of one another. The following is a version of Algorithm 1 modified for the symmetric spectral decomposition.

Algorithm 4

Input: a constant, symmetric, spectral decomposition $A_0 = \hat{X}_0 S_0 \hat{X}_0^{\mathrm{T}}$ and a constant matrix $A_1 = A_1^{\mathrm{T}} \in \mathbb{R}^{n \times n}$

Output: a symmetric, spectral decomposition $A_1 = \hat{X}_1 S_1 \hat{X}_1^{\mathrm{T}}$ that approximates a point on the minimal variation path through $A_0 = \hat{X}_0 S_0 \hat{X}_0^{\mathrm{T}}$

1. Obtain a gregarious, constant spectral decomposition $\hat{X}_0^{\mathrm{T}} A_1 \hat{X}_0 = V \Lambda V^{\mathrm{T}}$ by any good numerical method, e.g., [4, 5, 7, 16].
2. Determine the multiplicities of the eigenvalues of Λ.
3. Select a permutation matrix P_{L} that minimizes $\|\Phi^{\perp}_{\mathrm{L},\Lambda}(P_{\mathrm{L}} V)\|$.
4. Use Lemma 12 to evaluate $Z_{\mathrm{L}} = \Omega(\Phi_{\mathrm{L},\Lambda}(P_{\mathrm{L}} V))^{\mathrm{T}}$.
5. Set $\hat{X}_1 \leftarrow \hat{X}_0 V Z_{\mathrm{L}} P_{\mathrm{L}}$; $\quad S_1 \leftarrow P_{\mathrm{L}}^{\mathrm{T}} \Lambda P$

A particular case of the symmetric eigenvalue problem is the dual of the singular value decomposition

$$A(t) = \begin{bmatrix} 0 & E(t) \\ E(t)^{\mathrm{T}} & 0 \end{bmatrix}. \tag{68}$$

The singular value decomposition of $E(t)$ could be constructed from the eigenvalue-eigenvector decomposition of $A(t)$. So, to treat $X(t)$ and $Y(t)$ more symmetrically one can adapt Algorithm 4 for the computation of the analytic spectral decomposition of (68).

If only one orthogonal factor or the basis of only some singular subspaces of $E(t)$ is required, then Algorithms 1,2 and 3 can be made more efficient by storing and updating only the one factor or only the appropriate columns of X or Y.

3.5 Numerical experience

To demonstrate the procedure, we tested Algorithm 3 augmented with a simple halving/doubling variable step size strategy on several examples. We used the error estimate in Algorithm 3 to adjust the step size so that in any one step, the estimated error was less than 10^{-7}. We also restricted the step size so that at any call to Algorithm 1 the output orthogonal factors and the input orthogonal factors differed in norm by no more than the ad-hoc constant 1/2. In each case, we sampled values of a minimum variation ASVD at 101 equally spaced points over the interval $[-1, 1]$, and calculated central difference approximations to the first and second derivatives of $S(t)$, $\widehat{X}(t)$ and $\widehat{Y}(t)$. The experiments were run under MATLAB [19] on an Olivetti M24 (PC/XT compatible) with math co-processor. The unit roundoff was approximately 10^{-16}.

3.5.1 Example 1

The first example is Example 1 from the introduction with initial condition at $t_0 = -1$ given by

$$E(-1) = \begin{bmatrix} \cos(-1) & \sin(-1) \\ -\sin(-1) & \cos(-1) \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} \cos(-1) & \sin(-1) \\ -\sin(-1) & \cos(-1) \end{bmatrix}.$$

Due to minor rounding errors, the computed values of the minimal variation path differed from (1) by no more than 10^{-14}. Note that these errors are almost as small as the errors that would occur by rounding the exact minimum variation path to finite precision.

3.5.2 Example 2

This is Example 2 from Sect. 2 with initial condition at $t_0 = -1$ given by

$$E(-1) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -2 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Although $t = -1$ is a nongeneric point, the initial condition lies on an ASVD, so there is a minimum variation SVD that interpolates the initial condition. In this toy problem, no rounding errors corrupted the computed values of $\widehat{X}$ and $\widehat{Y}$.

3.5.3 Example 3

This is Example 3 from Sect. 2 with initial condition at $t_0 = -1$ given by

$$E(-1) = \begin{bmatrix} \cos(-1) & -\sin(-1) \\ \sin(-1) & \cos(-1) \end{bmatrix} \begin{bmatrix} e^{-1} \\ 0 \end{bmatrix} [\ 1\ ].$$

There is no ASVD of $E(t)$ that goes past $t = 0$, so this is a severe test of the procedure. The computed values of the minimal variation differed from (9) by no more than 10^{-14} until the minimum allowed step size was reached approximately at $t = -.03$ and the integration process was abandoned. The extremely small step size is an indication that an ASVD does not exist.

3.5.4 Example 4

This is Example 5.6 from [9]:

$$E(t) = \begin{bmatrix} 2-t & 0 & 0 & t & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & t/2 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

with initial condition $E(-1) = U\Sigma V^{\mathrm{T}}$ where

$$U = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\Sigma = \begin{bmatrix} 3.1623 & 0 & 0 & 0 & 0 \\ 0 & 1.1180 & 0 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

and

$$V = \begin{bmatrix} 0.9487 & 0 & 0 & 0.3162 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0.8944 & 0 & 0 & 0.4472 \\ -0.3162 & 0 & 0 & 0.9487 & 0 \\ 0 & -0.4472 & 0 & 0 & 0.8944 \end{bmatrix}.$$

Two singular values of $E(t)$ are identically zero; one singular value is greater than 1.4 (on $[-1, 1]$); one singular value is identically equal to one; and one singular value is slightly greater than one and is tangent to the line $y = 1$ at the nongeneric point $t = 0$. The nonzero singular values are displayed in Fig. 1.

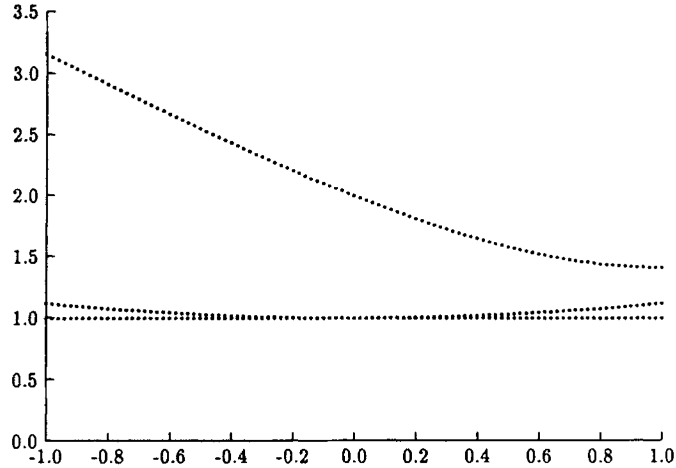

Fig. 1. Nonzero singular values from Example 4

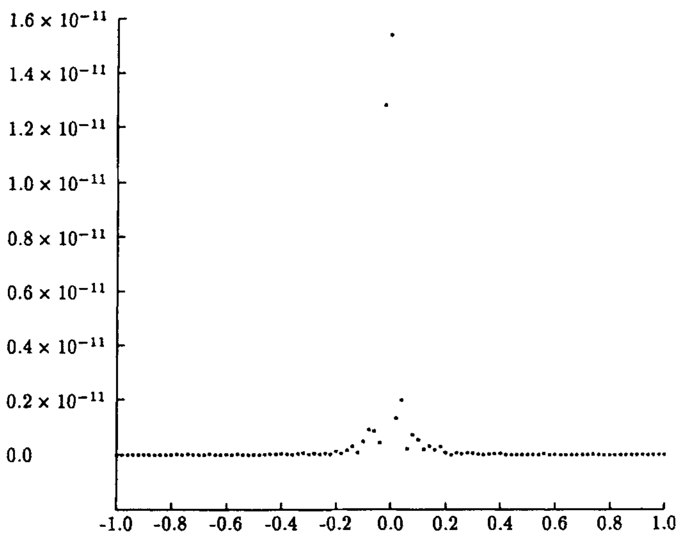

Fig. 2. Errors in $\hat{X}(t)$ from Example 4

In the minimal variation ASVD through this initial condition, $\hat{X}(t)$ is constant. The calculated values of $\hat{X}(t)$ differed from the initial condition by less than 1.6×10^{-11}. This is well under the requested local truncation error of 10^{-7}, but larger than the rounding errors in the previous examples. The computed values of $\hat{X}(t)$ remain constant to within an error of 10^{-14} until t approaches the nongeneric point $t = 0$. The singular subspaces become increasingly illconditioned as t approaches 0, because two singular values approach each other [13, p. 225]. The effect of rounding errors on the computed values of $\widehat{X}$ and $\widehat{Y}$ become greater and greater. Until the two converging singular values are close enough to be clustered as a double singular value, there is nothing the extrapolated Euler procedure can do to remove the rounding error generated perturbations in these subspaces. Once t has passed through the region of illcondition, the computed values of $\widehat{X}(t)$ settle back to an approximate constant.

Figure 2 is a graph of the errors in the computed values of $\|\widehat{X}(t)\|$ at the 101 test points. Note the scale of the ordinate. The peak around $t = 0$ is the effect of rounding errors on the ill-conditioned singular subspaces near the nongeneric point $t = 0$. The local truncation error of the numerical method contributes only to the error at $t = 0$.

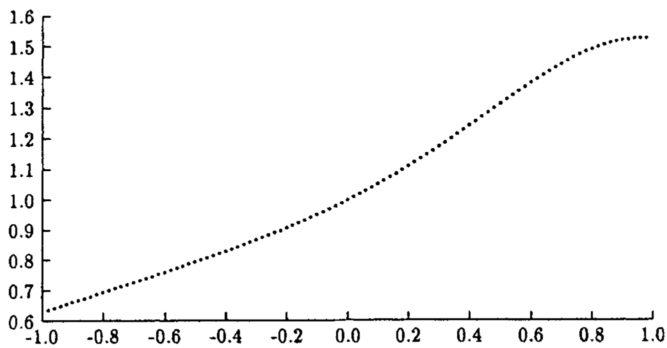

Fig. 3. $\|d\widehat{Y}/dt\|$ from Example 4

Figure 3 is a graph of the approximations to $\|d\widehat{Y}/dt\|$ obtained by a central difference approximation at the 99 interior test points. Despite rounding errors, multiple singular values and integration through the nongeneric point at $t = 0$, the empirical observation that $\|d\widehat{Y}/dt\|$ is smooth agrees with the theoretical expectation.

3.5.5 Example 5

To force the numerical method to resolve a nontrivial amount of nonuniqueness at every step, this example has multiple singular value paths and nongeneric points $t = -1, 0, 1$. The matrix $E(t)$ is constructed from the ad-hoc ASVD $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ where $Y(t) = I$,

$$S(t) = \begin{bmatrix} -t & 0 & 0 & 0 \\ 0 & -t & 0 & 0 \\ 0 & 0 & t^2 & 0 \\ 0 & 0 & 0 & t^2 \end{bmatrix}$$

$X(t) = \exp(tK)$ and $K \in \mathbb{R}^{4\times 4}$ is the skew symmetric matrix

$$K = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 2 & 0 \\ 0 & -2 & 0 & 3 \\ 0 & 0 & -3 & 0 \end{bmatrix}.$$

We use initial condition $E(-1) = U\Sigma V^{\mathrm{T}}$ where $U = \exp(-K)$, $\Sigma = S(-1)$ and $V = I$. Although $t = -1$ is not generic, the initial condition lies on an ASVD, so there exists a minimal variation ASVD, $E(t) = \hat{X}(t)S(t)\hat{Y}(t)$ through $E(-1) = U\Sigma V^{\mathrm{T}}$.

Corollary 9 implies that

$$\hat{X}(t) = \exp(tK)\exp((t+1)L^{\mathrm{T}})$$

and

$$\hat{Y}(t) = \exp((t+1)L^{\mathrm{T}})$$

where $L \in \mathbb{R}^{4\times 4}$ is the skew symmetric matrix

$$L = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 \\ 0 & 0 & -3 & 0 \end{bmatrix}.$$

The orthogonal factors of the minimum variation ASVD have variations $Vrn(\hat{X}(t)) = 5.65$ and $Vrn(\hat{Y}(t)) = 8.94$. The orthogonal factors of the original ASVD have variations $Vrn(X(t)) = 10.58$ and $Vrn(Y(t)) = 0$.

The values of $\hat{X}(t)$ computed by our program differed from the exact values by less than 1.6×10^{-10}. The error estimate in Algorithm 3 tends to be conservative, so we are not surprised that the observed errors are significantly smaller than the requested local truncation error of 10^{-7}. Because this example has multiple singular values, the local truncation error of the numerical method dominated the rounding errors.

4 Conclusions

A real analytic singular value decomposition (ASVD) of a path of matrices $E(t)$ is a real analytic path of factorization $E(t) = X(t)S(t)Y(t)^{\mathrm{T}}$ where $X(t)$ and $Y(t)$ are orthogonal and $S(t)$ is diagonal. If $E(t) \in \mathbb{R}^{m\times m}$ is analytic on $[a, b]$ and

$$E(t_0) = X_0 S_0 Y_0^{\mathrm{T}} \tag{69}$$

is any singular value decomposition at a generic point $t = t_0$, there is a unique ASVD $E(t) = \hat{X}(t)S(t)\hat{Y}(t)$ that interpolates (69), minimizes

$$Vrn(\hat{X}(t)) = \int_a^b \left\| \frac{d\hat{X}}{dt} \right\| dt, \tag{70}$$

and minimizes $Vrn(\widehat{Y}(t))$ subject to (70) being minimum. For some values of t, the diagonal entries of $S(t)$ may be negative and may not be in nonincreasing order.

An extrapolated-Euler-like method that treats the computation of the minimal variation SVD as the solution of a differential equation has proven to be an effective method of tracking the minimal variation SVD.

The techniques used for the singular value decomposition extend to the symmetric eigenvalue problem.

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