

SMOOTH SINGULAR VALUE DECOMPOSITION ON SYMPLECTIC GROUP AND LYAPUNOV EXPONENTS APPROXIMATION

L. DIECI AND L. LOPEZ

ABSTRACT. In this work we give a constructive argument to establish existence of a smooth singular value decomposition (SVD) for a generic C^k symplectic function X . We rely on the explicit structure of the polar factorization of X in order to justify the form of the SVD. Our construction gives a new algorithm to find the SVD of X , which we have used to approximate the Lyapunov exponents of a Hamiltonian differential system. Algorithmic details and an example are given.

1. INTRODUCTION

We consider a matrix valued function $X \in C^k(\mathbb{R}^+, \mathbb{R}^{m \times m})$, $k \geq 1$, belonging to the symplectic group \mathcal{S} . That is, for all $t \geq 0$, we have

$$(1) \quad X^T(t) J X(t) = J, \quad \text{with} \quad J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}.$$

Here, $m = 2n$, of course. For us¹, X is a fundamental matrix solution of a Hamiltonian system:

$$(2) \quad \dot{X} = C(t)X, \quad \text{where} \quad C^T(t)J + JC(t) = 0, \quad \forall t.$$

As a consequence of (1) (respectively, (2)), there are several relations which need to be satisfied by a symplectic (respectively, Hamiltonian) matrix valued function. Writing X (and similarly for C) in block form as $X = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix}$, where the partitioning is that inherited from J , i.e., all blocks are in $\mathbb{R}^{n \times n}$, the following facts are trivially verified.

Example 1.

(i) *If X is symplectic, it must satisfy the following relations*

$$X_{11}^T X_{21} = X_{21}^T X_{11}, \quad X_{22}^T X_{12} = X_{12}^T X_{22}, \quad X_{11}^T X_{22} - X_{21}^T X_{12} = I_n.$$

(ii) *If C is Hamiltonian, it must satisfy*

$$C_{22} = -C_{11}^T, \quad C_{12} = C_{12}^T, \quad C_{21} = C_{21}^T.$$

In [3], we studied the SVD of a generic function evolving on the Lorentz group. Our purpose in this work is to provide an explicit characterization of a singular value decomposition in \mathcal{S} of a generic function $X \in \mathcal{S}$. To arrive at a proper definition of genericity, we will first consider the polar factorization of X .

1991 *Mathematics Subject Classification.* 15A18, 65F99, 65L07.

Key words and phrases. symplectic group, singular values, Lyapunov exponents.

This work was supported in part under Grants NSF-FRG-0139895 and Italian COFIN2003 entitled *Dynamical Systems on Matrix Manifolds*.

¹In fact, without loss of generality

In Section 2, we discuss the polar decomposition of a function $X \in \mathcal{S}$, and further give an inertia diagonalization result for a generic positive definite function in \mathcal{S} . In Section 3 we will arrive at an SVD-like in \mathcal{S} of X , and derive a set of differential equations satisfied by the SVD factors of X . In Section 4, we give an application: by using the explicit form of the SVD of X we will approximate the Lyapunov exponents of a dynamical system with fundamental matrix solution X satisfying (2).

Notation. We will write $A > 0$ for a matrix (or matrix valued function) which is positive definite. For us, this will always be also symmetric.

2. POLAR DECOMPOSITION AND INERTIA DIAGONALIZATION

Consider a C^k function $X \in \mathcal{S}$ and its polar factorization of X : $X = QP$, with Q orthogonal and $P > 0$. Since X is full rank for all t , it is well known that Q and P are unique ([8, Corollary 7.3.3]) and also C^k functions ([4]). Furthermore, they are also in \mathcal{S} , see [9, 16].

We now derive the structure of the symmetric factor in the polar factorization of $X \in \mathcal{S}$.

Lemma 2. *Let $P \in \mathcal{S}$, $P > 0$. Then P must have the following form:*

$$(3) \quad P = \begin{pmatrix} A + BA^{-1}B & BA^{-1} \\ A^{-1}B & A^{-1} \end{pmatrix},$$

where $A > 0$ and $B = B^T$. Furthermore, any P partitioned as in (3), and with $B = B^T$, is positive definite if $A > 0$.

Proof. Write

$$P = \begin{pmatrix} P_{11} & P_{12} \\ P_{12}^T & P_{22} \end{pmatrix}$$

with $P = P^T$ and $P^T JP = J$.

- Since $P > 0$, then $P_{22} > 0$, and we may define $A^{-1} = P_{22}$.
- Implicitly define B from $A^{-1}B = P_{12}^T$. This gives $P_{22}B = P_{12}^T$, so that $B = P_{22}^{-1}P_{12}^T$. Now, $P_{22}^{-1}P_{12}^T = P_{12}P_{22}^{-1} \Leftrightarrow P_{12}^TP_{22} = P_{22}P_{12}$ which is true because of symplecticity. Therefore, $B = B^T$.
- At this point, we can set $BA^{-1} = P_{12}$, that is $B = P_{12}P_{22}^{-1}$.
- Finally:

$$\begin{aligned} A + BA^{-1}B &= P_{11} \Leftrightarrow P_{22}^{-1} + P_{12}P_{22}^{-1}P_{12}^T = P_{11} \Leftrightarrow I + P_{22}P_{12}P_{22}^{-1}P_{12}^T = P_{22}P_{11} \\ &\Leftrightarrow I + P_{12}^TP_{22}P_{22}^{-1}P_{12}^T = P_{22}P_{11} \Leftrightarrow P_{22}P_{11} = I + P_{12}^TP_{12} \Leftrightarrow P_{11}P_{22} = I + P_{12}^2 \end{aligned}$$

and the last equality is true because of symplecticity. Thus $P > 0$, symplectic, is of the form (3) with $A > 0$ and $B = B^T$.

Next, we verify the claim about $P > 0$ if $A > 0$. Let $\begin{bmatrix} x \\ y \end{bmatrix}$ be a general vector in \mathbb{R}^m , where both $x, y \in \mathbb{R}^n$. Then, we have

$$\begin{bmatrix} x^T & y^T \end{bmatrix} P \begin{bmatrix} x \\ y \end{bmatrix} = x^T Ax + (Bx + y)^T A^{-1}(Bx + y) > 0.$$

□

Next, we present a “diagonalization” result via an inertia symplectic transformation for the symplectic symmetric positive definite P of Lemma 2.

Lemma 3. *Let $P > 0$ be a $C^k(\mathbb{R}^+, \mathbb{R}^{m \times m})$ function of the form (3) and assume that all eigenvalues of $A^{-1}B$ are distinct for all t . Then there exists a nonsingular $Y \in C^k(\mathbb{R}^+, \mathbb{R}^{n \times n})$ such that*

$$(4) \quad Y^T A Y = I, \quad Y^T B Y = E,$$

where the function E is diagonal. It follows that P in (3) decomposes as

$$(5) \quad P = T \begin{pmatrix} I + E^2 & E \\ E & I \end{pmatrix} T^T,$$

where $T = \begin{pmatrix} Y^{-T} & 0 \\ 0 & Y \end{pmatrix}$ is symplectic.

Proof. First, let us take the Choleski factorization of A : $A = LL^T$. It is known (see [1]) that L is a C^k function. Next, observe that since

$$A^{-1}B = L^{-T}L^{-1}B = L^{-T}(L^{-1}BL^{-T})L^T$$

then the eigenvalues of $L^{-1}BL^{-T}$ are distinct. Let $H = L^{-1}BL^{-T}$. It follows from [4] that the symmetric function H has a C^k Schur decomposition. That is, there exists orthogonal $Q \in C^k(\mathbb{R}^+, \mathbb{R}^{n \times n})$ such that $Q^T HQ = E$, with E diagonal. At this point, we simply set $Y = L^{-T}Q$ to obtain (4).

Now, from (4) it follows easily that

$$\begin{aligned} A^{-1} &= YY^T, \quad A^{-1}B = YY^T Y^{-T} E Y^{-1} = Y E Y^{-1} \\ BA^{-1} &= Y^{-T} E Y^{-1} Y Y^{-1} Y^T = Y^{-T} E Y^T \\ A + BA^{-1}B &= Y^{-T}(I + E^2)Y^{-1}, \end{aligned}$$

and (5) follows at once. \square

The key assumption in Lemma 3 is that all eigenvalues of $A^{-1}B$ be distinct for all t . Next, we show that this is a honest assumption, in that it is satisfied by a generic positive definite function $P \in \mathcal{S}$. Genericity must be understood in the topological sense. That is, we consider the space of $C^k(\mathbb{R}^+, \mathbb{R}^{n \times n})$ functions, endowed with the Whitney (or fine) topology; see [10]. Then, a property within the space of C^k functions is generic if the set of elements that do not have this property is a countable union of nowhere dense sets.

Lemma 4. *Consider the pencil (A, B) , where both A and B are symmetric C^k functions and A is also positive definite. Then, generically, the function $A^{-1}B$ has distinct eigenvalues for all t . In particular, E in (4)-(5) has distinct diagonal entries.*

Proof. Let $A = LL^T$ be the Choleski decomposition of A . Then, L is a C^k function (e.g., see [1]). Now, consider the following similarity transformation of $A^{-1}B$:

$$L^T(A^{-1}B)L^{-T} = L^{-1}BL^{-T}.$$

The right-hand-side in this above expression is a symmetric, generic, C^k function. Therefore, from [4], we know that –generically– $L^{-1}BL^{-T}$ has distinct eigenvalues for all t , and thus so does $A^{-1}B$. Finally, from the proof of Lemma 3, E is similar to $A^{-1}B$. \square

3. SMOOTH SVD IN THE SYMPLECTIC GROUP

Clearly, it is simple to recover an SVD of X from an ordered Schur decomposition of the symmetric positive definite function P : If we have $P = ZEZ^T$, with $Z^TZ = I$ and E diagonal, then we have the SVD of X , $X = (QZ)EZ^T$. Our goal in this section is to justify the existence of a C^k Schur decomposition of $P \in \mathcal{S}$ of the form (3), and we want it to be with orthogonal factors in \mathcal{S} . However, we cannot do it for a generic C^k function in the sense of Lemma 4. Indeed, our construction will be restricted to a subclass of generic symplectic positive definite functions, which we call *dichotomic* functions. Although our interest here has been on C^k functions, also the analytic case is important, in which case² a symplectic SVD result is forthcoming ([13]).

Definition 5. *A positive definite function $P \in \mathcal{S}$ is called dichotomic if all of its eigenvalues are different from 1 for all t .*

Since all eigenvalues of $P \in \mathcal{S}$ appear as $\{\lambda, 1/\lambda\}$, the eigenvalues of a dichotomic function $P > 0$ can be put in two disjoint groups of n eigenvalues each, reciprocal of one another: n eigenvalues will be greater than 1, the other n will be between 0 and 1. This is the reason for the name “dichotomic”.

In particular, a “generic dichotomic” function $P \in \mathcal{S}$, $P > 0$, has distinct eigenvalues for all t .

3.1. Two stage decomposition. We will now see how to obtain the eigendecomposition of a generic dichotomic $P \in \mathcal{S}$, $P > 0$, and hence the SVD of $X \in \mathcal{S}$. We will describe this as a two stage process, motivated by the next informal consideration.

Observation. A function P of the form (3) has $n^2 + n$ degrees of freedom (i.e., the nonredundant entries of A and B in (3)). In a Schur decomposition of such P , we have n positive eigenvalues to determine (the other n are reciprocal of the first n), and so we have n^2 degrees of freedom to get the orthogonal factor, call it Q . We will look for Q as $Q = Q_1Q_2$, where Q_1 will need to block-diagonalize P , and Q_2 will need to diagonalize the diagonal blocks. To be precise, we will want to have symplectic and orthogonal $Q_1 \in C^k(\mathbb{R}^+, \mathbb{R}^{m \times m})$ such that, for all $t \geq 0$:

$$Q_1(t)^T P(t) Q_1(t) = \begin{pmatrix} S(t) & 0 \\ 0 & S^{-1}(t) \end{pmatrix},$$

and the block S is necessarily symmetric positive definite. Afterwards, we will seek $U \in C^k(\mathbb{R}^+, \mathbb{R}^{n \times n})$ such that, for all $t \geq 0$:

$$U(t)^T S(t) U(t) = \text{diag}(\sigma_1(t), \dots, \sigma_n(t)).$$

We will then set $Q_2 = \begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix}$. Now, finding U , in general, will require to fix $n(n-1)/2$ degrees of freedom, like describing any general $(n \times n)$ orthogonal function. Thus, to find Q_1 , we have at our disposal $n(n+1)/2$ degrees of freedom. This is just enough to block diagonalize P .

Now, if X is the solution of (2), and $X = QP$ is its polar decomposition with factors in \mathcal{S} , then P will be the solution of the system

$$(6) \quad \dot{P} = F(t)P, \quad \text{where} \quad F^T(t)J + JF(t) = 0, \quad \forall t,$$

²Niloufer Mackey pointed this out to us after we had completed our work

and in fact the coefficient F is given by $F(t) = Q^T(t)C(t)Q(t) - Q^T(t)\dot{Q}(t)$, for all t .

Next, we want to take the block diagonalization of P : $Q_1^T(t)P(t)Q_1(t) = \begin{pmatrix} S(t) & 0 \\ 0 & S^{-1}(t) \end{pmatrix}$, for all t , with Q_1 at once orthogonal and symplectic. The following result characterizes the group and the algebra of orthogonal and symplectic functions. The proof is trivial and hence omitted.

Lemma 6. *A function Q belongs to the intersection of the orthogonal and symplectic groups if and only if it has the following structure:*

$$Q = \begin{pmatrix} Q_{11} & Q_{12} \\ -Q_{12} & Q_{11} \end{pmatrix}$$

with

$$Q_{11}^T Q_{11} + Q_{12}^T Q_{12} = I_n, \quad Q_{11}^T Q_{12} = Q_{12}^T Q_{11}.$$

Moreover, a C^1 function Q is orthogonal and symplectic if and only if the function $H := Q^T \dot{Q}$ belongs to the algebra of Hamiltonian and skew-symmetric functions. For all t , such a function H must have the block form $H(t) = \begin{pmatrix} H_{11}(t) & H_{12}(t) \\ -H_{12}(t) & H_{11}(t) \end{pmatrix}$, where $H_{11}^T(t) = -H_{11}(t)$ and $H_{12}^T(t) = H_{12}(t)$.

To obtain the (block) eigendecomposition of P , we restrict to P dichotomic. We will need the following Lemma.

Lemma 7. *Let $P > 0$ be symplectic and dichotomic. Suppose that there exist Q_{11} and Q_{12} such that*

$$P \begin{bmatrix} Q_{11} \\ -Q_{12} \end{bmatrix} = \begin{bmatrix} Q_{11} \\ -Q_{12} \end{bmatrix} S,$$

where $Q_{11}^T Q_{11} + Q_{12}^T Q_{12} = I_n$ and $\sigma(S) = \{\lambda \in \sigma(P) : \lambda > 1\}$. Then, we also have

$$P \begin{bmatrix} Q_{12} \\ Q_{11} \end{bmatrix} = \begin{bmatrix} Q_{12} \\ Q_{11} \end{bmatrix} S^{-1},$$

and $Q_{11}^T Q_{12} = Q_{12}^T Q_{11}$. Therefore, by letting $Q_1 := \begin{bmatrix} Q_{11} & Q_{12} \\ -Q_{12} & Q_{11} \end{bmatrix}$, we have

$$Q_1^T P Q_1 = \begin{bmatrix} S & 0 \\ 0 & S^{-1} \end{bmatrix},$$

with Q_1 symplectic and orthogonal.

Proof. From $P \begin{bmatrix} Q_{11} \\ -Q_{12} \end{bmatrix} = \begin{bmatrix} Q_{11} \\ -Q_{12} \end{bmatrix} S$, using the fact that $P^{-1} = J^{-1}PJ$, we immediately obtain that $P \begin{bmatrix} Q_{12} \\ Q_{11} \end{bmatrix} = \begin{bmatrix} Q_{12} \\ Q_{11} \end{bmatrix} S^{-1}$. Now, we let Q_1 be defined as in the statement of the Lemma, and show that it is orthogonal. Writing Q_1 as groups of columns: $Q_1 := [C_1 \ C_2]$, we have to show that $C_1^T C_2 = 0$. We have

$$P C_1 = C_1 S, \quad \text{and} \quad P C_2 = C_2 S^{-1},$$

as well as $C_1^T C_1 = C_2^T C_2 = I$, so that we have at once

$$C_1^T C_2 = (C_1^T P C_2) S, \quad \text{and} \quad C_2^T C_1 = (C_2^T P C_1) S^{-1},$$

from which we get that

$$(C_1^T P C_2) S - S^{-T} (C_2^T P C_1) = 0$$

which gives $C_1^T P C_2 = 0$ since S and S^{-1} have no common eigenvalues. Therefore, $C_1^T C_2 = 0$ and Q_1 is orthogonal and symplectic. \square

We can now block-diagonalize P .

Theorem 8. *Let $P \in C^k$, $k \geq 1$, be the solution of (6): $\dot{P} = F(t)P$, subject to initial condition $P(0) = P_0$, with P_0 symplectic positive definite, and assume that P is dichotomic. Then, there exist $Q_1 \in C^k$, symplectic and orthogonal, such that for all $t \geq 0$:*

$$(7) \quad Q_1^T P Q_1 := D = \begin{bmatrix} S & 0 \\ 0 & S^{-1} \end{bmatrix},$$

where we require that the function $S > 0$ has eigenvalues greater than 1.

Proof. From [16], it is possible to obtain the decomposition for P_0 : $P_0 = Q_0 \begin{bmatrix} S_0 & 0 \\ 0 & S_0^{-1} \end{bmatrix} Q_0^T$ with Q_0 orthogonal and symplectic and $S_0 > 0$ with eigenvalues greater than 1. Let $Q_1(0) = Q_0$ and $S(0) = S_0$.

We impose on Q_1 the structure

$$(8) \quad Q_1 = \begin{bmatrix} Q_{11} & Q_{12} \\ -Q_{12} & Q_{11} \end{bmatrix},$$

with $Q_{11}^T Q_{11} + Q_{12}^T Q_{12} = I_n$, and obtain differential equations defining Q_{11} and Q_{12} in such a way that for all t we have $P(t) \begin{bmatrix} Q_{11}(t) \\ -Q_{12}(t) \end{bmatrix} = \begin{bmatrix} Q_{11}(t) \\ -Q_{12}(t) \end{bmatrix} S(t)$. Because of Lemma 7, by finding such Q_{11} and Q_{12} , we will have completed the proof.

The differential equation we will solve for $\begin{bmatrix} Q_{11} \\ -Q_{12} \end{bmatrix}$ is:

$$(9) \quad \frac{d}{dt} \begin{bmatrix} Q_{11} \\ -Q_{12} \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} \\ -Q_{12} & Q_{11} \end{bmatrix} \begin{bmatrix} H_{11} \\ H_{21} \end{bmatrix},$$

where H_{11} is an arbitrary (but sufficiently smooth) skew-symmetric function, which we can set to 0. Instead, H_{21} will be the solution of the linear system

$$(10) \quad S^{-1} H_{21} - H_{21} S + (Q_1^T F Q_1)_{21} S = 0,$$

and we observe that H_{21} exists, unique, since S and S^{-1} have no common eigenvalues. Before justifying these relations, let us show that the solution H_{21} of (10) is symmetric, a fact which is not immediately obvious.

We show that $H_{21}^T = H_{21}$. First of all, recall that F is Hamiltonian, see Example 1. This fact, and the fact that Q_1 has the structure in (8), give that $\tilde{F}_{21} := (Q_1^T F Q_1)_{21}$ is symmetric. Now, to solve (10), at each t , we take the Schur decomposition of the matrix $S(t)$: $W^T S W = \Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$ with $\lambda_1 > \dots > \lambda_n > 1$, and rewrite (10) for the new variable $\hat{H}_{21} = W^T H_{21} W$: With $\hat{F}_{21} = W^T \tilde{F}_{21} W$, this gives $\Lambda^{-1} \hat{H}_{21} - \hat{H}_{21} \Lambda + \hat{F}_{21} \Lambda = 0$. Now, examining the (i, j) and (j, i) entries of this equation, we immediately obtain that $\hat{H}_{21} = \hat{H}_{21}^T$ and thus also $H_{21}^T = H_{21}$.

Next, we justify the equations (9) and (10). With the form of Q_1 we imposed, (9) follows from the reasoning below. From the relation $\dot{P} = F(t)P$, using the implicit function theorem on the relations $Q_1^T P Q_1 = D$, $Q_1^T Q_1 = I$, we get

$$(11) \quad \dot{Q}_1^T P Q_1 + Q_1^T \dot{P} Q_1 + Q_1^T P \dot{Q}_1 = \dot{D}.$$

From (11), we let $H := Q_1^T \dot{Q}_1$ and partition it in a similar way to how F is. Rewrite (11) as

$$-HD + (Q_1^T F Q_1)D + DH = \dot{D},$$

and using the 0-structure of \dot{D} relative to its (2,1) block, we get (10). The block H_{11} is not uniquely determined, and we will set it to 0. So, we will eventually have the following system of differential equations which define Q_1 and S

$$\dot{Q}_1 = Q_1 H, \quad Q_1(0) = Q_0, \quad H = \begin{bmatrix} 0 & -H_{21}^T \\ H_{21} & 0 \end{bmatrix},$$

with H_{21} given above, and

$$(12) \quad \dot{S} = (Q_1^T F Q_1)S, \quad S(0) = S_0,$$

with an obvious analog for S^{-1} . Of course, only one of the equations for S or S^{-1} is needed. \square

The final thing to do is the Schur decomposition of the block S . To derive differential equations for this scope, we will use the assumption of genericity of the function S . In particular, this will imply that the eigenvalues of $S(t)$ are distinct for all t . In this case, the following result is well known (e.g., see [4] and also [11]), and its proof is therefore omitted.

Theorem 9. *Let $S \in C^k(\mathbb{R}^+, \mathbb{R}^{n \times n})$, $k \geq 1$, $S > 0$, with distinct eigenvalues for all $t \geq 0$, satisfy the differential equation*

$$\dot{S} = B(t)S, \quad S(0) = S_0.$$

Then, there exists $U \in C^k$, orthogonal, such that $U^T(t)S(t)U(t) = \Lambda(t)$, where $\Lambda(t) = \text{diag}(\lambda_1(t), \dots, \lambda_n(t))$, with $\lambda_1(t) > \dots > \lambda_n(t)$, for all $t \geq 0$. Moreover, U satisfies the differential equation $\dot{U} = UK$, where the entries of the skew-symmetric function K are defined as

$$(13) \quad k_{ij}(t) = -(U^T(t)B(t)U(t))_{ij} \frac{\lambda_i(t)}{\lambda_i(t) - \lambda_j(t)},$$

for all $t \geq 0$, and $i = 1, \dots, n-1$, $j = i+1, \dots, n$, with the rest defined by skew-symmetry.

3.2. All at once. In the above, we have separated different phases of the SVD, to clarify at which point the assumptions we made become necessary. However, in practice, when seeking the SVD of a symplectic X , we will proceed finding at once all the factors. Here below we summarize this process.

We seek U and V , in $C^k(\mathbb{R}^+, \mathbb{R}^{2n \times 2n})$, symplectic and orthogonal, and $\Sigma \in C^k(\mathbb{R}^+, \mathbb{R}^{2n \times 2n})$, diagonal of the form $\Sigma = \begin{bmatrix} \Lambda & 0 \\ 0 & \Lambda^{-1} \end{bmatrix}$ such that $XV = U\Sigma$, where X solves (2) and $\Lambda = \text{diag}(\sigma_1, \dots, \sigma_n)$. Since we will seek for U and V of the form

$$U = \begin{bmatrix} U_{11} & U_{12} \\ -U_{12} & U_{11} \end{bmatrix}, \quad V = \begin{bmatrix} V_{11} & V_{12} \\ -V_{12} & V_{11} \end{bmatrix},$$

we only need to find the reduced decomposition

$$(14) \quad X \begin{bmatrix} V_{11} \\ -V_{12} \end{bmatrix} = \begin{bmatrix} U_{11} \\ -U_{12} \end{bmatrix} \Lambda.$$

Formally setting $H := U^T \dot{U}$ and $K := V^T \dot{V}$, both skew-symmetric, and partitioning similarly to U and V , we will eventually solve the following differential equations to find U and V :

$$(15) \quad \begin{aligned} \frac{d}{dt} \begin{bmatrix} U_{11} \\ -U_{12} \end{bmatrix} &= \begin{bmatrix} U_{11} & U_{12} \\ -U_{12} & U_{11} \end{bmatrix} \begin{bmatrix} H_{11} \\ H_{21} \end{bmatrix}, \\ \frac{d}{dt} \begin{bmatrix} V_{11} \\ -V_{12} \end{bmatrix} &= \begin{bmatrix} V_{11} & V_{12} \\ -V_{12} & V_{11} \end{bmatrix} \begin{bmatrix} K_{11} \\ K_{21} \end{bmatrix}. \end{aligned}$$

To find expressions defining H_{12} , K_{12} , we will use the 0-structure in the defining decomposition $XV = U\Sigma$. So doing, we get that

$$-\begin{bmatrix} 0 & \Lambda \\ \Lambda & 0 \end{bmatrix} \begin{bmatrix} H_{12} \\ K_{12} \end{bmatrix} + \begin{bmatrix} H_{12} \\ K_{12} \end{bmatrix} \Lambda^{-1} = \begin{bmatrix} (U^T CU)_{12} \Lambda^{-1} \\ \Lambda (U^T CU)_{21}^T \end{bmatrix},$$

from which we uniquely find H_{12} and K_{12} . [We remark that $(U^T CU)_{21}^T = (U^T CU)_{21}$.] In fact, for $i, j = 1, \dots, n$, we have

$$(16) \quad \begin{aligned} (H_{12})_{ij} &= \frac{((U^T CU)_{12})_{ij} + \sigma_i^2 \sigma_j^2 ((U^T CU)_{21}^T)_{ij}}{1 - \sigma_i^2 \sigma_j^2} \\ (K_{12})_{ij} &= \frac{\sigma_i \sigma_j}{1 - \sigma_i^2 \sigma_j^2} [((U^T CU)_{12})_{ij} + ((U^T CU)_{21}^T)_{ij}]. \end{aligned}$$

From the relation $\dot{\Lambda} = (U^T CU)_{11} \Lambda + \Lambda K_{11} - H_{11} \Lambda$, since $\Lambda = \text{diag}(\sigma_1, \dots, \sigma_n)$, we get

$$(17) \quad \dot{\sigma}_i = ((U^T CU)_{11})_{ii} \sigma_i, \quad i = 1, \dots, n,$$

and the following expressions for the entries of the skew-symmetric H_{11} and K_{11} , for $i = 1, \dots, n$, $j = i+1, \dots, n$:

$$(18) \quad \begin{aligned} (H_{11})_{ij} &= \frac{1}{\sigma_j^2 - \sigma_i^2} [\sigma_j^2 ((U^T CU)_{11})_{ij} + \sigma_i^2 ((U^T CU)_{11})_{ji}] \\ (K_{11})_{ij} &= \frac{\sigma_i \sigma_j}{\sigma_j^2 - \sigma_i^2} [((U^T CU)_{11})_{ij} + ((U^T CU)_{11})_{ji}]. \end{aligned}$$

4. APPROXIMATION OF LYAPUNOV EXPONENTS

An application of the SVD of a fundamental matrix solution $X \in \mathcal{S}$ satisfying (2) is in the approximation of its Lyapunov exponents. We refer to [14] for formal definitions and justifications. Presently, we recall (e.g., see [7]) that if σ_i , and their reciprocals $1/\sigma_i$, $i = 1, \dots, n$, are the continuous singular values of X , then the Lyapunov exponents can be obtained as

$$(19) \quad \lambda_i = \lim_{t \rightarrow \infty} \frac{1}{t} \ln(\sigma_i(t)), \quad \text{and} \quad -\lambda_i, \quad i = 1, \dots, n.$$

Of course, in practice we will approximate the Lyapunov exponents on a finite interval $[0, T]$ as $\lambda_i \approx \frac{1}{T} \ln \sigma_i(T)$. As alternative to SVD based techniques, one can of course consider QR method; e.g., see [12] for a QR method tailored to symplectic functions.

In our case of $X \in \mathcal{S}$, we will only compute the (distinct) singular values less than 1 and thus just the n negative Lyapunov exponents. [So doing, we avoid working with quantities that blow up as time increases.] To compute these n singular values, we should solve the

analogous differential equation to (17), which however we will solve for the logarithms. That is, we will end up solving

$$(20) \quad \frac{d}{dt}v_i = (S_{11})_{ii}, \quad i = 1, \dots, n,$$

with $v_i = \ln(\sigma_i)$, $i = 1, \dots, n$, which amounts to a quadrature and where $S = U^T C U$. Similarly, rather than using (16) and (18) we will actually use

$$(21) \quad \begin{aligned} (H_{12})_{ij} &= \frac{1}{2}[-\coth(v_i + v_j)((S_{12})_{ij} + (S_{21})_{ji}) + (S_{12})_{ij} - (S_{21})_{ji}] \\ (K_{12})_{ij} &= -\frac{1}{2} \frac{1}{\sinh(v_i + v_j)} [(S_{12})_{ij} + (S_{12})_{ji}], \end{aligned}$$

for $i, j = 1, \dots, n$, and

$$(22) \quad \begin{aligned} (H_{11})_{ij} &= \frac{1}{2}[\coth(v_j - v_i)((S_{11})_{ij} + (S_{11})_{ji}) + (S_{11})_{ij} - (S_{11})_{ji}] \\ (K_{11})_{ij} &= \frac{1}{2} \frac{1}{\sinh(v_j - v_i)} [(S_{11})_{ij} + (S_{11})_{ji}], \end{aligned}$$

for $i = 1, \dots, n$, and $j = i + 1, \dots, n$, with the rest defined by skew-symmetry. The ordinary differential equation in (20) has been integrated by the Euler explicit method while the matrix ODEs in (15) have been solved by an exponential integrator (of order one) in order to preserve both the orthogonality and symplecticity of the matrices U and V during the evolution.

Remark 10. *We have not paid any attention to efficient computations, and our experiments are only meant to be illustrative. More refined implementations may make use of efficient techniques for computing the exponential of Hamiltonian and skew-symmetric matrices (e.g., see [2] for the case of skew-symmetric matrices), as well as make use of higher order integration schemes.*

In the experiments below, we took initial conditions (ICs) $X_0 = U_0 \Sigma_0 V_0$ where U_0 and V_0 are random orthogonal and symplectic matrices and $\Sigma_0 = \text{diag}(\Lambda_0, \Lambda_0^{-1})$ is a diagonal matrix with $\Lambda_0 = \text{diag}(\sigma_1^0, \dots, \sigma_n^0)$, and where $0 < \sigma_n^0 < \dots < \sigma_1^0 < 1$ are random as well.

Example 11. We take a system in the form (2) with $n = 2$, by defining $C(t) = \hat{C} + D(t)$, where

$$\begin{aligned} \hat{C}_{11} &= \begin{pmatrix} 2.5 & 1 \\ 2 & -2 \end{pmatrix}, & \hat{C}_{12} &= \begin{pmatrix} 2 & 4 \\ 4 & 1 \end{pmatrix}, & \hat{C}_{21} &= \begin{pmatrix} 2 & 5 \\ 5 & 2 \end{pmatrix}, \\ D_{11}(t) &= \begin{pmatrix} \frac{1}{(1+t^2)} & 0 \\ 0 & \frac{1}{(1+t^2)} \end{pmatrix}, & D_{12}(t) &= \begin{pmatrix} \frac{2}{(1+t^3)} & 0 \\ 0 & \frac{2}{(1+t)} \end{pmatrix}, & D_{21}(t) &= \begin{pmatrix} \frac{2}{(1+t^2)} & \frac{1}{(1+t^2)} \\ \frac{1}{(1+t^2)} & 0 \end{pmatrix}. \end{aligned}$$

The Lyapunov exponents of the system are the real parts of the eigenvalues of \hat{C} , that is $\lambda_1 = 7.432699$, $\lambda_2 = 2.237180$ together with $-\lambda_1$, $-\lambda_2$. We use the SVD method with time step $h = 0.001$, and integrate (15) and (20) up to the final time of $T = 10^4$. In Table 1 we show results of the approximate Lyapunov exponents $\frac{1}{T} \ln \sigma_i(T)$, $i = 1, 2$, for several values of T . As a measure of comparison, in Table 1 we also show the approximations obtained by using the continuous QR method (see [6]) which is based on continuously finding the factorization $X = QR$. In this case, we only approximate the two dominant exponents, and thus work directly on a system half the size (i.e., X here is in $\mathbb{R}^{4 \times 2}$). Lyapunov exponents are now approximated as $\frac{1}{T} \ln R_{ii}(T)$, $i = 1, 2$. Again, ICs have been chosen at random, and integration for the orthonormal factor Q has been done with a simple projected forward Euler scheme. From the results of this simulation, it is apparent that the SVD and QR methods are comparable in terms of accuracy (perhaps, the SVD

TABLE 1. Approximate exponents: SVD and QR

T	λ_1 -SVD	λ_2 -SVD	λ_1 -QR	λ_2 -QR
0.1	8.6371	4.1396	-0.0225	-0.8031
1	8.7579	1.6901	8.3651	1.0050
10	7.7949	2.1626	7.5039	2.0898
100	7.4720	2.2080	7.4623	2.1690
1000	7.4377	2.2332	7.4346	2.2353
10000	7.4333	2.2367	7.4333	2.2363

method is a bit more accurate for small values of T). On the other hand, the QR method is much less expensive, by a factor of about 8, precisely the difference caused by the linear algebra reduction achieved by halving the size of the problem (our implementation of the exponential integrator is forcing a cost of $O(m^3)$ per step).

Example 12. This second example is the familiar Hènon-Heiles problem, for which computation of the Lyapunov exponents was also done in [12]. We have the Hamiltonian

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3}q_2^3,$$

and the associated dynamical system $\dot{x} = J\nabla H(x(t))$, where ∇ is the gradient and $x = (q_1, q_2, p_1, p_2)$. That is, we have

$$(23) \quad \begin{aligned} q_1 &= p_1 \\ q_2 &= p_2 \\ \dot{p}_1 &= -q_1(1 + 2q_2) \\ \dot{p}_2 &= -q_2 - q_1^2 + q_2^2. \end{aligned}$$

Exact solution is not known, so we must solve (23) in order to obtain the associated linearized problem. We integrate for the trajectory x with the leapfrog scheme. For comparison with the results in [12], we performed experiments with each of the initial conditions (IC) in Table 2 with q_1 always given by 0:

TABLE 2. Initial conditions.

IC	q_2	p_2	p_1
1	0.2	0.02	0.463609
2	0.33	0.14	0.381389
3	0.015	0.25	0.432755
4	0.20	0.14	0.442417
5	-0.15	0.02	0.474183
6	0.25	0.30	0.328506

In Table 3 we show the approximate Lyapunov exponents at the final time $T = 10^4$, obtained integrating the ODEs in (15) and (20) with time step $h = 0.001$. Exponential notation is used throughout. In spite of the crudeness of our numerical implementation, the results are in good agreement with those in [12].

TABLE 3. Approximate Lyapunov exponents.

IC	λ_1	λ_2
1	7.42E-04	6.97E-04
2	7.97E-04	3.86E-04
3	8.31E-04	6.52E-05
4	3.93E-02	4.89E-04
5	5.48E-02	7.04E-04
6	5.48E-02	6.97E-04

5. CONCLUSIONS

Using the polar decomposition of a generic C^k symplectic function X we have derived a constructive argument to establish existence of a smooth singular value decomposition (SVD) for X where both factors are in the symplectic group. The generic dichotomic assumption on the polar factor of X has been essential in our discussion. Under this assumption, our construction gives a new algorithm to find the SVD of X , which—as illustration—we have used to approximate the Lyapunov exponents of Hamiltonian differential systems. Combining the results in this work with those derived in [3] for the Lorentz group, and by using the analysis in [5], one can consider the SVD of a function X evolving on a quadratic group generated by any orthogonal matrix H .

In terms of cost, our simple implementation of the SVD examined in this paper is not competitive with the tried and true QR methods, for the computation of Lyapunov exponents. On the other hand, unlike the case of QR methods, with our SVD technique one is able to obtain complete information on the fundamental solution matrix, without explicitly resolving undesired growth behaviors.

REFERENCES

- [1] J.L. Chern and L. Dieci. Smoothness and periodicity of some matrix decompositions. *SIAM J. Matrix Anal. Appl.*, Vol. 22 (2001), pp. 772–792.
- [2] N. Del Buono, L. Lopez and R. Peluso. Computation of the exponential of large sparse skew-symmetric matrices. *SIAM J. Scient. Comp.*, to appear (2005).
- [3] L. Dieci, C. Elia and L. Lopez. Smooth SVD on the Lorentz group with application to computation of Lyapunov exponents. *Journal of Computational and Applied Mathematics*, Vol. 164–165 (2004), pp. 255–264.
- [4] L. Dieci and T. Eirola. On smooth decompositions of matrices. *SIAM J. Matrix Anal. Appl.*, Vol. 20 (1999), pp. 800–819.
- [5] L. Dieci and L. Lopez. Lyapunov exponents of systems evolving on quadratic groups. *SIAM J. Matrix Anal. Appl.*, Vol. 24 (2003), pp. 1175–1185.
- [6] L. Dieci and E. Van Vleck. Computation of a few Lyapunov exponents for continuous and discrete dynamical systems. *Appl. Num. Math.*, Vol. 17 (1995), pp. 275–291.
- [7] K. Geist, U. Parlitz and W. Lauterborn. Comparison of different methods for computing Lyapunov exponents. *Prog. Theor. Phys.*, Vol. 83 (1990), pp. 875–893.
- [8] R.A. Horn and C.R. Johnson. *Matrix Analysis*. Cambridge University Press, New-York, 1985.
- [9] N. Higham, N. Mackey, S. Mackey and F. Tisseur. Computing the Polar Decomposition and the Matrix Sign Decomposition in Matrix Groups. *SIAM J. Matrix Anal. Appl.*, Vol. 25 (2004), pp. 1178–1192.
- [10] M.W. Hirsch. *Differential topology*. Springer-Verlag, New-York, 1976.
- [11] T. Kato. *Perturbation theory for linear operators*. Springer-Verlag, Berlin, 1995.
- [12] B. Leimkuhler and E. Van Vleck. Orthosymplectic integration of linear Hamiltonian systems. *Numer. Math.*, Vol. 77 (1997), pp. 269–282.
- [13] N. Mackey, S. Mackey and V. Mehrmann, Analytic SVD of symplectic matrices. *Personal communication* (2005).

- [14] V.I. Oseledec. A multiplicative ergodic theorem. Lyapunov characteristic numbers for dynamical systems. *Trans. Moscow Mathem. Society*, Vol. 19 (1968), pp. 197–231.
- [15] K. Wright. Differential equations for the analytical singular value decomposition of a matrix. *Numer. Math.*, Vol. 63 (1992), pp. 283–295.
- [16] H. Xu. An SVD-Like matrix decomposition and its applications. *Linear Algebra and Its Applications*, Vol. 368 (2003), pp. 1–24.

SCHOOL OF MATHEMATICS, GEORGIA TECH, ATLANTA, GA 30332 U.S.A.

E-mail address: dieci@math.gatech.edu

DIPARTIMENTO DI MATEMATICA, UNIV. OF BARI, I-70100, BARI, ITALY

E-mail address: lopezl@dm.uniba.it