Exponential polar factorization of the fundamental matrix of linear differential systems

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Abstract

We propose a new constructive procedure to factorize the fundamental real matrix of a linear system of differential equations as the product of the exponentials of a symmetric and a skew-symmetric matrix. Both matrices are explicitly constructed as series whose terms are computed recursively. The procedure is shown to converge for sufficiently small times. In this way, explicit exponential representations for the factors in the analytic polar decomposition are found. An additional advantage of the algorithm proposed here is that, if the exact solution evolves in a certain Lie group, then it provides approximations that also belong to the same Lie group, thus preserving important qualitative properties.

Keywords: Exponential factorization, polar decomposition
MSC (2000): 15A23, 34A45, 65L99

1 Introduction

Given the non-autonomous system of linear ordinary differential equations

$$\frac{dU}{dt} = A(t)\,U, \qquad U(0) = I \tag{1}$$

with $A(t)$ a real analytic $N \times N$ matrix, the Magnus expansion allows one to represent the fundamental matrix $U(t)$ locally as

$$U(t) = \exp(\Omega(t)), \qquad \Omega(0) = O, \tag{2}$$

where the exponent $\Omega(t)$ is given by an infinite series

$$\Omega(t) = \sum_{m=1}^{\infty} \Omega_m(t) \tag{3}$$

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whose terms are linear combinations of integrals and nested commutators involving the matrix A at different times [13]. The series converges in the interval $t \in [0, \tau)$ such that $\int_0^\tau \|A(s)\| ds < \pi$ and the sum $\Omega(t)$ verifies $\exp \Omega(t) = U(t)$. Different approximations to the solution of (1) are obtained when the series of Ω is truncated, all of them preserving important qualitative properties of the exact solution. Magnus expansion has been widely used as an analytic tool in many different areas of physics and chemistry, and also numerical integrators have been constructed which have proved to be highly competitive with other, more conventional numerical schemes in terms of accuracy and computational cost (see [2] and references therein).

Although the representation (2)-(3) and the approximations obtained when the series is truncated has several advantages, it is not always able to reproduce all the qualitative features of $U(t)$. In particular, suppose that the matrix-valued function $A(t)$ is periodic with period T. Then the Floquet theorems ensures the factorization of the solution as a periodic part and a purely exponential factor: $U(t) = P(t) \exp(tF)$, where F and P are $N \times N$ matrices, $P(t+T) = P(t)$ for all t and F is constant. It is clear, then, that the Magnus expansion does not explicitly provide this structure. In that case, however, it is possible to reformulate the procedure so that both matrices $P(t)$ and F can be constructed recursively [4].

Another example concerns symplectic matrices. As is well known, the most general $2N \times 2N$ symplectic matrix M can be written as the product of two exponentials of elements in the symplectic group Lie algebra as $M = \exp(X) \exp(Y)$, and each of the elements is of a special type, namely $X = JS^a$ and $Y(t) = JS^c$, where J is the standard canonical matrix,

$$J = \begin{pmatrix} O_N & I_N \\ -I_N & O_N \end{pmatrix},$$

S^a is a real symmetric matrix that anti commutes with J and S^c is a real symmetric matrix that commutes with J [8]. Since X is symmetric and Y is skew-symmetric, notice that the factorization $\exp(X) \exp(Y)$ is a special type of polar decomposition for the matrix M. According with this property, if $A(t)$ belongs to the symplectic Lie algebra $\mathfrak{sp}(2N)$, i.e., it verifies $A^T J + JA = O$, then the fundamental solution $U(t)$ evolves in the symplectic group $\mathrm{Sp}(2N)$ (i.e., $U^T(t) J U(t) = J$ for all t) and therefore admits a factorization

$$U(t) = \exp(X(t)) \exp(Y(t)), \tag{4}$$

where $X(t) = JS^a(t)$ is a symmetric matrix and $Y(t) = JS^c(t)$ is skew-symmetric. A natural question is whether the Magnus expansion can be adapted to treat this problem in order to provide explicit analytic expressions for both $X(t)$ and $Y(t)$, just as in the case of a periodic matrix $A(t)$. More generally, one might try to adapt the Magnus expansion to construct explicitly a polar factorization of the form (4) for the fundamental matrix of (1). In other words, the idea is then to build explicitly the solution of (1) as (4) with both matrices $X(t)$ and $Y(t)$ constructed as series of the form

$$X(t) = \sum_{i \geq 1} X_i(t), \qquad Y(t) = \sum_{i \geq 1} Y_i(t). \tag{5}$$

This issue is addressed in the sequel. More specifically, we present a procedure that allows us to compute recursively X_i, Y_i in terms of nested integrals and nested commutators involving the matrix $A(t)$. Moreover, these series are shown to be convergent, at least for sufficiently small times. Thus, in the convergence domain, we have explicit exponential representations for the factors $H(t)$ and $Q(t)$ in the analytic polar decomposition of $U(t)$:

$$U(t) = H(t)\,Q(t). \tag{6}$$

As is well known, given an arbitrary time-varying nonsingular real analytic matrix function $U(t)$ on an interval $[a, b]$ so that $U(t)$, $\dot{U}(t)$ and $U(t)^{-1}$ are bounded, there exists an analytic polar decomposition (6), with $Q(t)$ orthogonal, $H(t)$ symmetric (but not definite) and both are real analytic on $[a, b]$ [15].

Polar decomposition of time-varying matrices has proved to be useful in several contexts. Thus, for instance, it appears in numerical methods for computing analytic singular value decompositions [15] and as a path to inversion of time dependent nonsingular square matrices [10]. Polar decomposition is also used in computer graphics and in the study of stress and strain in continuous media [14]. Since both factors possess best approximation properties, it can be applied in optimal orthogonalization problems [11].

Theoretical general results on decompositions of a time varying matrix $U(t)$ of class $\mathcal{C}^k$ can be found in [7], where sufficient conditions for existence of QR, Schur, SVD and polar factorizations are given and differential equations for the factors are derived.

The procedure we present here for computing the factorization (4) for the fundamental matrix of (1) has several additional advantages. First, even when the series are truncated, the structure of the polar decomposition still remains for the resulting approximations. Second, the algorithm can be easily implemented in a symbolic algebra package and may be extended without difficulty to get convergent approximations to the analytic polar decomposition of a more general class of nonsingular time dependent matrices and also of the exponential of constant matrices. Third, if $A(t)$ belongs to a certain matrix Lie subalgebra, so that $U(t)$ evolves in the corresponding Lie group, it provides approximations in this Lie group, and thus they preserve important qualitative features of the exact solution. The symplectic case considered before is a case in point here. Fourth, if $A(t)$ depends on some parameters, this procedure leads to approximate factorizations to the exact solution involving directly these parameters, which in turn allows one to analyze different regions of the parameter space with just one calculation. In this sense, it differs from other more numerically oriented techniques for computing the polar decomposition existing in the literature (e.g. [3, 10, 15]).

It is important to stress that the formalism proposed here is not specifically designed to get efficient numerical algorithms for computing the analytic polar decomposition of an arbitrary matrix $U(t)$, but instead it is oriented to get a factorization of the form (4) for the fundamental matrix of eq. (1) which could be specially well adapted when the coefficient matrix $A(t)$ involves one or more parameters and belongs to some special matrix Lie subgroup.

2 Constructing the exponential polar factorization

2.1 Equations satisfied by $X(t)$ and $Y(t)$

The first step in the procedure is to establish the differential equations satisfied by both $X(t)$ and $Y(t)$ in the factorization $U(t) = \mathrm{e}^{X(t)}\mathrm{e}^{Y(t)}$. This is done by differentiating (4), taking into account the expression for the derivative of a matrix exponential [2, 12]:

$$\frac{d}{dt}\exp(\Omega(t)) = d\exp_{\Omega(t)}(\dot{\Omega}(t))\,\exp(\Omega(t)) = \exp(\Omega(t))\,d\exp_{-\Omega(t)}(\dot{\Omega}(t)),$$

where

$$d\exp_{\Omega(t)}(\dot{\Omega}(t)) \equiv \sum_{k=0}^{\infty}\frac{1}{(k+1)!}\,\mathrm{ad}_{\Omega}^{k}\,\dot{\Omega}. \tag{7}$$

Here ad_A stands for the adjoint operator of A, which acts according to

$$\mathrm{ad}_A B = [A,B], \qquad \mathrm{ad}_A^j B = [A, \mathrm{ad}_A^{j-1}B], \qquad \mathrm{ad}_A^0 B = B, \qquad j = 1,2,\ldots, \tag{8}$$

where $[A,B] = AB - BA$ denotes the commutator. After inserting the corresponding expressions into (1) we get

$$d\exp_X \dot{X}\,\mathrm{e}^{X(t)}\mathrm{e}^{Y(t)} + \mathrm{e}^{X(t)}d\exp_Y \dot{Y}\mathrm{e}^{Y(t)} = A(t)\mathrm{e}^{X(t)}\mathrm{e}^{Y(t)}, \tag{9}$$

or equivalently

$$\mathrm{e}^{-X(t)}\left(A(t) - d\exp_X \dot{X}\right)\mathrm{e}^{X(t)} = d\exp_Y \dot{Y}. \tag{10}$$

In general, $A(t)$ can be decomposed in a unique way into its symmetric and skew-symmetric part:

$$A(t) = P(t) + K(t), \quad \text{where} \quad P(t) = \frac{1}{2}(A + A^T), \quad K(t) = \frac{1}{2}(A - A^T).$$

If we denote by $\mathfrak{k}$ the set of skew-symmetric matrices and by $\mathfrak{p}$ the set of symmetric matrices of a given dimension N, it is clear that the following commutation relations hold for arbitrary elements in each set:

$$[\mathfrak{k},\mathfrak{k}] \subseteq \mathfrak{k}, \qquad [\mathfrak{k},\mathfrak{p}] \subseteq \mathfrak{p}, \qquad [\mathfrak{p},\mathfrak{p}] \subseteq \mathfrak{k}.$$

Therefore, since Y and $\dot{Y}$ are skew-symmetric, then $d\exp_Y \dot{Y} \in \mathfrak{k}$, and so the left hand side of eq. (10) also belongs to $\mathfrak{k}$. We must analyze this term and separate its symmetric contribution, which obviously has to vanish.

If we denote, for simplicity, $u \equiv \mathrm{ad}_X$, then

$$\begin{aligned}
&\mathrm{e}^{-X(t)}A(t)\,\mathrm{e}^{X(t)} = \mathrm{e}^{-\mathrm{ad}_X}A(t) = \mathrm{e}^{-\mathrm{ad}_X}K(t) + \mathrm{e}^{-\mathrm{ad}_X}P(t)\\
&= \cosh(u)\,(K) - \sinh(u)\,(K) + \cosh(u)\,(P) - \sinh(u)\,(P)\\
&= -\sinh(u)\,(K) + \cosh(u)\,(P) \qquad (\in \mathfrak{p})\\
&\quad + \cosh(u)\,(K) - \sinh(u)\,(P) \qquad (\in \mathfrak{k})
\end{aligned}$$

where the functions involving u have to be understood as formal power series. On the other hand,

$$
\begin{aligned}
&\mathrm{e}^{-X(t)} d\exp_X \dot{X}\, \mathrm{e}^{X(t)} = d\exp_{-X} \dot{X} = \sum_{j=0}^{\infty} \frac{(-1)^j}{(j+1)!}\, \mathrm{ad}_X^j \dot{X} \\
=&\sum_{p=0}^{\infty} \frac{(-1)^{2p}}{(2p+1)!}\, \mathrm{ad}_X^{2p} \dot{X} + \sum_{p=0}^{\infty} \frac{(-1)^{2p+1}}{(2p+2)!}\, \mathrm{ad}_X^{2p+1} \dot{X} \\
=&\frac{1}{u}\, \sinh(u)\, (\dot{X}) && (\in \mathfrak{p}) \\
+&\frac{1}{u}\, (1-\cosh(u))\, (\dot{X}) && (\in \mathfrak{k})
\end{aligned}
$$

In consequence,

$$
-\sinh(u)\, (K) + \cosh(u)\, (P) - \frac{1}{u} \sinh(u)\, (\dot{X}) = O \tag{11}
$$

and finally we arrive at the differential equation satisfied by X:

$$
\dot{X} = -u\, K + u\, \frac{\cosh(u)}{\sinh(u)}\, P, \qquad X(0) = O. \tag{12}
$$

Observe that this equation only involves $X(t)$. Explicitly, it reads

$$
\dot{X} = -\mathrm{ad}_X K + \sum_{k=0}^{\infty} \frac{2^{2k} B_{2k}}{(2k)!} \mathrm{ad}_X^{2k} P, \qquad X(0) = O, \tag{13}
$$

with B_j denoting the Bernoulli numbers [16].

In a similar way, we can obtain the equation satisfied by $Y(t)$. Specifically, by considering the projection of equation (10) into $\mathfrak{k}$ one has

$$
d\exp_Y \dot{Y} = \cosh(u)\, (K) - \sinh(u)\, (P) + \frac{\cosh(u) - 1}{u}\, \dot{X}, \tag{14}
$$

where, as before, $u \equiv \mathrm{ad}_X$. Inserting equation (11) into (14) results in

$$
d\exp_Y \dot{Y} = K + \frac{1 - \cosh(u)}{\sinh(u)}\, P \tag{15}
$$

and finally

$$
\dot{Y} = d\exp_Y^{-1} \left(K + \frac{1 - \cosh(u)}{\sinh(u)}\, P \right), \qquad Y(0) = O, \tag{16}
$$

where

$$
d\exp_Y^{-1} V = \sum_{j=0}^{\infty} \frac{B_j}{j!}\, \mathrm{ad}_Y^j V \equiv \frac{\mathrm{ad}_Y}{\mathrm{e}^{\mathrm{ad}_Y} - 1} V.
$$

By considering the power series of the function $(1-\cosh u)/\sinh u$, we can write

$$
\dot{Y} = \sum_{j=0}^{\infty} \frac{B_j}{j!}\, \mathrm{ad}_Y^j \left(K - 2 \sum_{k=2}^{\infty} \frac{(2^k - 1) B_k}{k!}\, \mathrm{ad}_X^{k-1} P \right), \qquad Y(0) = O. \tag{17}
$$

Notice that solving for $Y(t)$ requires to previously compute $X(t)$. As a matter of fact, it can be shown that, unless A is a constant matrix, one cannot write a differential equation for Y independent of X. In spite of that, in the sequel we show that it is indeed possible to construct both $X(t)$ and $Y(t)$ as power series by recurrence.

2.2 Constructing the series of $X(t)$ and $Y(t)$

To solve equation (13), let us introduce a parameter $\epsilon > 0$ and replace $A(t)$ in equation (1) by $\epsilon A(t)$. Then, the corresponding decomposition (4) reads

$$U(\epsilon, t) = \mathrm{e}^{X(\epsilon,t)}\, \mathrm{e}^{Y(\epsilon,t)}$$

and the goal is to determine the matrices $X(\epsilon, t)$, $Y(\epsilon, t)$ perturbatively as an infinite series in ϵ:

$$X(\epsilon, t) = \sum_{n=1}^{\infty} \epsilon^n X_n(t), \qquad Y(\epsilon, t) = \sum_{n=1}^{\infty} \epsilon^n Y_n(t), \tag{18}$$

so that we will recover the factorization (4) when $\epsilon = 1$. The equation satisfied by $X(\epsilon, t)$ is obviously

$$\frac{\partial X}{\partial t} = -\epsilon\, \mathrm{ad}_X K + \sum_{k=0}^{\infty} \frac{2^{2k} B_{2k}}{(2k)!}\, \mathrm{ad}_X^{2k}(\epsilon P), \qquad X(\epsilon, 0) = O. \tag{19}$$

Up to order ϵ^n we have

$$\begin{aligned}
\frac{\partial}{\partial t} X(\epsilon, t) &= \sum_{j=1}^{n} \epsilon^j \dot{X}_j(t) + \mathcal{O}(\epsilon^{n+1}) \\
\mathrm{ad}_X(\epsilon K) &= \sum_{j=1}^{n-1} \epsilon^{j+1} \mathrm{ad}_{X_j} K + \mathcal{O}(\epsilon^{n+1}) \\
\sum_{j=1}^{n-1} \frac{2^j B_j}{j!}\, \mathrm{ad}_X^j(\epsilon P) &= \sum_{l=2}^{n} \epsilon^l \sum_{j=1}^{l-1} \frac{2^j B_j}{j!} \sum_{\substack{k_1+\cdots+k_j=l-1 \\ k_1\geq 1,\ldots,k_j\geq 1}} \mathrm{ad}_{X_{k_1}} \cdots \mathrm{ad}_{X_{k_j}} P + \mathcal{O}(\epsilon^{n+1}).
\end{aligned}$$

Then, by inserting these expressions into (19) and equating powers of ϵ (see e.g. [5] for more details) we get

$$\begin{aligned}
\dot{X}_1(t) &= P(t) \qquad\qquad (20) \\
\dot{X}_n(t) &= -\mathrm{ad}_{X_{n-1}(t)} K(t) + \sum_{j=2}^{n-1} c_j \sum_{\substack{k_1+\cdots+k_j=n-1 \\ k_1\geq 1,\ldots,k_j\geq 1}} \mathrm{ad}_{X_{k_1}(t)} \cdots \mathrm{ad}_{X_{k_j}(t)} P(t),
\end{aligned}$$

for $n \geq 2$. Alternatively, for the series $C = \sum_{n\geq 1} C_n$ and the matrix B we can introduce the operator $S_n^{(j)}(t, C, B)$ defined as

$$\begin{aligned}
S_n^{(1)}(t, C, B) &= [C_{n-1}, B], \\
S_n^{(j)}(t, C, B) &= \sum_{m=1}^{n-j} [C_m, S_{n-m}^{(j-1)}(t, C, B)], \qquad 2 \leq j \leq n-1.
\end{aligned} \tag{21}$$

Then, from expression (20) and the initial condition $X(0) = O$, we get

$$\begin{aligned} X_1(t) &= \int_0^t P(s)ds \\ X_n(t) &= -\int_0^t S_n^{(1)}(\tau, X, K)\, d\tau + \sum_{j=2}^{n-1} c_j \int_0^t S_n^{(j)}(\tau, X, P)\, d\tau. \end{aligned} \tag{22}$$

Proceeding in a similar way for the $Y(\epsilon, t)$ series, and after some elementary algebra, one arrives at

$$\begin{aligned} Y_1(t) &= \int_0^t K(s)ds \\ Y_n(t) &= \sum_{j=1}^{n-1} \frac{B_j}{j!} \int_0^t S_n^{(j)}(\tau, Y, K)\, d\tau - 2\sum_{j=1}^{n-1} \int_0^t d_{j+1} S_n^{(j)}(\tau, X, P)\, d\tau \\ &\quad -2\sum_{j=2}^{n-1}\sum_{s=1}^{j-1}\sum_{p=1}^{n-j} \frac{B_s}{s!} d_{p+1} \int_0^t S_j^{(s)}(\tau, Y, S_{n-j+1}^{(p)}(\tau, X, P))d\tau, \end{aligned} \tag{23}$$

where

$$c_j = \frac{2^j B_j}{j!}, \qquad d_j = \frac{(2^j - 1)B_j}{j!}.$$

Notice that the expressions for $X_n(t)$ and $Y_n(t)$ only involve the evaluation of integrals of nested commutators of K, P and terms of the series that have been already computed.

2.3 Convergence of the series $X(t)$ and $Y(t)$

We next analyze the convergence of the series (18) (with $\epsilon = 1$) obtained with the procedure (22)-(23). For that purpose we consider the usual 2-norm in the space of matrices. Then, for two generic matrices A and B, we have

$$\|\mathrm{ad}_A B\| = \|[A, B]\| \leq 2\,\|A\|\,\|B\|, \qquad \text{so that} \qquad \|\mathrm{ad}_A\| \leq 2\,\|A\|. \tag{24}$$

Moreover, the 2-norm is unitarily invariant, so that, in general,

$$\left\|\mathrm{e}^{\mathrm{ad}_A} B\right\| = \|\mathrm{e}^A B\, \mathrm{e}^{-A}\| = \|B\|. \tag{25}$$

Consider first the differential equation (12), or equivalently (13), where $u \equiv \mathrm{ad}_X$, and in particular the series $u\frac{\cosh(u)}{\sinh(u)}P$. It is clear that

$$\begin{aligned} \left\|u\frac{\cosh(u)}{\sinh(u)}P\right\| &= \left\|\frac{u}{2\sinh(u)}(\mathrm{e}^u P + \mathrm{e}^{-u}P)\right\| \leq \frac{1}{2}\left\|\frac{u}{\sinh(u)}\right\| \left(\|\mathrm{e}^u P\| + \|e^{-u}P\|\right) \\ &\leq \frac{1}{2}\left\|\frac{u}{\sinh(u)}\right\| (\|P\| + \|P\|) \equiv \|h(u)\|\|P\|. \end{aligned}$$

Here we have used the unitary invariance of the 2-norm (property (25)). Since $X(t)$ is a symmetric matrix, then it is orthogonally diagonalizable. The same

is true for $u = \mathrm{ad}_X$, considered as a $n^2 \times n^2$ matrix, as shown in the Appendix. In addition, if X has n eigenvalues $\{\lambda_i \,|\, i = 1, ..., n\}$, then ad_X has the n^2 eigenvalues $\{\lambda_j - \lambda_k \,|\, j, k = 1, ..., n\}$ [17]. Therefore

$$h(u) = \frac{u}{\sinh u} = S^T \, h(D) \, S, \qquad \text{with} \quad D = \mathrm{diag}\,(\lambda_j - \lambda_k), \quad \lambda_i \in \mathbb{R}$$

and S is an orthogonal matrix, so that

$$\|h(u)\| = \left\| S^{-1} \, h(D) \, S \right\| = \|h(D)\| = \max\{|h(\lambda_j - \lambda_k)|\} \leq 1$$

since $\left| \frac{x}{\sinh(x)} \right| \leq 1$ for all $x \in \mathbb{R}$. In consequence, by integrating (12) we have

$$\begin{aligned} \|X(t)\| &\leq \int_0^t \left\| (-u\,K + u \frac{\cosh(u)}{\sinh(u)} \, P) \right\| \leq \int_0^t (2\,\|X\|\|K\| + \|P\|)\, ds \\ &\leq \int_0^t \|A(s)\|\, ds + \int_0^t 2\|A(s)\|\, \|X(s)\|\, ds \end{aligned} \tag{26}$$

Direct application of Gronwall's lemma [9] leads then to

$$\|X(t)\| \leq f(t) + \int_0^t 2\|A(s)\| f(s) \exp\left(\int_s^t 2\|A(v)\| dv \right) ds,$$

where

$$f(t) \equiv \int_0^t \|A(s)\|\, ds. \tag{27}$$

In consequence, $\|X(t)\|$ is bounded as long as $f(t)$ is bounded.

Let us turn now out attention to the series $Y(t)$. To analyze its (absolute) convergence, the following generalization of Gronwall's lemma will be useful [1].

Lemma 1 *Let $y(t)$, $v(t)$ be positive continuous functions in $t_0 \leq t \leq T$, where $C = const \geq 0$, the functions $y(t)$, $v(t)$ are continuous and non-negative, and $g(y)$ is a non-negative non-decreasing continuous function with $g(y) > 0$ for $y > 0$. Then, the inequality*

$$y(t) \leq C + \int_{t_0}^t v(s) g(y(s)) ds, \qquad t_0 \leq t \leq T$$

implies the inequality

$$y(t) \leq G^{-1} \left(G(C) + \int_{t_0}^t v(s) ds \right),$$

where

$$G(u) = \int_{u_0}^u \frac{ds}{g(s)}, \qquad u_0 > 0$$

for all $t \in [t_0, T)$ such that the function

$$G(C) + \int_{t_0}^t v(s) ds$$

belongs to the domain of the function G^{-1}.

Our starting point in this case is equation (16), or equivalently

$$Y(t) = \int_0^t d\exp_Y^{-1}\left(K\ \tanh\frac{u}{2}P\right)\,ds, \tag{28}$$

whence

$$\|Y(t)\| \le \int_0^t \left\|d\exp_{Y(s)}^{-1} B(s)\right\|\,ds, \qquad \text{with} \qquad B(s) \equiv K(s) - \tanh\frac{u}{2}\,P(s).$$

Here both $Y(t)$ and $B(t)$ are skew-symmetric matrices. We can write

$$d\exp_Y^{-1} B = \frac{\mathrm{ad}_Y}{\mathrm{e}^{\mathrm{ad}_Y}-1}B = \mathrm{e}^{-\mathrm{ad}_{Y/2}}\frac{\mathrm{ad}_Y}{\mathrm{e}^{\mathrm{ad}_{Y/2}}-\mathrm{e}^{-\mathrm{ad}_{Y/2}}}B = \mathrm{e}^{-v/2}\frac{v/2}{\sinh(v/2)}B$$

where $v \equiv \mathrm{ad}_Y$. In consequence, by applying property (25), it follows that

$$\left\|d\exp_Y^{-1} B\right\| = \left\|\frac{v/2}{\sinh(v/2)}\,B\right\| \le \frac{\|Y\|}{\sin\|Y\|}\,\|B\|$$

Notice that we cannot apply here the same procedure to bound $\|h(v)\|$ as we did before for $\|h(u)\|$, since it is not guaranteed that v is a diagonalizable matrix. In any case, it holds that

$$\|Y(t)\| \le \int_0^t g\left(\|Y(s)\|\right)\,\|B(s)\|\,ds \quad \le \int_0^t g\left(\|Y(s)\|\right)\,\left(\|K(s)\| + \left\|\tanh\frac{u}{2}\,P(s)\right\|\right)ds$$

with

$$g(x) = \frac{x}{\sin x},$$

a non-negative non-decreasing continuous function, with $g(x) > 0$, for $x \in (0,\pi)$. Now we have to bound the series $\tanh(u/2)P$. Proceeding as we did with function $h(u)$, it is clear that

$$\left\|\tanh\frac{u}{2}\right\| = \left\|S_1^T\left(\tanh D_1\right)S\right\| = \max\{|\tanh(\lambda_j-\lambda_k)/2|\} \le 1$$

and thus

$$\left\|\tanh\frac{u}{2}\,P\right\| \le \|P\|.$$

In consequence,

$$\|Y(t)\| \le \int_0^t g\left(\|Y(s)\|\right)\,\left(\|K(s)\| + \|P(s)\|\right)ds \quad \le 2\int_0^t g\left(\|Y(s)\|\right)\|A(s)\|\,ds.$$

Lemma 1 can now be readily applied to the function $y(t) = \|X(t)\|$, so that

$$\|Y(t)\| < G^{-1}\left(2\int_0^t \|A(s)\|ds\right),$$

with $G(u) = \int_{u_0}^u (1/g(s))ds$ for all t such that

$$2\int_0^t \|A(s)\|ds < G(\pi) = \int_0^\pi \frac{1}{g(s)}ds = \int_0^\pi \frac{\sin s}{s}ds = \mathrm{Si}(\pi).$$

In other words, the series $Y(t)$ is absolutely convergent for $t < T$ such that

$$\int_0^T \|A(s)\| ds < \frac{1}{2}\,\mathrm{Si}(\pi) = 0.92596852\ldots \tag{29}$$

We have thus completed the proof of the following

Theorem 2 *The fundamental matrix of $\dot{U} = A(t)U$, where $A(t)$ is a real analytic matrix, can be factorized as*

$$U(t) = \exp(X(t))\,\exp(Y(t)), \tag{30}$$

where $X(t)$ is symmetric, $Y(t)$ is skew-symmetric and the series

$$X(t) = \sum_{i\geq 1} X_i(t), \qquad Y(t) = \sum_{i\geq 1} Y_i(t), \tag{31}$$

whose terms are given recursively by (22)-(23), converge at least in the interval $t \in [0, T)$ such that

$$\int_0^T \|A(s)\| ds < \frac{1}{2}\,Si(\pi).$$

As a consequence, in the convergence domain of the series (31) we get explicitly an analytic polar decomposition of the fundamental matrix $U(t)$ in the form (30).

Example 1. Let us illustrate now with a simple example how the recurrence (22)-(23) works in practice to compute the polar factorization (30) and the domain (and rate) of convergence of the series. We take for simplicity the following coefficient matrix

$$A(t) = \begin{pmatrix} 4\alpha\cos t & 1 \\ \mathrm{e}^{-\beta t} & \alpha\sin t \end{pmatrix} \tag{32}$$

depending on two parameters $\alpha > 0$, $\beta > 0$. In this case

$$P(t) = \begin{pmatrix} 4\alpha\cos t & \frac{1}{2}(1+\mathrm{e}^{-\beta t}) \\ \frac{1}{2}(1+\mathrm{e}^{-\beta t}) & \alpha\sin t \end{pmatrix}, \; K = \frac{1}{2}(1-\mathrm{e}^{-\beta t}) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{33}$$

We have computed with the recurrence (22)-(23) the terms $X_n(t)$ and $Y_n(t)$ up to $n = 6$ with *Mathematica* and then we have determined the approximate solution $U_{\mathrm{ap}}(t) = \exp(X^a(t))\exp(Y^a(t))$ with the truncated series

$$X^a(t) = \sum_{i=1}^{n} X_i(t), \qquad Y^a(t) = \sum_{i=1}^{n} Y_i(t). \tag{34}$$

With this time dependence, it is possible to evaluate all the integrals appearing in the expansion analytically up to the order considered. Finally we have obtained the error with respect to the exact solution by calculating the Frobenius

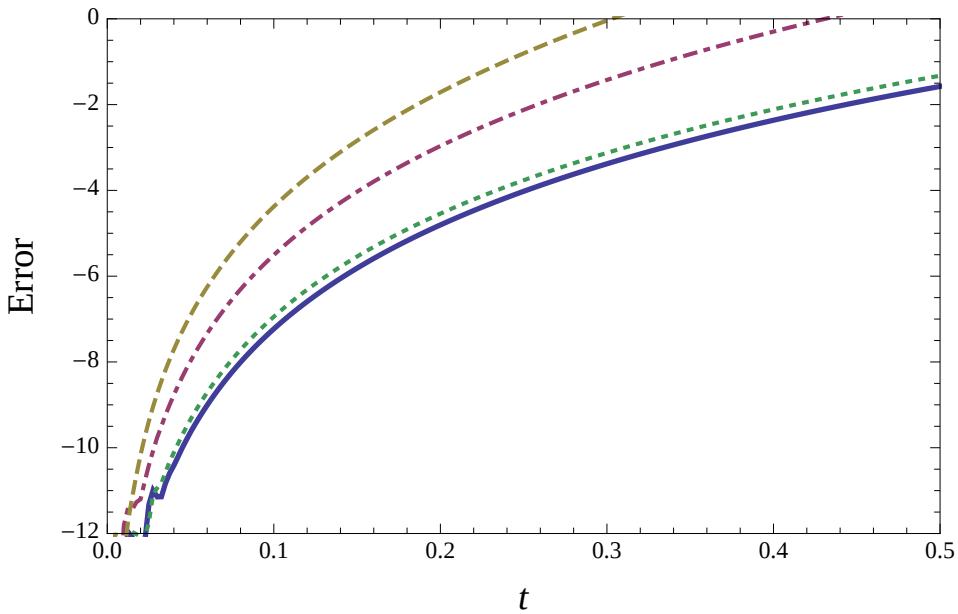

Figure 1: Error with respect to the exact result in logarithmic scale for Example 1 obtained with the exponential polar factorization for different values of the parameters: $\alpha = 1$, $\beta = 2$ (solid line); $\alpha = 2$, $\beta = 2$ (dot-dashed line); $\alpha = 3$, $\beta = 2$ (dashed line), and $\alpha = 1$, $\beta = 4$ (dotted line).

norm of the difference between the exact solution and the approximation, i.e., $\|U_{\rm ex}(t) - U_{\rm ap}(t)\|_F$, as a function of time for different values of the parameters. In Figure 1 we represent this error in logarithmic scale when: $\alpha = 1$, $\beta = 2$ (solid line); $\alpha = 2$, $\beta = 2$ (dot-dashed line); $\alpha = 3$, $\beta = 2$ (dashed line), and $\alpha = 1$, $\beta = 4$ (dotted line). The exact solution is computed numerically by *Mathematica* for each value of the parameters. Notice that the accuracy of the results increasingly deteriorates with higher values of α. This is consistent with the estimates provided by Theorem 2 for the convergence domain of the expansion: $T = 0.22196$, $T = 0.11438$, $T = 0.07674$ and $T = 0.22324$, respectively, for the values of the parameters considered. Even for larger values of t we get reasonable approximations to the exact result in all cases.

3 Generalizations

3.1 Exponential polar factorization for an arbitrary initial condition

So far we have only considered the case when the initial condition $U(0) = I$. Suppose one is interested in obtaining a similar representation of the solution of the general initial value problem

$$\frac{dU}{dt} = A(t)\,U, \qquad U(0) = U_0. \tag{35}$$

Although we can write the solution as $U(t) = \mathrm{e}^{X(t)}\,\mathrm{e}^{Y(t)}\,U_0$ with $X(t)$, $Y(t)$ constructed as the series (5) for the fundamental matrix, it is clear that this is does not correspond to a polar decomposition of $U(t)$.

Two different possibilities may be considered if the polar decomposition of the initial value, $U_0 = H_0 Q_0$, is available. The first consists in constructing a solution of the form

$$U(t) = \mathrm{e}^{X(t)} H_0\,\mathrm{e}^{Y(t)} Q_0.$$

In this case, by following a similar approach as in section 2, one gets the differential equations to be satisfied by each factor $X(t)$ and $Y(t)$, which turn out to be different from (12) and (16), respectively. Then, new recurrences have to be designed to construct the corresponding series (5).

The second procedure is more restrictive, in the sense that it requires computing previously a symmetric matrix X_0 and a skew-symmetric matrix Y_0 such that $H_0 = \exp X_0$, $Q_0 = \exp Y_0$ or alternatively $U_0 = \mathrm{e}^{X_0}\,\mathrm{e}^{Y_0}$. Then, equations (12) and (16) still apply, with initial conditions $X(0) = X_0$, $Y(0) = Y_0$, respectively. Therefore, the same recurrences obtained for the fundamental matrix directly apply, so that the series (5) are determined as

$$\begin{aligned}
X_1(t) &= X_0 + \int_0^t P(\tau)d\tau \\
X_n(t) &= -\int_0^t S_n^{(1)}(\tau, X, K)\,d\tau + \sum_{j=2}^{n-1} c_j \int_0^t S_n^{(j)}(\tau, X, P)\,d\tau \\
Y_1(t) &= Y_0 + \int_0^t K(\tau)d\tau \\
Y_n(t) &= \sum_{j=1}^{n-1} \frac{B_j}{j!} \int_0^t S_n^{(j)}(\tau, Y, K)\,d\tau - 2\sum_{j=1}^{n-1} \int_0^t d_{j+1} S_n^{(j)}(\tau, X, P)\,d\tau \\
&\quad -2\sum_{j=2}^{n-1}\sum_{s=1}^{j-1}\sum_{p=1}^{n-j} \frac{B_s}{s!} d_{p+1} \int_0^t S_j^{(s)}(\tau, Y, S_{n-j+1}^{(p)}(\tau, X, P))d\tau, \qquad n \geq 2
\end{aligned} \tag{36}$$

with $X_n(0) = Y_n(0) = O$ for $n \geq 2$.

This second procedure can also be applied for computing the exponential polar factorization of a given analytic nonsingular matrix $U(t)$ with $t \in [0, T]$. as long as $\dot{U}(t)U^{-1}(t) \equiv A(t)$.

Example 2. We carry out this procedure with the symplectic matrix

$$U(t) = \frac{1}{\sqrt{8}} \begin{pmatrix} 3\cos\omega t + 1 & 3\sin\omega t \\ -3\sin\omega t & 3\cos\omega t - 1 \end{pmatrix}. \tag{37}$$

A simple calculation shows that

$$A(t) = \dot{U}(t)U^{-1}(t) = \frac{3\omega}{8} \begin{pmatrix} \sin\omega t & 3 + \cos\omega t \\ -3 + \cos\omega t & -\sin\omega t \end{pmatrix} \in \mathfrak{sp}(2)$$

so that it is appropriate to consider a basis in the Lie algebra $\mathfrak{sp}(2)$. A possible option is given by the matrices

$$T_1 = J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad T_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad T_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

They satisfy the commutation rules

$$[T_1, T_2] = 2T_3, \qquad [T_2, T_3] = -2T_1, \qquad [T_3, T_1] = 2T_2.$$

In terms of this basis, one has $A(t) = P(t) + K$, with

$$P(t) = \frac{3\omega}{8}(\cos\omega t\, T_2 + \sin\omega t\, T_3), \qquad K = \frac{9\omega}{8} T_1,$$

and since

$$U_0 = U(0) = \begin{pmatrix} \sqrt{2} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix}, \qquad \text{then} \qquad X_0 = \log\sqrt{2}\, T_3, \qquad Y_0 = O.$$

Applying recurrence (36) one arrives at

$$X(t) = b_2(t)\, T_2 + b_3(t)\, T_3, \qquad Y(t) = b_1(t) T_1$$

where $b_1(t)$, $b_2(t)$ and $b_3(t)$ are complicated expressions depending on $\sin(n\,\omega\, t)$, $\cos(n\,\omega\, t)$ $(n = 1, \ldots)$, powers of $\omega\, t$ and products of these functions. A straightforward calculation shows that

$$\mathrm{e}^X = \cosh\eta\, I + \frac{\sinh\eta}{\eta}(b_2 T_2 + b_3 T_3), \qquad \mathrm{e}^Y = \cos b_1\, I + \sin b_1\, T_1,$$

where $\eta = \sqrt{b_2^2 + b_3^2}$. Therefore, by construction, $\exp(X(t))$ and $\exp(Y(t))$ are both symplectic, as well as the approximation $U_{\mathrm{ap}}(t) = \mathrm{e}^{X(t)}\mathrm{e}^{Y(t)}$.

In Figure 2 we represent the difference (in logarithmic scale) between the polar factors computed with the recurrence (36) up to $n = 8$ with *Mathematica* and the exact values $H(t)$ and $Q(t)$ as a function of time, i.e., $\|\exp(X(t)) - H(t)\|$ (solid line) and $\|\exp(Y(t)) - Q(t)\|$ (dashed line) for two different values of the parameter of the problem, $\omega = 2$ (bottom) and $\omega = 3$ (top). Since in this case we know the exact solution (37), $H(t)$ and $Q(t)$ can be computed from its corresponding singular value as follows [3]: if $U_{\mathrm{ex}}(t) = \widehat{X}(t) S(t) \widehat{Y}(t)^T$ is the corresponding singular value decomposition, then $Q(t) = \widehat{X}(t)\widehat{Y}(t)^T$, $H(t) = \widehat{X}(t) S(t) \widehat{X}(t)^T$. Notice that error in the determination of the $\exp Y$ factor is almost one order of magnitude smaller than the corresponding to $\exp X$ for the values analyzed. The approximation is more accurate for $\omega = 2$. This is consistent with the convergence domain guaranteed by Theorem 2: $T \approx 0.30865$ for $\omega = 2$ and $T \approx 0.20577$ for $\omega = 3$.

Since $A(t)$ is periodic with period $\tau = 2\pi/\omega$, Floquet's theorem allows one to express the fundamental matrix as $U(t) = Q(t)\exp(tF)$, where $Q(t+\tau) = Q(t)$ and F is a constant matrix. Notice that the polar factorization considered here differs from Floquet: $X(t)$ is not periodic and the function $b_1(t)$ is not linear in t.

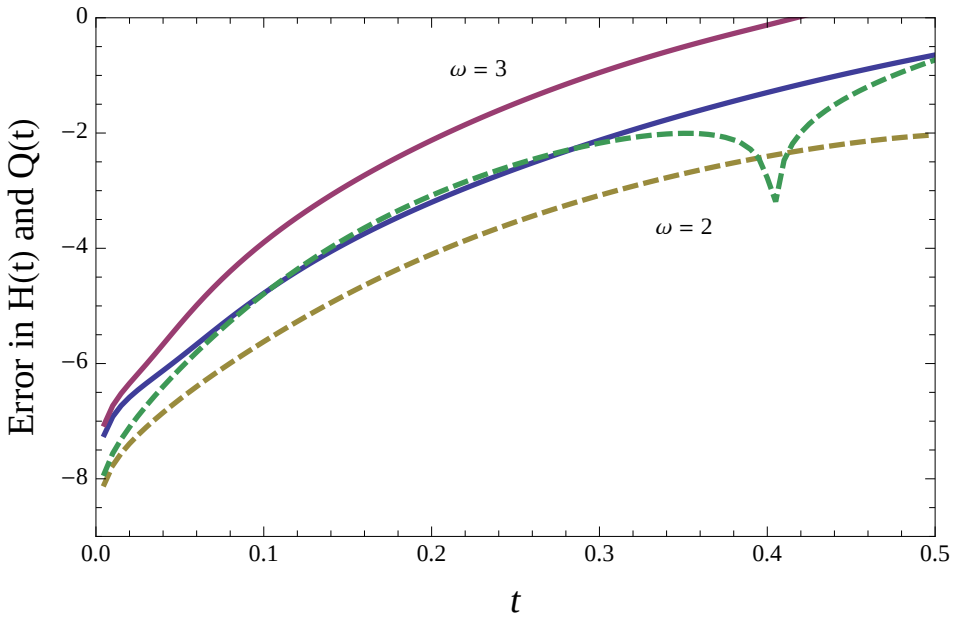

Figure 2: Error with respect to the exact polar factors $H(t)$ (solid line) and $Q(t)$ (dashed line) in logarithmic scale for Example 2 obtained with the exponential polar factorization based on the recurrence (36) with $n = 8$ terms. Two values of the parameter ω are considered.

3.2 Polar decomposition of the matrix exponential

Theorem 2 guarantees that the fundamental matrix of $\dot{U} = A(t)U$ admits a polar decomposition of the form $U(t) = \mathrm{e}^{X(t)}\,\mathrm{e}^{Y(t)}$ for sufficiently small values of t. Obviously, if A is constant, then we can write $\mathrm{e}^{tA} = \mathrm{e}^{X(t)}\,\mathrm{e}^{Y(t)}$ and the computation with the recursion (22)-(23) simplifies considerably. It is possible to implement this recurrence in a symbolic algebra package and obtain analytic expressions for both $X(t)$ and $Y(t)$ up to very high order. We have done so in *Mathematica* up to $n = 15$ and rewritten the terms in the Hall basis of the free Lie algebra generated by the symbols P and K with the algorithm and code developed in [6]. The computation requires modest memory requirements and takes a few minutes in a personal computer. The symmetry properties of both P and K lead to some simplifications in the expression of the terms X_j and Y_j. Thus, all terms $Y_{2n}(t) = 0$, as noticed in [18], whereas half the coefficients in the Hall basis of both X_{2n+1} and Y_{2n+1} vanish. Moreover, the number of vanishing coefficients for X_{2n} for the first values of n, $n \geq 2$, is $1, 4, 14, 49, 165, 576$ out of $3, 9, 30, 99, 335, 1161$ elements. For the sake of illustration, the last coefficient of X_{15} in the Hall basis is $t^{15}\,65981/52306974720$, i.e., the last term in the expression of $X_{15}(t)$ reads

$$t^{15}\,\frac{65981}{52306974720}\,[[[K,[P,K]],[K,[K,[P,K]]]],[[K,[P,[P,K]]],[K,[K,[P,K]]]]],$$

whereas the last coefficient of Y_{15} is zero. Thus, the procedure developed here allows one to express e^{tA} directly as the product of the exponential of two series

$X(t)$ and $Y(t)$ and get some insight into the structure of these series without using the Baker–Campbell–Hausdorff theorem. Moreover, by considering the 2-norm, Theorem 2 guarantees convergence of this factorization for $0 \leq t \leq T$ such that

$$T = \frac{1}{2(\|P\| + \|K\|)} \operatorname{Si}(\pi).$$

4 Concluding remarks

We have presented a procedure to construct a factorization of the fundamental matrix $U(t)$ of the linear system (1) as the product of the exponentials of a symmetric matrix $X(t)$ and a skew-symmetric matrix $Y(t)$. Both matrices $X(t)$ and $Y(t)$ are constructed as series of the form $X(t) = \sum_{i\geq 1} X_i(t)$, $Y(t) = \sum_{i\geq 1} Y_i(t)$, and a recursion has been obtained for determining the expressions of the terms X_i, Y_i. This is done by solving iteratively the differential equations that $X(t)$ and $Y(t)$ obey. In addition, sufficient conditions have been provided for the absolute convergence of the series. This fact guarantees that if $U(t)$ evolves in a Lie group, then the proposed approximation also belongs to the Lie group. In the particular case of the symplectic group, the procedure allows one in a natural way to write the matrix as the product of two exponentials of elements in the corresponding Lie algebra [8].

The approach can be easily adapted when an arbitrary initial condition $U(0) = U_0$ is considered, and also for an arbitrary nonsingular matrix $U(t)$ such that $\dot{U}U^{-1} = A$. If $A(t)$ depends on some parameters, the procedure allows one to construct approximations involving directly these parameters, and thus the analysis of the parameter space can be carried out with only one calculation.

In this work we have only considered the 'left' polar decomposition $U(t) = \mathrm{e}^{X(t)}\,\mathrm{e}^{Y(t)}$. It is clear that a similar approach could also be applied to get a factorization in the reverse order, i.e., the 'right' polar decomposition $U(t) = \mathrm{e}^{\widetilde{Y}(t)}\,\mathrm{e}^{\widetilde{X}(t)}$, with $\widetilde{Y}(t)$ skew-symmetric and $\widetilde{X}(t)$ symmetric. It turns out, however, that in contrast with the case considered here, the differential equations satisfied by $\widetilde{X}(t)$ and $\widetilde{Y}(t)$ involve both series $\widetilde{X}(t)$ and $\widetilde{Y}(t)$, and thus the analysis is more complicated.

Acknowledgements

This work has been partially supported by Ministerio de Ciencia e Innovación (Spain) under project MTM2010-18246-C03-02 (co-financed by FEDER Funds of the European Union).

A Appendix

In this appendix we show that if X is an orthogonally diagonalizable $n \times n$ matrix, then the linear operator ad_X can be represented by an orthogonally diagonalizable $n^2 \times n^2$ matrix.

Let $\{u_1, \ldots, u_n\}$ be an orthonormal basis of (right) eigenvectors of X in $\mathbb{R}^n$, and $\{v_1, \ldots, v_n\}$ an orthonormal basis of left eigenvectors of X. Then, clearly,

$$Xu_i = \lambda_i u_i, \qquad v_j^T X = \lambda_j v_j^T,$$

where $\lambda_1, \lambda_2, \ldots$ denote the eigenvalues of X. Next we form the $n \times n$ matrices $\hat{S}_{ij} = u_i v_j^T$, $i, j = 1, \ldots, n$. Then

$$\begin{aligned} \mathrm{ad}_X \hat{S}_{ij} &= [X, \hat{S}_{ij}] = X\hat{S}_{ij} - \hat{S}_{ij}X = Xu_i v_j^T - u_i v_j^T X \\ &= \lambda_i u_i v_j^T - \lambda_j u_i v_j^T = (\lambda_i - \lambda_j)\hat{S}_{ij} \equiv \mu_{ij}\hat{S}_{ij}. \end{aligned}$$

In other words, $\hat{S}_{ij}$ is an eigenvector of ad_X with eigenvalue $\mu_{ij} = \lambda_i - \lambda_j$.

If we arrange the elements of $\hat{S}_{ij}$ in one column (by appending to the first column all the other columns), then $\hat{S}_{ij}$ can be interpreted as a vector of n^2 components. Let $S_{ij} \in \mathbb{R}^{n^2}$ denote this vector. By the same token, the linear mapping ad_X can be represented by a matrix of dimension $n^2 \times n^2$, say U. This matrix is singular, since for $X \neq 0$, $UX = 0$.

Now we construct a matrix S whose columns are eigenvectors of U arranged as follows:

$$S = (S_{11}\, S_{12}\, \cdots S_{1n}\, S_{21}\, S_{22}\, \cdots S_{2n}\, \cdots S_{n1}\, S_{n2}\, \cdots S_{nn})\,.$$

It turns out that S is orthogonal, since their columns are orthonormal vectors:

$$(S_{ij})^T (S_{kl}) = \left(u_i v_j^T\right)^T \left(u_k v_l^T\right) = v_j u_i^T u_k v_l^T = \delta_{jl}\delta_{ik}.$$

Therefore

$$S^T U S = D = \mathrm{diag}(\mu_{11}, \mu_{12}, \ldots)$$

and U is orthogonally diagonalizable.

References

[1] I. Bihari. A generalization of a lemma of Bellman and its application to uniqueness problems of differential equations. *Acta Math. Acad. Sci. Hungar.* **7** (1956), 81-94.

[2] S. Blanes, F. Casas, J.A. Oteo and J. Ros. The Magnus expansion and some of its applications. *Phys. Rep.* **470** (2009), 151-238.

[3] A. Bunse-Gerstner, R. Byers, V. Mehrmann and N.K. Nichols. Numerical computation of an analytic singular value decomposition of a matrix valued function. *Numer. Math.* (1991), 1-40.

[4] F. Casas, J.A. Oteo and J. Ros. Floquet theory: exponential perturbative treatment. *J. Phys. A: Math. Gen.* **34** (2001), 3379-3388.

[5] F. Casas. Numerical integration methods for the double-bracket flow. *J. Comput. Appl. Math.* **166** (2004), 477-495.

[6] F. Casas and A. Murua. An efficient algorithm for computing the Baker–Campbell–Hausdorff series and some of its applications. *J. Math. Phys.* **50** (2009), 033513.

[7] L. Dieci and T. Eirola. On smooth decompositions of matrices. *SIAM J. Matrix Anal. Appl.* **20** (1999) 800-819.

[8] A.J. Dragt. Lectures on Nonlinear Orbit Dynamics. In: *Physics of High Energy Particle Accelerators.* R.A. Carrigan, F.R. Huson, M Month. American Institute of Physics (1982), 147-313.

[9] T.M. Flett. *Differential Analysis.* Cambridge University Press (1980).

[10] N.H. Getz and J.E. Marsden. Dynamical methods for polar decomposition and inversion of matrices. *Lin. Alg. Appl.* **258** (1997), 311-343.

[11] N.J. Higham. *Functions of Matrices. Theory and Computation.* SIAM (2008).

[12] A. Iserles, H.Z. Munthe-Kaas, S.P. Nørsett and A. Zanna. Lie-group methods. *Acta Numerica* **9** (2000), 215-365.

[13] W. Magnus. On the exponential solution of differential equations for a linear operator. *Commun. Pure Appl. Math.* **VII** (1954), 649-673.

[14] J.E. Marsden and T.J.R. Hughes. *Mathematical Foundations of Elasticity.* Dover (1983).

[15] V. Mehrmann and W. Rath. Numerical methods for the computation of analytic singular value decompositions. *Electr. Trans. Numer. Anal.* **1** (1993), 72-88.

[16] F.W.J. Olver, D.W. Lozier, R.F. Boisvert, and C.W. Clark (Eds). *NIST Handbook of Mathematical Functions.* Cambridge University Press (2010).

[17] W. Rossmann. *Lie Groups. An Introduction through Linear Groups.* Oxford University Press (2002).

[18] A. Zanna. Recurrence relations and convergence theory of the generalized polar decomposition on Lie groups. *Math. Comp.* **73** (2004), 761–776.