CONTINUATION OF SINGULAR VALUE DECOMPOSITIONS

LUCA DIECI, M. GRAZIA GASPARO, AND ALESSANDRA PAPINI

Abstract. In this work we consider computing a smooth path for a (block) singular value decomposition of a full rank matrix valued function. We give new theoretical results and then introduce and implement several algorithms to compute a smooth path. We illustrate performance of the algorithms with a few numerical examples.

1. Introduction

Frequently, one needs to find decompositions of nearby matrices, for example their *singular value decomposition*, SVD. Of course, it is quite natural to inquire whether or not one can use the work done to obtain the SVD of a matrix to obtain the SVD of a nearby matrix. In general, it is hard to imagine that this will be possible, unless the factors themselves will be close, not just the matrices. A reasonable mathematical framework to study this problem is the following: We consider a matrix valued function depending smoothly on a real parameter: $A : t \in [0,1] \to \mathbb{R}^{m\times n}$, $m \geq n$, and assume that A is of full rank n for all t. [Of course, the restriction to the interval $[0,1]$ is for convenience only. Any interval, even the entire real line, is in principle allowed]. Under certain nondegeneracies conditions on A, which will guarantee that our goal is feasible, our task in this work is to compute a smooth path of block singular value decompositions (SVDs) for A.

We must make two immediate observations: (i) In general, see [6], the factors vary less smoothly than the original function A, and (ii) moreover, even when the factors themselves can be chosen to vary as smoothly as A, the standard algorithms used in matrix computations do not generally deliver these smoothly varying factors.

Let us now summarize the problem that we consider and our computational goal.

(P) Given a matrix valued function $A \in \mathcal{C}^s([0,1], \mathbb{R}^{m\times n})$, $s \geq 1$, $m \geq n$, of rank n. Suppose that A has p groups of singular values ($p \leq n$) which stay disjoint and vary continuously for all t, call them $\Sigma_1, \dots, \Sigma_p$. We want to transform A with orthogonal transformations $U \in \mathcal{C}^s([0,1], \mathbb{R}^{m\times m})$ and $V \in \mathcal{C}^s([0,1], \mathbb{R}^{n\times n})$ so that $U^TAV = \begin{bmatrix} S \\ 0 \end{bmatrix}$, where $S = \mathrm{diag}(S_i,\ i = 1, \dots, p)$, the diagonal blocks S_i are symmetric positive definite, and the eigenvalues of the S_i coincide with the Σ_i, $i = 1, \dots, p$.

1991 *Mathematics Subject Classification.* 65F15, 65F99.

Key words and phrases. Continuation, singular value decomposition, symmetric function, tridiagonal and bidiagonal forms, Riccati equations.

This work was supported in part under NSF Grant DMS-0139895, and INDAM-GNCS and MIUR Rome-Italy .

In the above problem, the limiting cases are $p = 1$ and $p = n$. In case $p = 1$, we are effectively obtaining the decomposition $A = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} S \\ 0 \end{bmatrix} V^T$, from which we can read off the polar decomposition of A, namely $A = (U_1 V^T)(V S V^T)$, and a smooth basis for the left null space $\mathcal{N}(A^T)$, namely U_2. In case $p = n$, we are obtaining the complete SVD of A.

Remark 1.1. In the study of dynamical systems, a situation of interest is that of $p = 2$, corresponding to the singular values less than 1, respectively greater than 1: E.g., this is the case for hyperbolic fixed points. However, in general, it is not at all clear to us how to choose p a priori, though some indication may be provided by an initial SVD of $A(0)$. In future work, we anticipate removing all together the assumption of distinct singular values.

The theoretical justification of feasibility of the task can be found in [4, 6] for the $\mathcal{C}^s$ case, and in [3] for the analytic case. Earlier contributions on this topic are also found in the book of Kato [12] and the work [9]. Numerical studies have mostly focused on the analytic case: [3, 13] use least variation ideas based on the early work of Rheinboldt, [14], while [16] explicitely integrates the differential equations associated with the analytic path. These early numerical techniques have merits as well as drawbacks. In our opinion, the main merit of the algebraic techniques of [3, 13] is that one ends up (conceptually) with the exact factors, and the main drawback is that it is not clear how to proceed adaptively in time, i.e., where to seek the SVDs. The technique of Wright, [16], on the other hand, is amenable to adaptive time stepping, but fails to produce exact factors. Conceivably, both the algebraic technique of [3, 13] and the differential equation technique of [16] may be adapted to remedy their shortcomings; e.g., renewed effort is being spent on self correcting integration techniques, see [2]. However, our point of view is to combine the merits of the above approaches, thereby providing exact factors while adaptively choosing the time sequence where the factors are found, along the lines of our works [7, 8]. Indeed, the present work is most closely related to [8]. In the present work, we make several new theoretical and algorithmic contributions, in particular: We give new constructive results to obtain smooth orthonormal bases for $\mathcal{N}(A^T)$, smooth polar factorizations, smooth bidiagonalizations. Also our algorithms and implementations are new.

A plan of this work is as follows. In the next section we give theoretical results on smoothness of SVD-like and related decompositions. In particular, we give **constructive** results on how to obtain a smooth factorization like $U^T A V = \begin{bmatrix} P \\ 0 \end{bmatrix}$ with P positive definite, from which we easily read off a smooth orthonormal basis for $\mathcal{N}(A^T)$, and we also give some new results on smooth tridiagonalization of symmetric functions and on smoothness of bidiagonalization of unsymmetric functions, adapting results of [8] related to Hessenberg forms. In §3 we discuss our algorithms and give implementation details. In §4 we present numerical results on some test cases.

2. SVD and related decompositions

The following well known result gives the theoretical justification of our goal. We present it in a form adapted from [4, Theorem 2.4].

Theorem 2.1. *Let A be a $\mathcal{C}^s$, $s \geq 1$, matrix valued function, $t \in [0,1] \to A(t) \in \mathbb{R}^{m\times n}$, $m \geq n$, of rank n, having p disjoint groups of singular values ($p \leq n$) that vary continuously for all t: $\Sigma_1, \dots, \Sigma_p$. Let $z = m - n$. Consider the function $M \in \mathcal{C}^s([0,1], \mathbb{R}^{(m+n)\times(m+n)})$ given by*

$$M(t) = \begin{bmatrix} 0 & A(t) \\ A^T(t) & 0 \end{bmatrix}. \tag{2.1}$$

Then, there exists orthogonal $Q \in \mathcal{C}^s([0,1], \mathbb{R}^{(m+n)\times(m+n)})$ of the form

$$Q(t) = \begin{bmatrix} U_2(t) & U_1(t)/\sqrt{2} & U_1(t)/\sqrt{2} \\ 0 & V(t)/\sqrt{2} & -V(t)/\sqrt{2} \end{bmatrix} \tag{2.2}$$

such that

$$Q^T(t)M(t)Q(t) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & S(t) & 0 \\ 0 & 0 & -S(t) \end{bmatrix} \tag{2.3}$$

where S is $S = \mathrm{diag}(S_i,\ i = 1, \dots, p)$, and each S_i is symmetric positive definite, and its eigenvalues coincide with the Σ_i, $i = 1, \dots, p$. In (2.2), we have $U_2 \in \mathcal{C}^s([0,1], \mathbb{R}^{m\times z})$, $U_1 \in \mathcal{C}^s([0,1], \mathbb{R}^{m\times n})$, and $V \in \mathcal{C}^s([0,1], \mathbb{R}^{n\times n})$. Equivalently, if we let $U = \begin{bmatrix} U_1 & U_2 \end{bmatrix}$, then

$$U^T(t)A(t)V(t) = \begin{bmatrix} S(t) \\ 0 \end{bmatrix}, \tag{2.4}$$

with the previous form of S.

Proof. The proof is a straightforward adaptation of the proof of [4, Theorem 2.4] and is therefore omitted. □

It is worth stressing that Theorem 2.1 goes both ways. That is, if we have Q giving the form (2.3), then Q is of the form (2.2) and we can recover the SVD for A in (2.4). On the other hand, from the SVD in (2.4), partitioning $U = \begin{bmatrix} U_1 & U_2 \end{bmatrix}$, we can recover Q as in (2.2) and (2.3). Of course, in practice we do not work with M, but only with A, thereby avoiding doubling the dimension of the problem.

2.1. **The left null–space: $\mathcal{N}(A^T)$.** First of all, we now show how we can (and do) obtain a smooth transformation which gives explicitly an orthonormal basis for the left null–space $\mathcal{N}(A^T)$, i.e., U_2 in (2.2).

Suppose that at $t = t_0$ (initially $t_0 = 0$), we have $\widetilde{U}(t_0)$, $\widetilde{V}(t_0)$ and $\widetilde{A}_1(t_0)$ such that $\widetilde{U}^T(t_0)A(t_0)\widetilde{V}(t_0) = \begin{bmatrix} \widetilde{A}_1(t_0) \\ 0 \end{bmatrix}$, where $\widetilde{A}_1(t_0) \in \mathbb{R}^{n\times n}$ is invertible. Let $t_1 > t_0$ be such that, for $t \in [t_0, t_1]$, the function $\widetilde{A}(t) = \widetilde{U}^T(t_0)A(t)\widetilde{V}(t_0)$ has the leading $(n \times n)$-block invertible. In other words, letting $\widetilde{A}(t) = \begin{bmatrix} \widetilde{A}_{11}(t) \\ \widetilde{A}_{21}(t) \end{bmatrix}$, where for all $t \in [t_0, t_1]$ $\widetilde{A}_{11}(t) \in \mathbb{R}^{n\times n}$ and $\widetilde{A}_{21}(t) \in \mathbb{R}^{z\times n}$, we have that $\widetilde{A}_{11}(t)$ is invertible. [Notice that, if t is sufficiently close to t_0, because of continuity we will have $\widetilde{A}_{21}(t) \approx 0$, and $\widetilde{A}_{11}(t)$ certainly invertible].

For all $t \in [t_0, t_1]$, we can annihilate $\widetilde{A}_{21}$ with a Gauss transformation:

$$\begin{bmatrix} I_n & 0 \\ -X_z(t) & I_z \end{bmatrix} \begin{bmatrix} \widetilde{A}_{11}(t) \\ \widetilde{A}_{21}(t) \end{bmatrix} = \begin{bmatrix} \widetilde{A}_{11}(t) \\ 0 \end{bmatrix} ,$$

so that $X_z : t \to \mathbb{R}^{z \times n}$ satisfies

$$X_z(t)\widetilde{A}_{11}(t) = \widetilde{A}_{21}(t) \qquad \text{or} \qquad \widetilde{A}_{11}^T(t)X_z^T(t) = \widetilde{A}_{21}^T(t) .$$

Observe that X_z is a $\mathcal{C}^s$ function as long as $\widetilde{A}_{11}$ remains invertible. Of course, for t close to t_0, we will have $X_z \approx 0$.

Next, for all $t \in [t_0, t_1]$, we seek to replace the smooth basis $\begin{bmatrix} -X_z^T(t) \\ I_z \end{bmatrix}$ for $\mathcal{N}(\widetilde{A}^T)$ by a smooth orthonormal basis while at the same time obtaining a smooth basis for its orthogonal complement. That is, we seek a smooth factorization of the function $\begin{bmatrix} -X_z(t)^T \\ I_z \end{bmatrix}$ in the form $\begin{bmatrix} -X_z(t)^T \\ I_z \end{bmatrix} = \begin{bmatrix} \widehat{U}_2(t) & Q_1(t) \end{bmatrix} \begin{bmatrix} R_1(t) \\ 0 \end{bmatrix}$, where $R_1(t) \in \mathbb{R}^{z \times z}$ is smooth and upper triangular (with positive diagonal) and $\begin{bmatrix} \widehat{U}_2(t) & Q_1(t) \end{bmatrix}$ is orthogonal and smooth. We remark that the existence of such smooth factorization is guaranteed since $\begin{bmatrix} -X_z(t)^T \\ I_z \end{bmatrix}$ is full rank (e.g., see [6]). Equivalently, premultiplying by $\left[\begin{smallmatrix} 0 & I_z \\ I_n & 0 \end{smallmatrix}\right]$, we seek

$$\begin{bmatrix} I_z \\ -X_z(t)^T \end{bmatrix} = \begin{bmatrix} 0 & I_z \\ I_n & 0 \end{bmatrix} \begin{bmatrix} \widehat{U}_2(t) & Q_1(t) \end{bmatrix} \begin{bmatrix} R_1(t) \\ 0 \end{bmatrix} . \tag{2.5}$$

One possible way to achieve (2.5) is to simply consider the enlarged function $\begin{bmatrix} I_z & 0 \\ -X_z^T & I_n \end{bmatrix}$, and then take the unique QR factorization (orthogonal/triangular) of this enlarged function by requiring the diagonal of the triangular factor to be positive. Since it is known that such QR factorization is smooth, we would be done. However, we do not want to explicitly take the QR factorization of the enlarged function $\begin{bmatrix} I_z & 0 \\ -X_z^T & I_n \end{bmatrix}$, since this would lead to an algorithm costing $O(m^3)$ flops. Using Householder reductions, which would only require working with $\begin{bmatrix} I_z \\ -X_z^T \end{bmatrix}$ while delivering a basis also for the orthogonal complement, must be discarded since generally Householder transformations do not give smooth bases. Our idea is to find a smooth QR–like factorization of the enlarged function $T := \begin{bmatrix} I_z & 0 \\ -X_z^T & I_n \end{bmatrix}$, while only working with $\begin{bmatrix} I_z \\ -X_z^T \end{bmatrix}$ one column at the time. We propose a construction based on the following Theorems.

Theorem 2.2. *Let $y : t \to \mathbb{R}^n$ be a $\mathcal{C}^s$ function. Then, the functions below have the stated form and all are $\mathcal{C}^s$ functions.*

(i) *Positive definite square root. If $y \neq 0$:*

$$(I + yy^T)^{1/2} = I + \alpha yy^T \quad \text{with} \quad \alpha = \frac{\sqrt{1+y^Ty}-1}{y^Ty}. \tag{2.6}$$

If $y = 0$, then the unique positive definite square root is the identity.

(ii) *Inverse (assume $\alpha y^T y \neq -1$):*

$$(I + \alpha yy^T)^{-1} = I - \beta yy^T \quad \text{with} \quad \beta = \frac{\alpha}{1+\alpha y^Ty}. \tag{2.7}$$

(iii) *Inverse square root:*

$$(I + yy^T)^{-1/2} = I - \beta yy^T, \tag{2.8}$$

where β is given in (2.7)*, with α given in* (2.6)*.*

Proof. If the stated expressions are correct, smoothness follows at once. Equation (2.7) is well known and easily verified. To verify (2.6), multiply both left and right hand sides by themselves: there are two possible choices for α, the given one ensures positive definiteness of the square root. Finally, to show (2.8) rewrite $(I + yy^T)^{-1/2} = \big((I + yy^T)^{1/2}\big)^{-1}$ and use (2.6) and (2.7). □

Theorem 2.3. *Let $y : t \to \mathbb{R}^n$ be a $\mathcal{C}^s$ function, and let $\widehat{L} : t \to \mathbb{R}^{n\times n}$ be an invertible $\mathcal{C}^s$ function. Let p be any of the values $p = z, z-1, \dots, 1$. Then, the $\mathcal{C}^s$ matrix valued function $L := \begin{bmatrix} 1 & 0 & 0 \\ 0 & I_{p-1} & 0 \\ y & 0 & \widehat{L} \end{bmatrix}$ admits the $\mathcal{C}^s$ factorization $L = QB$, where Q is orthogonal and given by*

$$Q = \begin{bmatrix} 1 & 0 & -y^T \\ 0 & I_{p-1} & 0 \\ y & 0 & I_n \end{bmatrix} \begin{bmatrix} (1+y^Ty)^{-1/2} & 0 & 0 \\ 0 & I_{p-1} & 0 \\ 0 & 0 & (I_n + yy^T)^{-1/2} \end{bmatrix}$$

and B is given by

$$B = \begin{bmatrix} (1+y^Ty)^{1/2} & 0 & (1+y^Ty)^{-1/2}y^T\widehat{L} \\ 0 & I_{p-1} & 0 \\ 0 & 0 & (I_n + yy^T)^{-1/2}\widehat{L} \end{bmatrix}.$$

In these formulas, the given square roots are always the unique positive definite square roots.

Proof. The given form of the factorization, as well as the orthogonality of Q, can be directly verified. The smoothness properties are a consequence of the stated form, smoothness of y, and the explicit expressions for functions of rank one updates given in Theorem 2.2. □

Now we can find the desired factorization (2.5). The construction rests on Theorem 2.3 and goes as follows. Let $(-X_z)^T$ be written column-wise as $(-X_z)^T = \begin{bmatrix} y_1 & y_2 & \dots & y_z \end{bmatrix}$. Let $L_j = \begin{bmatrix} 1 & 0 & 0 \\ 0 & I_{z-j} & 0 \\ y_j & 0 & I_n \end{bmatrix}$, $j = 1, \dots, z$, and rewrite T as $T = T_1 T_2 \dots T_z$, where

$$T_j = \begin{bmatrix} I_{j-1} & 0 \\ 0 & L_j \end{bmatrix} .$$

Using Theorem 2.3, factor $T_1 = Q_{11} B_1$, and notice that $B_1 T_2$ has the form (R_{11} is a scalar)

$$B_1 T_2 = \begin{bmatrix} R_{11} & * & * & * \\ 0 & 1 & 0 & 0 \\ 0 & 0 & I_{z-2} & 0 \\ 0 & \widehat{B}_1 y_2 & 0 & \widehat{B}_1 \end{bmatrix} .$$

So, we can again use Theorem 2.3 on the unreduced part of $B_1 T_2$, that is $\begin{bmatrix} 1 & 0 & 0 \\ 0 & I_{z-2} & 0 \\ \widehat{B}_1 y_2 & 0 & \widehat{B}_1 \end{bmatrix}$. Proceeding this way, we obtain (2.5).

At this point, we perform the transformation

$$\begin{bmatrix} Q_1^T(t) \\ \widehat{U}_2^T(t) \end{bmatrix} \widetilde{A}(t) = \begin{bmatrix} Q_1^T(t)\widetilde{A}(t) \\ 0 \end{bmatrix} \equiv \begin{bmatrix} \widetilde{A}_1(t) \\ 0 \end{bmatrix} \tag{2.9}$$

where $\widetilde{A}_1 \in \mathbb{R}^{n\times n}$ is an invertible $\mathcal{C}^s$ function for $t \in [t_0, t_1]$. From (2.9), recalling that $\widetilde{A}(t) = \widetilde{U}(t_0)^T A(t) \widetilde{V}(t_0)$, it is trivial to obtain a smooth orthonormal basis for $\mathcal{N}(A^T)$.

So, we have smoothly transformed the problem into a square problem. We now seek a smooth SVD for this square matrix valued function. We will do this in two different ways (see §3.2 and §3.3), and for one of them, see §3.2, the first step will be to transform $\widetilde{A}_1$ to a symmetric positive definite function. We discuss this next.

2.2. The polar form.

Now, suppose that at $t = t_0$ (initially $t_0 = 0$), we have $U_1(t_0)$, $V(t_0)$ and $P(t_0)$ such that $U_1^T(t_0)\widetilde{A}_1(t_0)V(t_0) = P(t_0)$, where $P(t_0)$ is symmetric positive definite. For $t \in [t_0, t_1]$, define $\widehat{A}_1(t) = U_1^T(t_0)\widetilde{A}_1(t)V(t_0)$ and notice that if t is close to t_0 then $\widehat{A}_1(t)$ is nearly symmetric positive definite.

We next present a constructive procedure to obtain a smooth decomposition

$$\widehat{U}_1^T(t)\widehat{A}_1(t)\widehat{V}(t) = P(t) , \tag{2.10}$$

with $\widehat{U}_1$ and $\widehat{V}$ orthogonal and P symmetric positive definite. Notice that the existence of (2.10) is guaranteed by Theorem 2.1; see also [6]. We remark that $\widehat{U}_1^T(t)$, $\widehat{V}(t)$, and $P(t)$, are not unique. The measure of non-uniqueness is given by a similarity transformation of (2.10) with an orthogonal function $Q(t)$; that is, with respect to a given choice of $\widehat{U}_1^T(t)$, $\widehat{V}(t)$, and $P(t)$, all other possibilities are in the equivalence class given by

$$\big(Q^T(t)\widehat{U}_1^T(t)\big)\widehat{A}_1(t)\big(\widehat{V}(t)Q(t)\big) = Q^T(t)P(t)Q(t) ,$$

where Q is an orthogonal $\mathcal{C}^s$ function. What is important is that –within this equivalence class– the function $Y(t) = \widehat{V}(t)\widehat{U}_1^T(t)$ is unique, and, moreover, that for t sufficiently close to t_0, $Y(t)$ is close to the identity. Thus, to find a smooth choice for $\widehat{U}_1^T(t)$ and $\widehat{V}(t)$, we will use the following procedure.

For all $t \geq t_0$, for which $(I + Y(t))$ is invertible, let us formally define the function

$$X(t) = (I - Y(t))(I + Y(t))^{-1}\,. \tag{2.11}$$

Observe that such X is a smooth function as long as $(I + Y(t))$ is invertible, which for us is guaranteed since we will always have Y close to the identity. Observe also that $X(t)$ is nothing but the Cayley transform of $Y(t)$, which is orthogonal, and hence $X(t)$ is skew-symmetric as long as it is defined. Our idea, then, is to find X, and from it recover smooth representatives $\widehat{U}_1$ and $\widehat{V}$. To find X we can use the following.

Theorem 2.4. *For $t \geq t_0$ such that the stated inverse in* (2.11) *is defined, $X(t)$ in* (2.11) *satisfies the Riccati equation*

$$(\widehat{A}_1 - \widehat{A}_1^T) + X(\widehat{A}_1 - \widehat{A}_1^T)X + X(\widehat{A}_1 + \widehat{A}_1^T) + (\widehat{A}_1 + \widehat{A}_1^T)X = 0\,. \tag{2.12}$$

Proof. From (2.10) we have

$$(\widehat{V}\widehat{U}_1^T)\widehat{A}_1 - \widehat{A}_1^T(\widehat{U}_1\widehat{V}^T) = 0\,. \tag{2.13}$$

Furthermore, inversion of the Cayley transform in (2.11) gives

$$\widehat{V}\widehat{U}_1^T = (I - X)(I + X)^{-1}\,, \quad \widehat{U}_1\widehat{V}^T = (I - X)^{-1}(I + X)\,.$$

Using this in (2.13), we obtain the result. □

Now, we stress once more that for t close to t_0, we expect the antisymmetric part of $\widehat{A}_1(t)$ to be near 0. So, at least for t sufficiently close to t_0, $X(t)$ is the isolated solution of (2.12) near 0 (e.g., see [5]), and it is a smooth function of t.

To rebuild smooth $\widehat{U}_1$ and $\widehat{V}$, we proceed as follows. Consider –for explanatory purposes only– the function $\widetilde{M}$ defined by

$$\widetilde{M}(t) = \begin{bmatrix} 0 & \widehat{A}_1(t) \\ \widehat{A}_1^T(t) & 0 \end{bmatrix}$$

and the orthogonal matrix $R_0 = \frac{1}{\sqrt{2}}\begin{bmatrix} I & -I \\ I & I \end{bmatrix}$, so that

$$R_0^T\widetilde{M}(t)R_0 = \frac{1}{2}\begin{bmatrix} \widehat{A}_1(t) + \widehat{A}_1^T(t) & \widehat{A}_1(t) - \widehat{A}_1^T(t) \\ -\widehat{A}_1(t) + \widehat{A}_1^T(t) & -\widehat{A}_1(t) - \widehat{A}_1^T(t) \end{bmatrix} \equiv \widehat{M}(t)\,. \tag{2.14}$$

Then, the Riccati equation satisfied by $X(t)$ arises from the following transformation

$$\begin{bmatrix} I_n & 0 \\ -X(t) & I_n \end{bmatrix}\widehat{M}(t)\begin{bmatrix} I_n & 0 \\ X(t) & I_n \end{bmatrix} = \begin{bmatrix} * & * \\ 0 & * \end{bmatrix}\,,$$

so that in the upper block we have clustered the positive eigenvalues of $\widehat{M}(t)$. [Recall that the eigenvalues of $\widehat{M}(t)$ come in $\pm$ pairs and that there are no 0 eigenvalues]. So, what we need to do is to replace $\begin{bmatrix} I_n \\ X \end{bmatrix}$ by a smooth orthonormal basis. This is trivially accomplished by taking the QR factorization of $\begin{bmatrix} I_n \\ X \end{bmatrix}$: $\begin{bmatrix} I_n \\ X \end{bmatrix} = Q_1R_1$, with $Q_1 \in \mathbb{R}^{2n\times n}$

orthonormal and $R_1 \in \mathbb{R}^{n\times n}$ upper triangular with positive diagonal. As it is well known (e.g., see [6]), these factors are smooth. At this point, we set

$$\widehat{Q}_1(t) \equiv R_0 Q_1$$

so that $\widehat{Q}_1 \in \mathcal{C}^s(\mathbb{R}, \mathbb{R}^{2n\times n})$ remains orthonormal. Finally, partitioning

$$\widehat{Q}_1(t) = \begin{bmatrix} \widehat{Q}_{11}(t) \\ \widehat{Q}_{21}(t) \end{bmatrix}$$

we choose

$$\widehat{U}_1(t) = \sqrt{2}\widehat{Q}_{11}(t)\,, \quad \widehat{V}(t) = \sqrt{2}\widehat{Q}_{21}(t)\,, \tag{2.15}$$

and we notice that our choice is such that for t sufficiently close to t_0, both $\widehat{U}_1(t)$ and $\widehat{V}(t)$ are close to I_n. With these choices, we have what we wanted

$$\widehat{U}_1^T(t)\big(U_1^T(t_0)\widetilde{A}_1(t)V(t_0)\big)\widehat{V}(t) = P(t)\,,$$

and we can update the orthogonal factors:

$$U_1(t) \leftarrow U_1(t_0)\widehat{U}_1(t)\ , \quad V(t) \leftarrow V(t_0)\widehat{V}(t)\,.$$

2.3. **Simplifying structure.** We conclude this section with results which justify some of the algorithmic choices to be explained in §3. Some results are about smooth tridiagonalization (with orthogonal functions) of a symmetric function, others are about smooth bi-diagonalization (with orthogonal transformations) of a general matrix valued function. We can think of the tridiagonalization result as being useful to find the Schur decomposition of the symmetric function $P(t)$ of (2.10), while we can think of the bidiagonalization result as being useful to directly find the SVD of the function $\widetilde{A}_1(t)$ in (2.9).

In the Theorems below we make assumptions about unreduced tridiagonal, respectively bidiagonal, structure. It is important to recall the implications of these assumptions. In particular, recall that:

- An unreduced symmetric tridiagonal matrix (or matrix valued function) has distinct eigenvalues;
- An unreduced bidiagonal matrix (or matrix valued function) has distinct singular values.

Theorem 2.5. *Let $P : t \to \mathbb{R}^{m\times m}$ be a $\mathcal{C}^s$ symmetric function. Then, P can be brought to tridiagonal form with a $\mathcal{C}^s$ orthogonal function Q if, for any given t, the matrices $P(t)$ can be brought to unreduced tridiagonal form with an orthogonal matrix whose first column is given by $Q(t)e_1$.*

Proof. This is an adaptation of [8, Theorem 2], which was concerned with unreduced smooth lower Hessenberg form in the non-symmetric case (obviously, a symmetric lower Hessenberg matrix is tridiagonal). We must only remark that the assumption in [8, Theorem 2] that the vector $Q(t)e_1$ be a constant vector is not necessary: Indeed, the arguments in the cited work go through immediately by requiring that $Q(\cdot)e_1 \in \mathcal{C}^s$. □

Theorem 2.6. *Let $\widetilde{A}_1 : t \to \mathbb{R}^{n\times n}$ be an invertible $\mathcal{C}^s$ function. Then, $\widetilde{A}_1$ can be brought to upper bidiagonal form, $U^T\widetilde{A}_1V$, with $\mathcal{C}^s$ orthogonal functions U and V if, for any given t, the matrices $\widetilde{A}_1(t)$ can be brought to unreduced upper bidiagonal form with orthogonal matrices whose first columns are $U(t)e_1 = \widetilde{A}_1(t)e_1/\left\|\widetilde{A}_1(t)e_1\right\|$, and $V(t)e_1 = e_1$.*

Proof. The statement is equivalent to the requirement that $\widetilde{A}_1\widetilde{A}_1^T$ can be smoothly brought to tridiagonal form with a function U whose first column, for all t, is given by $U(t)e_1 = \widetilde{A}_1(t)e_1/\left\|\widetilde{A}_1(t)e_1\right\|$, and the symmetric function $\widetilde{A}_1^T\widetilde{A}_1$ can be smoothly brought to tridiagonal form with a function V whose first column is e_1, for all t. Then, the result follows from Theorem 2.5 and the "uniqueness" of the orthogonal factors given by the implicit Q-theorem, see [11]. □

With an eye to the algorithms of §3, we now give two new theoretical results which simplify further the structure of a smooth unreduced tridiagonal, or bidiagonal, function by using smooth unit (block) lower triangular transformations. Besides our own algorithmic motivation, these results appear interesting on their own rights. The first Theorem below is a special case of [8, Theorem 6].

Theorem 2.7. *Let $H \in \mathcal{C}^s([0,1],\mathbb{R}^{n\times n})$, $s \geq 1$, be an unreduced symmetric tridiagonal function with p groups of eigenvalues $\Lambda_1(t),\dots,\Lambda_p(t)$, that vary continuously, of dimensions $n_1,\dots,n_p$, for all $t\in[0,1]$. Write H in block notation as* $H = \begin{bmatrix} H_{11} & H_{12} & 0 & \dots & 0 \\ H_{12}^T & H_{22} & H_{23} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & H_{p-2,p-1}^T & H_{p-1,p-1} & H_{p-1,p} \\ 0 & \dots & 0 & H_{p-1,p}^T & H_{pp} \end{bmatrix}$, *where each H_{ii} is unreduced symmetric tridiagonal of size n_i, $i = 1,\dots,p$, and $H_{i,i+1}$ are of the form* $\begin{bmatrix} 0 & 0 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 0 \\ * & 0 & \dots & 0 \end{bmatrix}$. *Then, there exists a real valued $\mathcal{C}^s$ function T, of the form*

$$T = \begin{bmatrix} I & 0 & \dots & 0 \\ X_{21} & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ X_{p1} & \dots & X_{p,p-1} & I \end{bmatrix}, \tag{2.16}$$

with diagonal identity blocks of dimension n_i, $i = 1,\dots,p$, such that, for all t,

$$T^{-1}(t)H(t)T(t) =: B(t) = \begin{bmatrix} B_{11} & B_{12} & 0 & \dots & 0 \\ 0 & B_{22} & B_{23} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & B_{p-1,p-1} & B_{p-1,p} \\ 0 & \dots & 0 & 0 & B_{pp} \end{bmatrix}. \tag{2.17}$$

Here, $B_{i,i+1} = H_{i,i+1}$, $i = 1,\dots,p-1$, $B_{ii}(t)\in\mathbb{R}^{n_i\times n_i}$, and $\sigma(B_{ii}(t)) = \Lambda_i(t)$, $i = 1,\dots,p$. Further, each B_{ii}, $i = 1,\dots,p$, is in unreduced bordered tridiagonal structure, i .e., it is tridiagonal with first column and last row (possibly) filled in.

We next rephrase the above result in a slightly different form, which will be useful for the algorithms of the next Section.

Theorem 2.8. *Rewrite the function T of Theorem 2.7 as $T = T_1T_2\dots T_{p-1}$, where we have set*

$$T_k = \begin{bmatrix} I_{k_1} & 0 & 0 \\ 0 & I_{n_k} & 0 \\ 0 & X_{k+1:p,k} & I_{k_2} \end{bmatrix}, \quad k = 1,\dots,p-1,$$

and I_{k_1} is the identity block of dimension $k_1 = n_1 + \cdots + n_{k-1}$, and I_{k_2} of dimension $k_2 = n_{k+1} + \cdots + n_p$. If we set $B_1(t) = H(t)$, and then $B_{k+1}(t) = T_k^{-1}(t)B_k(t)T_k(t)$, $k = 1, \ldots, p-1$, then we have $B_p(t) = B(t)$ of Theorem 2.7 and moreover

$$B_k = \begin{bmatrix} B_{1:k-1,1:k-1} & B_{1:k-1,k:p} \\ 0 & \widehat{B}_k \end{bmatrix} , \quad \widehat{B}_k = \begin{bmatrix} \widehat{H}_{kk} & H_{k,k+1:p} \\ \widehat{H}_{k+1:p,k} & H_{k+1:p,k+1:p} \end{bmatrix} , \tag{2.18}$$

where $\widehat{B}_k = H_{k:p,k:p} - X_{k:p,k-1}H_{k-1,k:p}$.

Proof. This is a tedious, but otherwise simple, direct verification. □

Next is a result about reduction of a (block) bidiagonal structure.

Theorem 2.9. *Let $B \in \mathcal{C}^s([0,1], \mathbb{R}^{n\times n})$, $s \geq 1$, be an invertible unreduced bidiagonal function with p groups of singular values $\Sigma_1(t), \ldots, \Sigma_p(t)$, that vary continuously, of dimensions $n_1, \ldots, n_p$, for all $t \in [0,1]$. Write B in block notation as $B = \begin{bmatrix} B_{11} & B_{12} & 0 & \ldots & 0 \\ 0 & B_{22} & B_{23} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & B_{p-1,p-1} & B_{p-1,p} \\ 0 & \ldots & 0 & 0 & B_{pp} \end{bmatrix}$, where each B_{ii} is unreduced bidiagonal of size n_i, $i = 1, \ldots, p$, and $B_{i,i+1}$ are of the form $\begin{bmatrix} 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \ldots & \vdots \\ 0 & 0 & \ldots & 0 \\ * & 0 & \ldots & 0 \end{bmatrix}$. Then, there exist real valued $\mathcal{C}^s$ functions T_X and T_Y, of the form*

$$T_X = \begin{bmatrix} I & 0 & \ldots & 0 \\ X_{21} & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ X_{p1} & \ldots & X_{p,p-1} & I \end{bmatrix} , \quad T_Y = \begin{bmatrix} I & 0 & \ldots & 0 \\ Y_{21} & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ Y_{p1} & \ldots & Y_{p,p-1} & I \end{bmatrix} , \tag{2.19}$$

with diagonal identity blocks of dimension n_i, $i = 1, \ldots, p$, such that, for all t,

$$\begin{aligned} T_X^{-1}(t)B(t)T_Y(t) &= \begin{bmatrix} \widehat{B}_{11} & B_{12} & 0 & \ldots & 0 \\ 0 & \widehat{B}_{22} & B_{23} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & \widehat{B}_{p-1,p-1} & B_{p-1,p} \\ 0 & \ldots & 0 & 0 & \widehat{B}_{pp} \end{bmatrix} , \\ \text{and} \quad T_Y^{-1}(t)B^T(t)T_X(t) &= \begin{bmatrix} B_{11}^T & 0 & 0 & \ldots & 0 \\ 0 & B_{22}^T & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & B_{p-1,p-1}^T & 0 \\ 0 & \ldots & 0 & 0 & B_{pp}^T \end{bmatrix} . \end{aligned} \tag{2.20}$$

Moreover, $\sigma(\begin{bmatrix} 0 & \widehat{B}_{ii}(t) \\ B_{ii}^T(t) & 0 \end{bmatrix})$, $i = 1, \ldots, p$, is given by $\pm$ the singular values of Σ_i.

Proof. We write T_X as $T_X = T_{X_1}T_{X_2}\ldots T_{X_{p-1}}$, where we have set $T_{X_k} = \begin{bmatrix} I_{k_1} & 0 & 0 \\ 0 & I_{n_k} & 0 \\ 0 & X_{k+1:p,k} & I_{k_2} \end{bmatrix}$, with I_{k_1} the identity block of dimension $k_1 = n_1 + \cdots + n_{k-1}$, and I_{k_2} of dimension $k_2 = n_{k+1} + \cdots + n_p$. Similarly, we write $T_Y = T_{Y_1}\ldots T_{Y_{p-1}}$.

Now, the task of T_{X_1} and T_{Y_1} is to obtain

$$T_{X_1}^{-1}BT_{Y_1} = \begin{bmatrix} B_{11} + B_{1,2:p}Y_{2:p,1} & B_{1,2:p} \\ 0 & B_{2:p,2:p} - X_{2:p,1}B_{1,2:p} \end{bmatrix} , \quad T_{Y_1}^{-1}B^TT_{X_1} = \begin{bmatrix} B_{11}^T & 0 \\ 0 & B_{2:p,2:p}^T \end{bmatrix} ,$$

such that the eigenvalues of $\begin{bmatrix} 0 & B_{11}+B_{1,2:p}Y_{2:p,1} \\ B_{11}^T & 0 \end{bmatrix}$ are $\pm$ the singular values in Σ_1, and the eigenvalues of $\begin{bmatrix} 0 & B_{2:p,2:p}-X_{2:p,1}B_{1,2:p} \\ B_{2:p,2:p}^T & 0 \end{bmatrix}$ are $\pm$ the other singular values. Assuming that this is done, we would then have $\widehat{B}_{11} := B_{11} + B_{1,2:p}Y_{2:p,1}$, and would seek T_{X_2} and T_{Y_2} to achieve further reduction of the unreduced part, and so forth. The key observation is that $B_{2:p,2:p} - X_{2:p,1}B_{1,2:p}$ has the structure $\begin{bmatrix} \widetilde{B}_{22} & B_{2,3:p} \\ \widetilde{B}_{3:p,2} & B_{3:p,3:p} \end{bmatrix}$. Therefore, the complete proof will follow from this argument below.

Let $\widetilde{B}$ and B be of the form

$$\widetilde{B} = \begin{bmatrix} \widetilde{B}_{11} & B_{12} \\ \widetilde{B}_{21} & B_{22} \end{bmatrix} , \quad B^T = \begin{bmatrix} B_{11}^T & 0 \\ B_{12}^T & B_{22}^T \end{bmatrix} ,$$

where B_{11} and B_{22} are unreduced upper bidiagonal, and B_{12} is of the form $\begin{bmatrix} 0 & 0 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 0 \\ * & 0 & \dots & 0 \end{bmatrix}$. Let Σ_1 and Σ_2 be two groups making up the singular values of B, and moreover assume that $\widetilde{B}$ is such that the eigenvalues of $\begin{bmatrix} 0 & \widetilde{B} \\ B^T & 0 \end{bmatrix}$ are $\pm$ the singular values of B.

We seek $T_X = \begin{bmatrix} I & 0 \\ X & I \end{bmatrix}$ and $T_Y = \begin{bmatrix} I & 0 \\ Y & I \end{bmatrix}$ such that

$$T_X^{-1}\widetilde{B}T_Y = \begin{bmatrix} \widetilde{B}_{11} + B_{12}Y & B_{12} \\ 0 & B_{22} - XB_{12} \end{bmatrix} , \quad T_Y^{-1}B^TT_X = \begin{bmatrix} B_{11}^T & 0 \\ 0 & B_{22}^T \end{bmatrix} ,$$

and such that the eigenvalues of $\begin{bmatrix} 0 & \widetilde{B}_{11}+B_{12}Y \\ B_{11}^T & 0 \end{bmatrix}$ are $\pm$ the singular values in Σ_1, and the eigenvalues of $\begin{bmatrix} 0 & B_{22}-XB_{12} \\ B_{22}^T & 0 \end{bmatrix}$ are $\pm$ the singular values in Σ_2.

Now, in order to have T_X and T_Y as above, we need to satisfy the system

$$\begin{aligned} &\widetilde{B}_{21} + B_{22}Y - X\widetilde{B}_{11} - XB_{12}Y = 0 \\ &B_{12}^T + B_{22}^TX - YB_{11}^T = 0 . \end{aligned} \tag{2.21}$$

On the other hand, X and Y solve (2.21) if and only if (recall that B_{11} and B_{22} are nonsingular) they solve the two Riccati equations

$$\begin{aligned} &(\widetilde{B}_{21}B_{11}^T + B_{22}B_{12}^T) + (B_{22}B_{22}^T)X - X(\widetilde{B}_{11}B_{11}^T + B_{12}B_{12}^T) - X(B_{12}B_{22}^T)X = 0 \\ &(B_{22}^T\widetilde{B}_{21} + B_{12}^T\widetilde{B}_{11}) + (B_{22}^TB_{22} + B_{12}^TB_{12})Y - Y(B_{11}^T\widetilde{B}_{11}) - Y(B_{11}^TB_{12})Y = 0 , \end{aligned} \tag{2.22}$$

which is to say that $T_X^{-1}(\widetilde{B}B^T)T_X$ and $T_Y^{-1}(B^T\widetilde{B})T_Y$ are block upper triangular. Now, by direct verification we observe that both $(\widetilde{B}B^T)$ and $(B^T\widetilde{B})$ are unreduced lower Hessenberg. Thus, from [8, Theorem 6], there exist T_X and T_Y so that indeed $T_X^{-1}(\widetilde{B}B^T)T_X$ and $T_Y^{-1}(B^T\widetilde{B})T_Y$ are block upper triangular and furthermore

$$\sigma\big(T_X^{-1}(\widetilde{B}B^T)T_X\big)_{11} = \sigma\big(T_Y^{-1}(B^T\widetilde{B})T_Y\big)_{11}$$

and coincide with the squares of the singular values of Σ_1 and similarly

$$\sigma\big(T_X^{-1}(\widetilde{B}B^T)T_X\big)_{22} = \sigma\big(T_Y^{-1}(B^T\widetilde{B})T_Y\big)_{22}$$

and coincide with the squares of the singular values of Σ_2. But, since the eigenvalues of $\begin{bmatrix} 0 & \widetilde{B}_{11}+B_{12}Y \\ B_{11}^T & 0 \end{bmatrix}$ are $\pm$ the square roots of the eigenvalues of $\big(T_X^{-1}(\widetilde{B}B^T)T_X\big)_{11}$ and the eigenvalues of $\begin{bmatrix} 0 & B_{22}-XB_{12} \\ B_{22}^T & 0 \end{bmatrix}$ are $\pm$ the square roots of the eigenvalues of $\big(T_X^{-1}(\widetilde{B}B^T)T_X\big)_{22}$, the result follows. $\square$

3. Algorithms

Our algorithms follow closely the previous theoretical outline. We have implemented several variants of the basic techniques, thereby seeking a SVD with one block, or several blocks of disjoint singular values. We have further implemented variants in which we do perform prior reduction to tridiagonal, or bidiagonal, forms. We find it convenient to explain our algorithms by separately addressing the different modules.

At first, we will describe the algorithms "at regime", then we will discuss what we do the very first time, i.e., at $t = 0$, see Section 3.5. So, we can now assume that at the value t_0 we have reference decompositions for all the tasks to be outlined next, that we have chosen the stepsize h (see Section 3.4), and that we need to update the decompositions at the value $t = t_0 + h$.

The first thing that all the algorithms do is to reduce the rectangular problem to a square one.

3.1. **Left Null Space.** This part is in common to all algorithms, and it is done exactly as explained in §2.1. This computation gives us the matrix $\widetilde{A}_1(t)$ in (2.9). Of course, in the practical implementation, when using Theorem 2.3, all rank-one updates therein are computed with the aid of Theorem 2.2.

3.2. **Method 1.** This method starts with the reduction to symmetric positive definite form of §2.2.

3.2.1. *Algorithm Polar.* In this phase, we (smoothly) transform $\widetilde{A}_1(t)$ of (2.9) into $P(t)$. We do this exactly as explained in §2.2. Therefore, we seek $\widehat{U}_1(t)$ and $\widehat{V}(t)$ that give

$$\widehat{U}_1(t)^T\big(U_1^T(t_0)\widetilde{A}_1(t)V(t_0)\big)\widehat{V}(t) = P(t) \ ,$$

with $\widehat{U}_1(t)$ and $\widehat{V}(t)$ given by (2.15). The only thing we need to discuss is how we solve the Riccati equation (2.12), or $F(X) = 0$. This is a standard task, and we have implemented both a Newton and a stationary Newton iteration. To exemplify, recalling (2.14), given an initial guess $X^{(0)}$ and a value TOL for stopping the iteration, Newton's method is

$$\begin{aligned}
&\text{For } k = 0, \dots, K_{\text{Max}}, \quad \text{solve} \\
&-[\widehat{M}_{22} - X^{(k)}\widehat{M}_{12}]Y + Y[\widehat{M}_{11} + \widehat{M}_{12}X^{(k)}] = -F(X^{(k)})/2\,, \\
&\text{update } X^{(k+1)} \leftarrow X^{(k)} + Y\,. \quad \text{If } \frac{\|Y\|}{1 + \|X^{(k+1)}\|} \le \texttt{TOL} \text{ Stop}\,.
\end{aligned} \tag{3.1}$$

We stress that the solution X will be close to 0, for small continuation step h, and indeed $X = 0 + O(h)$. Thus, we could start the iteration in (3.1) with the initial guess $X^{(0)} = 0$. This corresponds to the *trivial predictor* in a standard continuation context. A much better choice is given by using the *tangent predictor*, which is obtained by solving

$$X^{(0)} \ : \ P(t_0)X^{(0)} + X^{(0)}P(t_0) \ = \ \widehat{M}_{21}(t) \ . \tag{3.2}$$

This choice of $X^{(0)}$ is $O(h^2)$-close to X. (Notice that $\widehat{M}_{21}(t) = -F(0)/2$).

At this point, we have $P(t)$ symmetric positive definite. In order to further obtain the (block) diagonalization of this, we have proceeded in two different ways. The first approach we implemented, see §3.2.2, mimicks the "block Schur approach" of [8]. This is certainly a sensible approach for the case of two blocks, since only one Riccati equation will have to be solved. However, if we need a block-diagonalization with, say, p blocks (and p is large), then several Riccati equations with no particularly exploitable structure will have to be solved, and this is an apparently expensive endeavor. Still, this technique will always work, as long as the assumption of having p disjoint blocks of singular values is satisfied and the continuation step h is sufficiently small. Moreover, with this technique, we only accumulate orthogonal transformations, which is a numerically stable accumulation. Nonetheless, to alleviate the expense of solving several Riccati equations with no particular structure, we also implemented a technique which performs initial reduction to tridiagonal form (see §3.2.3), prior to the block diagonalization phase (see §3.2.4), which we still carry out by solving Riccati equations. We will see below that the added tridiagonal structure will lead to very inexpensive solution of the resulting Riccati equations. The caveat of this latter technique is that it requires unreduced triadiagonal form, since its theoretical backing rests on Theorem 2.5. Moreover, now we will need to accumulate non-orthogonal transformations. Still, in spite of these theoretical difficulties, in many practical cases this technique works reliably and is indeed less expensive than the one of §3.2.2.

3.2.2. *Block Diagonalization 1.*
(i) First, we form $\widehat{S} := Q(t_0)^T P(t) Q(t_0)$, where $Q(t_0)$ is so that $S(t_0) := Q(t_0)^T P(t_0) Q(t_0)$ is symmetric block-diagonal. Therefore, $\widehat{S}$ is close to being symmetric block diagonal, for small h.
(ii) We annihilate the lower triangular entries of $\widehat{S}$ by using the transformation $T_1 = \begin{bmatrix} I & 0 & \cdots & 0 \\ X_{21} & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ X_{p1} & \cdots & X_{p,p-1} & I \end{bmatrix}$. Thus, we need to solve the following algebraic Riccati equations:

$$\begin{aligned} &\text{For } j = 1, 2, \ldots, p-1, \quad \text{let} \quad i = j+1. \,\text{Solve } F_j(X) = 0\ , \quad \text{where} \\ &F_j(X) = \widehat{S}_{i:p,j} + \widehat{S}_{i:p,i:p} X - X \widehat{S}_{jj} - X \widehat{S}_{j,i:p} X\ , \quad \text{let} \quad X_{i:p,j} = X \\ &\text{Update} \quad \widehat{S}_{1:j,j} \leftarrow \widehat{S}_{1:j,j} + \widehat{S}_{1:j,i:p} X_{i:p,j}\ , \quad \widehat{S}_{i:p,i:p} \leftarrow \widehat{S}_{i:p,i:p} - X_{i:p,j} \widehat{S}_{j,i:p}\ . \end{aligned} \tag{3.3}$$

(iii) Finally, we recover a Schur form by performing the QR factorization of T_1: $T_1 = Q_1 U_1$, where U_1 is upper triangular with positive diagonal entries. With this Q_1, we set $Q(t) = Q(t_0) Q_1$ and thus have $S(t) = Q(t)^T P(t) Q(t)$. By symmetry, and (block) upper triangularity, we must then have that $S(t)$ is indeed symmetric and block diagonal. We then proceed to a new step.

As usual, to solve the Riccati equations in (3.3), we can use a Newton, or a stationary Newton, iteration. We notice that we expect all $X_{i:p,j} \approx 0$, i.e., T_1 is near the identity. Thus, as starting guess, we may use the trivial predictors, though it is often more convenient to use the tangent predictors. To obtain these, we adopted the same procedure of [8]. In particular, see [8, Equations (9) and (10)].

3.2.3. *Algorithm Tridiagonal.* Here we (smoothly) transform $P(t)$ with orthogonal $Q(t)$ into unreduced tridiagonal form: $H(t) = Q^T(t) P(t) Q(t)$, assuming that such unreduced form exists (see Theorem 2.5). The procedure is straightforward. Letting $Q(t_0)$ be such that $H(t_0) = Q^T(t_0) P(t_0) Q(t_0)$ is in unreduced tridiagonal form, we seek the matrix Q_1 closest to the identity such that $H(t) = Q_1^T \big(Q^T(t_0) P(t) Q(t_0)\big) Q_1$ is unreduced tridiagonal.

To find Q_1 we use Householder transformations, and then adjust the signs of the columns of Q_1 by enforcing the diagonal entries of Q_1 to be positive.

3.2.4. *Block Diagonalization 2.* This algorithm starts with the unreduced tridiagonal $H(t)$ and finds the block-bidiagonal form of which in Theorem 2.7. Suppose we have $T(t_0)$ giving the reduction to block bidiagonal form for $H(t_0)$ in factored form as in Theorem 2.8: $T(t_0) = T_1(t_0)T_2(t_0)\dots T_{p-1}(t_0)$. Then, we seek $T_1, T_2, \dots, T_{p-1}$, of the form of which in Theorem 2.8 so that

$$T_{p-1}^{-1}T_{p-1}^{-1}(t_0)\cdots\big(T_2^{-1}T_2^{-1}(t_0)(T_1^{-1}T_1^{-1}(t_0)H(t)T_1(t_0)T_1)T_2(t_0)T_2\big)\cdots T_{p-1}(t_0)T_{p-1} \tag{3.4}$$

is in the form (2.17). Afterwards, we take the QR factorization of $T(t)$ and we are done.

To obtain the desired reduction from (3.4), we must solve several algebraic Riccati equations. With notation from (2.18), we need to solve:

$$\begin{aligned} &\text{For } k = 1, 2, \dots, p-1, \quad \text{let} \quad i = k+1. \text{ Solve } F_k(X) = 0\ , \quad \text{where} \\ &F_k(X) = \widehat{H}_{i:p,k} + H_{i:p,i:p}X - X\widehat{H}_{kk} - XH_{k,i:p}X\ , \quad \text{let} \quad X_{i:p,k} = X \\ &\text{Update:} \quad \widehat{B}_k \to \begin{bmatrix} B_{kk} & H_{k,i:p} \\ 0 & \widehat{B}_{k+1} \end{bmatrix}. \end{aligned} \tag{3.5}$$

Now, the main benefit of the prior tridiagonal reduction is that we have a very exploitable structure when solving these Riccati equations by Newton's method. Indeed, during Newton's method on (3.5) we need to solve Sylvester's equations like

$$-[H_{i:p,i:p} - X^{(0)}H_{k,i:p}]Y + Y[\widehat{H}_{kk} + H_{k,i:p}X^{(0)}] = -F(X^{(0)})\,, \tag{3.6}$$

where we can think of $\widehat{H}_{kk}$ as a small dimensional block (quite often it is just a number) and of $H_{i:p,i:p}$ as the large(r) block. Now, consider the (large) block $H_{i:p,i:p} - X^{(0)}H_{k,i:p}$. In general, of course, the symmetric tridiagonal structure of $H_{i:p,i:p}$ is lost; however, since $H_{k,i:p} = \begin{bmatrix} H_{k,k+1} & 0 & \dots & 0 \end{bmatrix}$ and $H_{k,k+1} = \begin{bmatrix} 0 & 0 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 0 \\ * & 0 & \dots & 0 \end{bmatrix}$, we end up with tridiagonal structure plus a possible fill-in of the first column. Likewise, looking at the block $\widehat{H}_{kk} + H_{k,i:p}X^{(0)}$, we now have that $\widehat{H}_{kk}$ is tridiagonal with first column filled in and thus the entire block becomes tridiagonal with first column and last row filled in. So, we have to solve Sylvester equations of the type $AY + YB = C$, where A is tridiagonal plus first column filled in, and the (small, dimension-wise) block B can be thought of as being in lower Hessenberg form. Thus, we can use the Hessenberg-Schur algorithm of [10], bringing B to lower Schur form, while maintaining A unchanged. Altogether we obtain an inexpensive solution process for the Riccati equations in (3.5) when compared to the Riccati equations in (3.3).

3.3. **Method 2.** This second method takes $\widetilde{A}_1(t)$ in (2.9) and finds its (block) SVD directly, without first reducing the problem to a symmetric one. Again, we have proceeded in two different ways. The first approach we implemented, "Block SVD 1" of §3.3.1, is the analog of the algorithm in §3.2.2, except that now we will work with different Riccati transformations on the right and on the left. Again motivated by reasons of efficiency, we also considered another approach, "Block SVD 2" in §3.3.3, which first bidiagonalizes $\widetilde{A}_1(t)$ and then finds its SVD by using bilateral Riccati transformations. The bidiagonalization algorithm itself is outlined in §3.3.2. Advantages and disadvantages of these two methods are similar to what we discussed for the different implementations of Method 1. In particular, "Block SVD 1" has the soundest theoretical backing and will always work as long as the assumption of having p disjoint blocks of singular values is satisfied and the continuation step h is sufficiently small. Moreover, only orthogonal transformations are accumulated. On the other hand, this technique is expensive when p is large, since Riccati equations with no particularly exploitable structure have to be solved. Instead, the method in §3.3.3, being preceded by bi-diagonalization of $\widetilde{A}_1(t)$, will allow to solve inexpensively the resulting Riccati equations. The price we pay now is that we need Theorem 2.6 to hold, hence we need unreduced bidiagonal form, and further we will also end up accumulating non-orthogonal transformations. Nonetheless, this technique seems to work well in practice.

3.3.1. *Block SVD 1.* For simplicity, we describe this method when we seek the block SVD of $\widetilde{A}_1(t)$ in two blocks. That is, we need to find orthogonal $U(t)$ and $V(t)$ such that $U^T(t)\widetilde{A}_1(t)V(t) = S(t) = \left[\begin{smallmatrix} S_1(t) & 0 \\ 0 & S_2(t) \end{smallmatrix}\right]$ where $S_1(t)$ and $S_2(t)$ are symmetric and positive definite. As usual, we assume to have $U(t_0)$ and $V(t_0)$ which achieved the decomposition at t_0 and we form $\widehat{A} := U^T(t_0)\widetilde{A}_1(t)V(t_0)$. Therefore, $\widehat{A}$ is close to being symmetric block diagonal, for small h. We write $\widehat{A}$ in block form as $\widehat{A} = \left[\begin{smallmatrix} \widehat{A}_{11} & E_{12} \\ E_{21} & \widehat{A}_{22} \end{smallmatrix}\right]$. Next, we seek U_1 and V_1 such that $U_1^T\widehat{A}V_1 = S(t)$.

To find U_1 and V_1 we proceed in two steps. First, we seek the transformations $T_X = \left[\begin{smallmatrix} I & 0 \\ X & I \end{smallmatrix}\right]$ and $T_Y = \left[\begin{smallmatrix} I & 0 \\ Y & I \end{smallmatrix}\right]$ to achieve the reductions of $\widehat{A}$ and $\widehat{A}^T$ to block triangular form:

$$T_X^{-1}\widehat{A}T_Y = \begin{bmatrix} \widehat{A}_{11}+E_{12}Y & E_{12} \\ 0 & \widehat{A}_{22}-XE_{12} \end{bmatrix} \quad T_Y^{-1}\widehat{A}^T T_X = \begin{bmatrix} \widehat{A}_{11}^T+E_{21}^T X & E_{21}^T \\ 0 & \widehat{A}_{22}^T-YE_{21}^T \end{bmatrix}, \tag{3.7}$$

where the blocking is such that the spectrum of $\left[\begin{smallmatrix} 0 & \widehat{A}_{11}+E_{12}Y \\ \widehat{A}_{11}^T+E_{21}^T X & 0 \end{smallmatrix}\right]$ is given by $\pm$ the eigenvalues of $S_1(t)$, and that of $\left[\begin{smallmatrix} 0 & \widehat{A}_{22}-XE_{12} \\ \widehat{A}_{22}^T-YE_{21}^T & 0 \end{smallmatrix}\right]$ is given by $\pm$ the eigenvalues of $S_2(t)$.

We point out that the requirement in (3.7) means that we have to solve the (coupled) Riccati equation(s):

$$\begin{bmatrix} 0 & E_{12}^T \\ E_{21} & 0 \end{bmatrix} + \begin{bmatrix} 0 & \widehat{A}_{22}^T \\ \widehat{A}_{22} & 0 \end{bmatrix}\begin{bmatrix} Y & 0 \\ 0 & X \end{bmatrix} - \begin{bmatrix} Y & 0 \\ 0 & X \end{bmatrix}\begin{bmatrix} 0 & \widehat{A}_{11}^T \\ \widehat{A}_{11} & 0 \end{bmatrix} - \begin{bmatrix} Y & 0 \\ 0 & X \end{bmatrix}\begin{bmatrix} 0 & E_{21}^T \\ E_{12} & 0 \end{bmatrix}\begin{bmatrix} Y & 0 \\ 0 & X \end{bmatrix} = 0. \tag{3.8}$$

Naturally, we can view (3.8) as a single Riccati equation associated to the problem

$$\begin{bmatrix} \begin{bmatrix} 0 & \widehat{A}_{11}^T \\ \widehat{A}_{11} & 0 \end{bmatrix} & \begin{bmatrix} 0 & E_{21}^T \\ E_{12} & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & E_{12}^T \\ E_{21} & 0 \end{bmatrix} & \begin{bmatrix} 0 & \widehat{A}_{22}^T \\ \widehat{A}_{22} & 0 \end{bmatrix} \end{bmatrix}.$$

In this light, the solvability theory for (3.8) is standard, see [15, 5]. We simply remark that the sought solution is the one for which X and Y are closest to 0.

We also observe that the transformations in (3.7) can be interpreted as follows. Let $\widehat{M} = \left[\begin{smallmatrix} 0 & \widehat{A} \\ \widehat{A}^T & 0 \end{smallmatrix}\right]$ and let $T = \left[\begin{smallmatrix} T_X & 0 \\ 0 & T_Y \end{smallmatrix}\right]$. Then, (3.7) arises from the requirement that $T^{-1}\widehat{M}T$ has the $(1,2)$ and $(2,1)$ blocks (block) upper triangular.

After X and Y are found, we take the QR factorizations of T_X and T_Y with the diagonal of the R-factors positive: $T_X = Q_X R_X$, $T_Y = Q_Y R_Y$, and let $Q = \left[\begin{smallmatrix} Q_X & 0 \\ 0 & Q_Y \end{smallmatrix}\right]$. Then, we realize (using simmetry of $\widehat{M}$ and the fact that R_X and R_Y are triangular) that we have the following structure

$$Q^T \widehat{M} Q = \begin{bmatrix} 0 & \left[\begin{smallmatrix} C_{11} & 0 \\ 0 & C_{22} \end{smallmatrix}\right] \\ \left[\begin{smallmatrix} C_{11}^T & 0 \\ 0 & C_{22}^T \end{smallmatrix}\right] & 0 \end{bmatrix} .$$

Finally, we bring C_{ii} into symmetric positive definite form as in (2.10). That is, we find, in the way described in Algorithm 3.2.1, $\widehat{U}_i, \widehat{V}_i$, $i = 1, 2$, such that

$$\widehat{U}_i^T C_{ii} \widehat{V}_i = S_i(t) \ , \ i = 1, 2 \, .$$

Finally, letting

$$U_1 = Q_X \begin{bmatrix} \widehat{U}_1 & 0 \\ 0 & \widehat{U}_2 \end{bmatrix} \ , \quad V_1 = Q_Y \begin{bmatrix} \widehat{V}_1 & 0 \\ 0 & \widehat{V}_2 \end{bmatrix} \ ,$$

we have that $U_1^T \widehat{A} V_1 = S(t)$ as desired.

Remark 3.1. If one needs to find the block SVD decomposition with several blocks, not just two, the procedure outlined above can be repeated on the unreduced part, prior to the final symmetrization step.

3.3.2. *Algorithm Bidiagonal.* Here we perform (smooth) bidiagonalization of $\widetilde{A}_1(t)$. That is, we find $\widetilde{U}_1(t)$ and $\widetilde{V}(t)$ such that

$$\widetilde{B}_1(t) = \widetilde{U}_1^T(t) \widetilde{A}_1(t) \widetilde{V}(t)$$

is in unreduced bidiagonal form, assuming that such unreduced form exists (see Theorem 2.6). The procedure is quite similar to the one of Algorithm 3.2.3. With obvious notation, we seek corrections $\widetilde{U}_1$ and $\widetilde{V}$, closest to the identity, such that

$$\widetilde{U}_1^T (\widetilde{U}_1^T(t_0) \widetilde{A}_1(t) \widetilde{V}(t_0)) \widetilde{V} = \widetilde{B}_1(t) \, ,$$

and then set $\widetilde{U}_1(t) = \widetilde{U}_1(t_0)\widetilde{U}_1$ and $\widetilde{V}(t) = \widetilde{V}(t_0)\widetilde{V}$. As in Algorithm 3.2.3, to find $\widetilde{U}_1$ and $\widetilde{V}$ we first use Householder transformations to achieve the bidiagonalization and then adjust the signs of the columns of $\widetilde{U}_1$ and $\widetilde{V}$ forcing the diagonals entries of $\widetilde{U}_1$ and $\widetilde{V}$ to be positive.

3.3.3. *Block SVD 2.* Now we assume that $\widetilde{B}_1(t)$ is in the unreduced upper bidiagonal form

$$\widetilde{B}_1(t) = \begin{bmatrix} b_{11} & b_{12} & 0 & \dots & 0 \\ 0 & b_{22} & b_{23} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \dots & \dots & \dots & b_{n-1,n-1} & b_{n-1,n} \\ 0 & \dots & \dots & 0 & b_{nn} \end{bmatrix} .$$

For completeness, we describe what we do when we seek a complete SVD of $\widetilde{B}_1(t)$. We will use the construction of Theorem 2.9.

So, we seek T_X and T_Y of the form

$$T_X = \begin{bmatrix} 1 & 0 & \dots & 0 \\ x_{21} & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ x_{n1} & \dots & x_{n,n-1} & 1 \end{bmatrix} , \quad T_Y = \begin{bmatrix} 1 & 0 & \dots & 0 \\ y_{21} & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ y_{n1} & \dots & y_{n,n-1} & 1 \end{bmatrix} ,$$

such that

$$T_X^{-1} \widetilde{B}_1 T_Y = \begin{bmatrix} \widehat{b}_{11} & b_{12} & 0 & \dots & 0 \\ 0 & \widehat{b}_{22} & b_{23} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \widehat{b}_{n-1,n-1} & b_{n-1,n} \\ 0 & \dots & 0 & 0 & \widehat{b}_{nn} \end{bmatrix} , \quad T_Y^{-1} \widetilde{B}_1^T T_X = \begin{bmatrix} b_{11} & 0 & 0 & \dots & 0 \\ 0 & b_{22} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & b_{n-1,n-1} & 0 \\ 0 & \dots & 0 & 0 & b_{nn} \end{bmatrix} ,$$

and further $\sigma(\begin{bmatrix} 0 & \widehat{b}_{ii} \\ b_{ii} & 0 \end{bmatrix}) = \pm\sigma_i$, $i = 1, \dots, n$. Once such T_X and T_Y have been found, we take their QR-factorizations: $T_X = Q_X R_X$, $T_Y = Q_Y R_Y$, where the triangular factors have positive diagonals. Since we must have that $\begin{bmatrix} Q_X^T & 0 \\ 0 & Q_Y^T \end{bmatrix} \begin{bmatrix} 0 & \widetilde{B}_1 \\ \widetilde{B}_1^T & 0 \end{bmatrix} \begin{bmatrix} Q_X & 0 \\ 0 & Q_Y \end{bmatrix}$ is symmetric, then elementary manipulations will give us that $Q_X^T \widetilde{B}_1 Q_Y$ is the sought SVD.

To obtain T_X and T_Y, we find it convenient to formulate the problem as a block symmetric tridiagonal one so that we can use the same implementation resulting from (3.4), in particular we can solve Riccati equatons similar to those in (3.5). To achieve this, we proceed as follows.

Take the symmetric permutation $P = [n+1, 1, n+2, 2, ...]$ and form (not explicitly)

$$H := P^T \begin{bmatrix} 0 & \widetilde{B}_1(t) \\ \widetilde{B}_1^T(t) & 0 \end{bmatrix} P \, .$$

Then, H is block symmetric tridiagonal with (2×2) blocks $H_{i,i} = \begin{bmatrix} 0 & b_{ii} \\ b_{ii} & 0 \end{bmatrix}$, $H_{i,i+1} = \begin{bmatrix} 0 & 0 \\ b_{i,i+1} & 0 \end{bmatrix}$. On this structure, we can solve Riccati equations like in (3.5) (with $p = n$ there) to obtain

$$T^{-1} H T = \begin{bmatrix} \widehat{H}_{11} & H_{12} & & & \\ & \widehat{H}_{22} & H_{23} & & \\ & & \ddots & \ddots & \\ & & & \widehat{H}_{n-1,n-1} & H_{n-1,n} \\ & & & & \widehat{H}_{nn} \end{bmatrix} ,$$

where the diagonal blocks are $\widehat{H}_{ii} = \begin{bmatrix} 0 & b_{ii} \\ \widehat{b}_{ii} & 0 \end{bmatrix}$ and $\sigma(\widehat{H}_{ii}) = \pm\sigma_i$, $i = 1, \dots, n$. Of course, in the case under scrutiny here, the solutions of the Riccati equations which we solve have a very special structure since, with the above P, we have that

$$P T P^T = \begin{bmatrix} T_X & 0 \\ 0 & T_Y \end{bmatrix} ,$$

where T_X and T_Y are precisely what we were looking for.

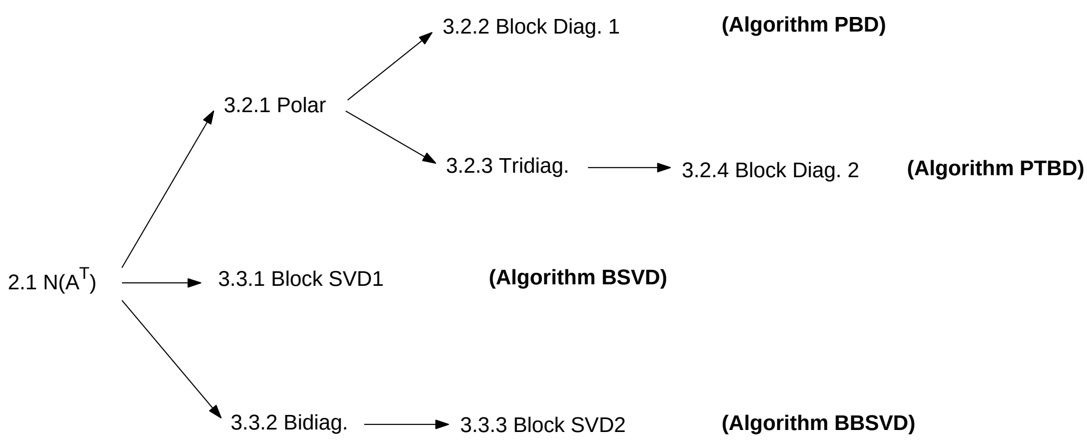
Remark 3.2. The above description holds essentially unchanged even if we do not seek a complete SVD, but just a block SVD in $p < n$ blocks. Of course, T_X and T_Y must be interpreted block-wise, and in the end result we will have that $\widehat{H}_{ii}$ are blocks whose eigenvalues are $\pm$ the singular values of the blocks S_i. Details of the changes, included the final symmetrization step, are obvious and will be omitted.

3.4. **Continuation.** To adaptively choose the step h, we adopt a common strategy in the continuation literature [1]. As in [8], we enlarge/restrict the stepsize based upon the number of Newton's iterations required for convergence.

3.5. **Initialization.** Here we describe what we do the very first time, i.e. at $t = 0$. In practice, all reference decompositions are obtained from an SVD of $A(0)$. That is, we find the SVD: $U(0)^T A(0)V(0) = \begin{bmatrix} \Sigma(0) \\ 0 \end{bmatrix}$. Then, we initialize the various algorithms as follows.

- Algorithm 3.1. We use $\widetilde{A}_1(0) = V(0)\Sigma(0)V^T(0)$. Therefore, we are using the reference decomposition $\begin{bmatrix} V(0) & 0 \\ 0 & I \end{bmatrix} U(0)^T A(0)I = \begin{bmatrix} \widetilde{A}_1(0) \\ 0 \end{bmatrix}$.
- Algorithm 3.2.1. Trivially, we use $P(0) = \widetilde{A}_1(0)$.
- Algorithm 3.2.2. We trivially have the Schur of $P(0)$ using $V(0)$, and from this we can group the columns of $V(0)$ as we need in order to enforce a reference eigenvalues' blocking.
- Algorithm 3.2.3. We use Householder transformations by fixing the first column of the accumulated orthogonal transformation in a basically arbitrary way.
- Algorithm 3.2.4. From a Schur form of $H(0)$ achieving the desired blocking, we then form the Riccati transformation $T(0)$.
- Algorithm 3.3.1. Again, reference factors are trivially obtained from the form of $\widetilde{A}_1(0) = V(0)\Sigma(0)V^T(0)$.
- Algorithm 3.3.2. To get $\widetilde{B}_1(0)$, we accumulate Householder transformations by fixing the first columns according to Theorem 2.6.
- Algorithm 3.3.3. Similarly to the initialization done for Algorithm 3.2.4, we form the Riccati transformations from the SVD of the bidiagonal $\widetilde{B}_1(0)$.

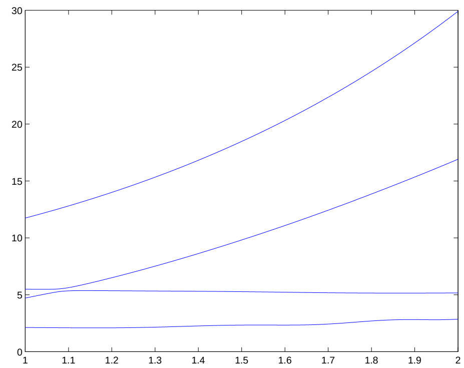
In the diagram below, we summarize the different Algorithms we implemented. We will refer to the names in parentheses in the next section.



4. Examples

Here we show performance of the various algorithms on the examples below. All algorithms have been implemented in `Matlab`.

Example 4.1. We have the function $A : t \in [1,2] \to A(t) \in \mathbb{R}^{6,4}$: $A(t) = \begin{bmatrix} 1-t & 1 & 1+t & \cos t^2 \\ -\sin(1+t) & 2 & 1 & 0 \\ 0 & 3 & 1+t^2 & -4t^2 \\ -t & 4e^t & 1 & 2 \\ 5 & 0 & 1 & e^{-t} \\ 2e^{1-t} & 0 & -\cos t^3 & 0 \end{bmatrix}$. The four singular values of A are distinct, though the second and third singular values come near each other at $t \approx 1.1$. See the figure on the right.



Example 4.2. Here we have $A : t \in [0, 1/2] \to A(t) \in \mathbb{R}^{10,7}$. $A(t)$ is built as $A(t) = U(t)\Sigma(t)V^T(t)$, where:

$$\Sigma(t) = \begin{bmatrix} D(t) \\ 0 \end{bmatrix}, D = \mathrm{diag}(40, 30, 20, 10, d_5, d_6, d_7)$$

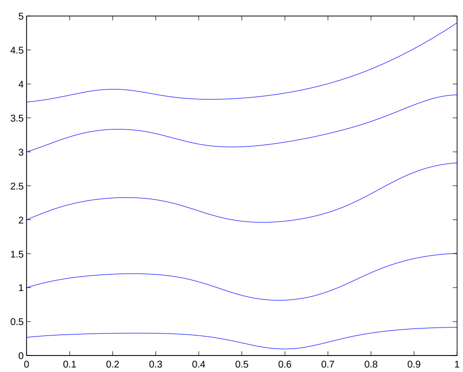
$$d_5(t) = 5 + (5-\alpha)\sin(2\pi t),\ d_6(t) = 5^t + 1,\ d_7(t) = 5^t, \alpha = 10^{-3}.$$

Also, we form U and V as exponentials of skew-symmetric functions as follows. We set $S(t,p)$ to be the (p,p) skew-symmetric function of entries

$$S_{ij} = \frac{(-1)^{i+j}(t-1)(t+3)^{j-i}}{j+1},\ S_{ji} = -S_{ij},\ j = 1, \dots, p;\ \ i = 1 \dots, j-1,$$

and then take $U(t) = e^{S(t,10)}$, $V(t) = e^{-S(t,7)}$.

Example 4.3. Here we have $A : t \in [0,1] \to A(t) \in \mathbb{R}^{5,5}$. $A(t)$ is built as $A(t) = U(t)P(t)U(t)$, where $P(t) = \mathrm{trid}(-1, a_{ii}, -1;\ i = 1, \dots, 5)$, $a_{11}(t) = 2 + 2.5t^2$, $a_{22} = a_{33} = a_{44} = 2$, $a_{55}(t) = 2 + \sin(2.5\pi t)$, and we take $U(t) = e^{\begin{bmatrix} 0 & 0 \\ 0 & S(t,4) \end{bmatrix}}$ where $S(t,4)$ is already defined in Example 4.2. The singular values are shown on the right.



Results of our experiments are summarized in Tables 1, 2 and 3. In the Tables, relatively to the Algorithm(s) we used, we give `Nsteps`, the required number of steps to complete the path, and `Nits`, the total number of iterations required for solving the relevant Riccati equations (this number is inclusive of the iterations performed also on unsuccessful steps). Wherever appropriate, in the columns `Nits` there are two numbers, the first refers to the number of iterations required to achieve the desired eigenvalues/singular values blocking, the second to the (largest) number of iterations required to achieve the positive definite form of Algorithm 3.2.1. Also, in the first two columns we report on results obtained when using the Euler (tangent) predictor, and in the third and fourth columns when using the trivial predictor, to solve the relevant Riccati equations, all of which have then been solved by Newton's method.

Finally, when using Algorithm 3.3.2, bidiagonalization, we fixed the first column of U and V as in Theorem 2.6, whereas when using Algorithm 3.2.3, tridiagonalization, we used as first column of Q the first unit vector in Examples 4.1 and 4.3, and the normalization of the vector (at two digits) $q = [\,-0.4,-1.7,0.1,0.3,-1.1,1.2,1.2\,]$ for Example 4.2.

In the Tables, the results relative to using Algorithms `PBD` and `BSVD` are for a block SVD in two blocks, while the results relative to using Algorithms `PTBD` and `BBSVD` are for a complete SVD. Dimensions of the blocks for the block-SVDs are 2 and 2 for Example 4.1, 4 and 3 for Example 4.2, and 2 and 3 for Example 4.3. The values of `Nits` relative to the algorithms which achieve a complete SVD refer to the average number of iterations required to solve the $(n-1)$ Riccati equations.

Table 1. Example 4.1.

Algorithm	Nsteps	Nits	Nsteps	Nits
PBD	23	68, 51	29	92, 77
PTBD	Fail	—	308	1050, 616
BSVD	23	68, 48	29	92, 69
BBSVD	32	97	395	1329

The failure in Table 1 refers to the fact that, although convergence takes place, a wrong ordering of singular values is produced.

Table 2. Example 4.2.

Algorithm	Nsteps	Nits	Nsteps	Nits
PBD	1825	3773, 7201	1823	5505, 7704
PTBD	1989	5063, 5342	6074	19178, 18232
BSVD	1841	6181, 6886	1810	6809, 5963
BBSVD	Fail	–	–	–

The failure in Table 2 is due to the lack of unreduced bidiagonal form. In general, this is a hard problem for all methods. The simple adaptive time stepping strategy we adopted attempted to take longer stepsizes to the detriment of robustness and to the net effect of repeated failures and large number of iterations. The large number of iterations of Algorithm `BSVD`, in comparison with Algorithm `PBD`, is explained by the fact that there are repeated failures to obtain the positive definite blocks: while in Algorithm `PBD` this is done first, in Algorithm `BSVD` this is done after having obtained the desired blocking, and hence it penalizes the overall number of iterations.

Table 3. Example 4.3.

Algorithm	Nsteps	Nits	Nsteps	Nits
PBD	25	68, 83	46	144, 167
PTBD	42	138, 118	200	711, 565
BSVD	27	93, 72	38	138, 127
BBSVD	29	88	134	465

Table 3 shows clearly the potential advantages of simplifying a priori the structure of the problem, as made evident by comparing the second and fourth rows of Table 3.

Remark 4.4. We now briefly summarize our computational experience, on the above problems and on other problems we solved as well.

(i) Algorithms PBD and BSVD are comparable, with a slight edge to Algorithm PBD. For a complete SVD, Algorithm BBSVD is usually better than Algorithm PTBD. These latter two Algorithms require unreduced bidiagonal, respectively tridiagonal, forms, a requirement which appears to be more than a theoretical restriction and has a clear practical impact as well. Still, whenever these unreduced tridiagonal or bidiagonal forms exist, Algorithms PTBD and BBSVD appear to be robust and accurate in spite of the fact that we are not controlling the conditioning of the underlying transformations.

(ii) In terms of cost, all methods share the initial cost of reduction to a square problem. After this phase, all methods have a leading flop count of $O(n^3)$, at least as long as Algorithms PBD and BSVD are used for two blocks. Of course, the constant hidden in the $O(n^3)$ term depends on the Algorithm. For example, and in the case of two equal sized blocks, Algorithms PBD and BSVD have roughly the same cost of about $200n^3$ flops per step. The costs of Algorithms PTBD and BBSVD, instead, differ substantially: Algorithm PTBD has a cost of about $190n^3$ flops per step, whereas Algorithm BBSVD has a cost of about $23n^3$ flops per step. All these flop counts are given under the assumption that the relevant Riccati equations need 3 full Newton iterations to converge, and that all predictors are tangent predictors.

5. Conclusions

We have considered computing a smooth path of (block) SVDs for a smooth full rank matrix valued function, $A : t \to A(t)$. We derived, justified, implemented, and provided limited comparison for, several algorithms. One may argue why not just to compute the SVD of $A(t)$, in the standard manner, at several t values, rather than using our smooth SVD techniques. After all, the asymptotic cost of our methods is not less than that of a standard SVD. But, we must stress that we provided at once not only the SVD of $A(t)$ at some t-values, but also adaptively decided **where** such SVDs are found. Our main underlying assumption is that there are p groups of singular value of $A(t)$ which stay disjoint for all t: these are the groups we track. In forthcoming extensions, we are considering degenerate situations, such as when A looses rank or there are merging singular values. This is particularly important in order to monitor possible bifurcations. Finally, our methods are not suitable for large and sparse problems, and development of methods suitable for large and sparse problems would also be an interesting endeavor.

References

[1] E. Allgower and K. Georg. Continuation and path following. *Acta Numerica*, pages 1–64, 1993.
[2] M. Baumann and U. Helmke. Diagonalization of time varying symmetric matrices. *Preprint, Univ. Wurzburg*, 2002.
[3] A. Bunse-Gerstner, R. Byers, V. Mehrmann, and N. K. Nichols. Numerical computation of an analytic singular value decomposition by a matrix valued function. *Numer. Math.*, 60:1–40, 1991.
[4] J.L. Chern and L. Dieci. Smoothness and periodicity of some matrix decompositions. *SIAM J. Matrix Anal. Appl.*, 22:772–792, 2001.

[5] J. W. Demmel. Three methods for refining estimates of invariant subspaces. *Computing*, 38:43–57, 1987.

[6] L. Dieci and T. Eirola. On smooth decomposition of matrices. *SIAM J. Matrix Anal. Appl.*, 20:800–819, 1999.

[7] L. Dieci and M. Friedman. Continuation of invariant subspaces. *Numerical Linear Algebra with Applications*, 8:317–327, 2001.

[8] L. Dieci and A. Papini. Continuation of eigendecompositions. *Future Generation Computer Systems*, 19:1125-1137, 2003.

[9] H. Gingold and P.F. Hsieh. Globally analytic triangularization of a matrix function. *Linear Algebra Appl.*, 169:75–101, 1992.

[10] G. H. Golub, S. Nash, and C. Van Loan. A Hessenberg-Schur method for the problem $AX + XB = C$. *IEEE Trans. Auto. Control*, 24:909–913, 1979.

[11] G. H. Golub and C. F. Van Loan. *Matrix Computations*. The Johns Hopkins University Press, 2nd edition, 1989.

[12] T. Kato. *Perturbation Theory for Linear Operators*. Springer-Verlag, Berlin, 1976. 2nd edition.

[13] V. Mehrmann and W. Rath. Numerical methods for the computation of analytic singular value decompositions. *Electronic Trans. Numerical Analysis*, 1:72–88, 1993.

[14] W. Rheinboldt. On the computation of multi-dimensional solution manifolds of parametrized equations. *Numer. Math.*, 53:165–181, 1988.

[15] G. W. Stewart. Error and perturbation bounds for subspaces associated with certain eigenvalue problems. *SIAM Review*, 15:727–764, 1973.

[16] K. Wright. Differential equations for the analytical singular value decomposition of a matrix. *Numer. Math.*, 63:283–295, 1992.

School of Mathematics, Georgia Institute of Technology, Atlanta, GA 30332, U.S.A.
E-mail address: dieci@math.gatech.edu

Dep. Energetica S. Stecco, Univ. of Florence, via C. Lombroso 6/17, 50134 Florence, Italy
E-mail address: gasparo@de.unifi.it

Dep. Energetica S. Stecco, Univ. of Florence, via C. Lombroso 6/17, 50134 Florence, Italy
E-mail address: papini@de.unifi.it