Letter to the Editor

Computing multiple integrals involving matrix exponentials

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Abstract

In this paper, a generalization of a formula proposed by Van Loan [Computing integrals involving the matrix exponential, IEEE Trans. Automat. Control 23 (1978) 395–404] for the computation of multiple integrals of exponential matrices is introduced. In this way, the numerical evaluation of such integrals is reduced to the use of a conventional algorithm to compute matrix exponentials. The formula is applied for evaluating some kinds of integrals that frequently emerge in a number of classical mathematical subjects in the framework of differential equations, numerical methods and control engineering applications.

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1. Introduction

This note deals with the computation of multiple integrals involving matrix exponentials, which frequently emerge in a number of classical mathematical subjects in the framework of differential equations, numerical methods, control engineering applications, etc. Specifically, integral of the form

$$\int_{0}^{t} \int_{0}^{s_1} \cdots \int_{0}^{s_{k-2}} e^{A_{11}(t-s_1)} A_{12} e^{A_{22}(s_1-s_2)} A_{23} \cdots e^{A_{kk}s_{k-1}} ds_{k-1} \cdots ds_1$$

will be considered, where $A_{ik}$ are $d_i \times d_k$ constant matrices, $t > 0$ and $k = 1, 2, \ldots$

At a glance, the analytical calculation of these integrals seems to be difficult. Nevertheless, in [19] a simple explicit formula in terms of certain exponential matrix was given. In that way, a number of distinctive integrals such as

$$\int_{0}^{t} e^{A_{11}s} A_{12} e^{A_{22}s} ds$$

and

$$\int_{0}^{t} \int_{0}^{s_1} e^{A_{11}s_1} A_{12} e^{A_{22}(s_1-s_2)} ds_2 ds_1$$

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can easily be computed as particular cases of the mentioned formula [19]. However, such formula is restricted to integrals with multiplicity \( k \leq 4 \), which obviously limits its usefulness range.

The proposal of this note is generalizing the formula introduced in [19] for any positive value of \( k \). This has been strongly motivated for the need of computing the integrals

\[
\int_0^t e^{F(t-s)}G(s)\,ds \quad (2)
\]

and

\[
\int_0^t e^{F(t-s)}G(s)G^T(s)e^{F^T(t-s)}\,ds \quad (3)
\]

where \( F \) is an \( r \times r \) constant matrix and \( G : \mathbb{R} \rightarrow \mathbb{R}^{r \times d} \) a smooth function. Integrals of the type (2) appear as a term in the analytical solution of linear time-depending control system [16], linear ordinary and delay differential equations [6]. Integrals like (3) are associated to the notions of controllability and observability Grammians of linear control systems [16]. They also appear as the covariance matrix of the solution of linear stochastic differential equations with time-depending additive noise [1] and, in the context of filtering theory, as the system noise covariance matrix of the extended Kalman filter for continuous-discrete state-space models with additive noise [10]. In addition, they arise in a number of numerical schemes for the integration of ordinary differential equations that are based on polynomial approximations for the remainder term of the variation of constant formula [9,8,7,3,4].

The paper has three sections. In the first one, the generalized formula is derived, whereas in the second one the formula is applied to the computation of the integrals (2) and (3). Last section deals with some computational aspects for implementing such a formula.

2. Main result

A simple way to compute single, double and triple integrals of the form is provided [19, Theorem 1]:

\[
B_{12}(t) = \int_0^t e^{A_{11}(t-u)}A_{12}e^{A_{22}u}\,du,
\]

\[
B_{13}(t) = \int_0^t \int_0^u e^{A_{11}(t-u)}A_{12}e^{A_{22}(u-r)}A_{23}e^{A_{33}r}\,dr\,du
\]

and

\[
B_{14}(t) = \int_0^t \int_0^u \int_0^r e^{A_{11}(t-u)}A_{12}e^{A_{22}(u-r)}A_{23}e^{A_{33}(r-w)}A_{34}e^{A_{44}w}\,dw\,dr\,du,
\]

in terms of a single exponential matrix, but not integrals of the form (1) with \( k \geq 5 \). Next theorem overcomes this restriction.

**Theorem 1.** Let \( d_1, d_2, \ldots, d_n \) be positive integers. If the \( n \times n \) block triangular matrix \( A = [A_{ij}]_{i,j=1:n} \) is defined by

\[
A = \begin{pmatrix}
A_{11} & A_{12} & \cdots & A_{1n} \\
0 & A_{22} & \cdots & A_{2n} \\
0 & 0 & \ddots & \vdots \\
0 & 0 & \cdots & A_{nn}
\end{pmatrix},
\]

where \( (A_{ij})_{l,j=1,n} \) are \( d_l \times d_j \) matrices such that \( d_l = d_j \) for \( l = j \), then for \( t \geq 0 \)

\[
e^{At} = \begin{pmatrix}
B_{11}(t) & B_{12}(t) & \cdots & B_{1n}(t) \\
0 & B_{22}(t) & \cdots & B_{2n}(t) \\
0 & 0 & \ddots & \vdots \\
0 & 0 & \cdots & B_{nn}(t)
\end{pmatrix},
\]
Then, by applying the identities (4–5) with triangular matrix $A_{1n}$ [19]. Suppose that they also hold for $n = m + 1$ block triangular matrix $A = \{(A_{ij})\}_{l,j=1:m+1}$.

Let us rewrite the matrix $A$ as the $2 \times 2$ block triangular matrix $\tilde{A} = [\tilde{A}_{ij}]_{i,j=1:2}$ defined by

$$\tilde{A} = \left( \begin{array}{cc} [(A_{ij})]_{l,j=1:m} & [(A_{l,m+1})]_{l=1:m} \\ 0 & A_{m+1,m+1} \end{array} \right),$$

and let $B(t) = [(B_{ij}(t))]_{l,j=1:m+1}$ be the $(m + 1) \times (m + 1)$ block triangular matrix given by

$$B(t) = e^{At} = e^{\tilde{A}t}.$$

Then, by applying the identities (4–5) with $n = 2$ to the matrix $\tilde{A}$ we obtain

$$[(B_{l,j}(t))]_{l,j=1:m} = e^{\tilde{A}_{11}t},$$

(6)

$$B_{m+1,m+1}(t) = e^{A_{m+1,m+1}t},$$

(7)

$$[(B_{l,m+1}(t))]_{l=1:m} = \int_0^t e^{\tilde{A}_{11}(t-s_1)} \tilde{A}_{12} e^{A_{m+1,m+1}s_1} \, ds_1.$$ 

(8)

Since $\tilde{A}_{11} = [(A_{ij})]_{l,j=1:m}$ then (6) and (7) imply that

$$B_{ll}(t) = e^{\tilde{A}_{11}t}, \quad l = 1, \ldots, m + 1,$$

(9)

$$B_{lj}(t) = \int_0^t M^{(l,j)}(t, s_1) \, ds_1 + \sum_{k=1}^{j-l-1} \int_0^t \int_0^{s_1} \ldots \int_0^{s_k} \sum_{l<i_1<\ldots<i_k<j} M^{(l,i_1,\ldots,i_k,j)}(t, s_1, \ldots, s_{k+1}) \, ds_{k+1} \ldots ds_1,$$

$$l = 1, \ldots, m - 1, \quad j = l + 1, \ldots, m.$$

(10)

On the other hand, since $e^{\tilde{A}_{11}(t-s_1)} = [(B_{l,j}(t-s_1))]_{l,j=1:m}$ and $\tilde{A}_{12} = [(A_{l,m+1})]_{l=1:m}$, the identity (8) implies the following expression for each block $B_{l,m+1}(t)$, $l = 1, \ldots, m$:

$$B_{l,m+1}(t) = \sum_{j=l}^{m} \int_0^t B_{l,j}(t-s_1) A_{j,m+1} e^{A_{m+1,m+1}s_1} \, ds_1,$$

$$l = 1, \ldots, m.$$
which by (9) and (10) gives

\[ B_{l,m+1}(t) = \int_0^t M^{(l,m+1)}(t,s_1)ds_1 + \sum_{j=l+1}^m \int_0^t \int_0^{t-s_1} M^{(l,j,m+1)}(t,s_1+s_2,s_1)ds_2ds_1 \]

\[ + \sum_{j=l+2}^m \sum_{k=1}^{j-1} \int_0^t \int_0^{t-s_1} \int_0^{s_2} \cdots \int_0^{s_{k+1}} \sum_{l<i_1<\cdots<i_k<j} \times M^{(l,i_1,\ldots,i_k,j,m+1)}(t,s_1+s_2,\ldots,s_1+s_k+2,s_1)ds_{k+2} \cdots ds_1. \] 

(11)

For each \( k = 0, 1, \ldots \) the change of variables \( u_1 = s_1 + s_2, u_2 = s_1 + s_3, \ldots, u_{k+1} = s_1 + s_k+2, u_k+2 = s_1 \) in each of the multiple integrals that appear in (11) yields

\[ B_{l,m+1}(t) = \int_0^t M^{(l,m+1)}(t,u_1)du_1 + \sum_{k=1}^{m-l} \int_0^t \int_0^{u_1} \cdots \int_0^{u_k} \sum_{l<i_1<\cdots<i_k<j} \times M^{(l,i_1,\ldots,i_k,j)}(t,u_1,\ldots,u_{k+1})du_{k+1} \cdots du_1, \]

which when combined with (9) and (10) shows that the identities (4) and (5) hold for \( n = m+1 \), and the proof concludes.

Now we are able to evaluate the integrals \( B_{12}(t), B_{13}(t), B_{14}(t) \) and the integrals

\[ B_{1k}(t) = \int_0^t \int_0^{s_1} \cdots \int_0^{s_{k-2}} e^{A_{11}(t-s_1)}A_{12}e^{A_{22}(s_1-s_2)}A_{23} \cdots e^{A_{k-2,k-1}}ds_{k-1} \cdots ds_1 \]

for \( k \geq 5 \) as well, all of them computed by just a single exponential matrix. This is, by applying the theorem above follows that the blocks \( B_{12}(t), B_{13}(t), \ldots, B_{1k}(t) \) are easily obtained from \( e^{tA} \), with

\[
A = \begin{bmatrix}
A_{11} & A_{12} & 0 & 0 & 0 \\
0 & A_{22} & A_{23} & 0 & 0 \\
0 & 0 & A_{33} & \ddots & 0 \\
0 & 0 & 0 & \ddots & A_{k-1,k} \\
0 & 0 & 0 & 0 & A_{kk}
\end{bmatrix}.
\]

3. Application of the generalized formula

This section is devoted to compute integrals of the form (2) and (3) by means of the theorem stated in the previous section.

Firstly, suppose that \( G(s) \) is a \( r \times d \) polynomial matrix function of degree \( p \). That is,

\[ G(s) = \sum_{i=0}^p G_is^i, \]

or equivalently,

\[ G(s) = G_0 + \int_0^s G_1 du + \sum_{i=2}^p \int_0^s \int_0^{u_1} \cdots \int_0^{u_{i-1}} (i!G_i) du_i du_{i-1} \cdots du_1. \]

Then, by Theorem 1 it is easy to check that

\[ \int_0^t e^{F(t-s)}G(s)ds = B_{1,p+2}(t), \]

(12)
where

\[
B(t) = [(B_{lj}(t))]_{l,j=1:p+2} = e^{A t},
\]

and the block triangular matrix \( A = [(A_{lj})]_{l,j=1:p+2} \) is given by

\[
A = \begin{pmatrix}
F & p!G_p & (p-1)!G_{p-1} & \cdots & G_1 & G_0 \\
0 & 0 & I_d & \cdots & 0 & 0 \\
0 & 0 & 0 & \ddots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \ddots & I_d & 0 \\
0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & \cdots & 0 & 0 & 0 \\
\end{pmatrix}.
\]

In a similar way, it is obtained that

\[
\int_0^t e^{F(t-s)}G(s)G^T(s)e^{F^T(t-s)}ds = B_{1,2p+2}(t)B^T_{11}(t),
\]

where \( B(t) = e^{A t} \) and the matrix \( A \) in this case is given by

\[
A = \begin{pmatrix}
F & H_{2p} & H_{2p-1} & \cdots & H_1 & H_0 \\
0 & -F^T & I_d & \cdots & 0 & 0 \\
0 & 0 & -F^T & \ddots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \ddots & I_d & 0 \\
0 & 0 & \cdots & 0 & -F^T & I_d \\
0 & 0 & \cdots & 0 & 0 & -F^T \\
\end{pmatrix},
\]

with

\[
H_i = \sum_{l+j=i} (l!j!)G_lG_j^T, \quad i = 0, \ldots, 2p.
\]

In case that \( G : \mathbb{R} \to \mathbb{R}^{r \times d} \) be a function with \( p \) continuous derivatives it can be approximated by means of its truncated Taylor expansion. That is,

\[
G(s) \approx \sum_{i=0}^p \frac{G_i}{i!}s^i,
\]

where the coefficient \( G_i \) is the \( i \)th derivative of \( G \) at \( s = 0 \). In this case, the above procedure to compute the integrals (12) and (13) for polynomial \( G \) will give a convenient way to approximate integrals like (2) and (3). In [15], such approximation for (3) was considered early and an upper bound for it was also given. However, no closed formula in terms of a simple exponential matrix was given for this approximation. Such is the main improvement of this paper in comparison with [15]. At this point it is worth remark that such approximations have been successfully applied to the computation of the predictions provided by the Local Linearization filters for non-linear continuous-discrete state-space models [12,13], as well as in [2,14] for computing other types of multiple integrals involving matrix exponentials. This evidences the practical usefulness of the result achieved in this paper.

4. Computational aspects

It is obvious that the main computational task on the practical application of Theorem 1 is the use of an appropriate numerical algorithm to compute matrix exponentials. For instance, those based on rational Padé approximations, the Schur decomposition or Krylov subspace methods (see [18,17] for excellent reviews on effective methods to compute matrix exponential). The choice of one of them will mainly depend on the size and structure of the matrix \( A \) in Theorem 1. In many cases, it is enough to use the algorithms developed in [5], which take advantage of the special structure of...
For a high dimensional matrix \( A \), Krylov subspace methods are strongly recommended. Nowadays, a number of professional mathematical softwares such as MATLAB 7.0 provide efficient and precise codes for computing matrix exponentials. Therefore, the numerical evaluation of the integrals under consideration can be carried out in an effective, accurate and simple way. In fact, some numerical experiments have been performed for an application of the classical result of Van Loan (i.e. integrals of type (1) for \( k \leq 4 \)). Specifically, in [11] were compared different numerical algorithms for the evaluation of some integrals of type (1) with \( k \leq 4 \). Those results could be easily extrapolated to our general setting since such a comparison was mainly focused on the dimension of the block triangular matrix \( A \).

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References