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Error analysis for exponential splitting based on the Generalized Polar Decomposition I: Local and global bounds

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Abstract

In this paper we consider splitting methods for the approximation of the exponential of a matrix from a Lie algebra to a Lie group. Particular attention is paid to splitting that arise from Generalized Polar Decompositions. We derive both local and global bounds for various methods. The theoretical results are finally discussed in several numerical experiments.

1 Introduction

Much research has been focused during recent years on the computation (either exact of approximated) of the matrix exponential, defined as

$$\mathrm{e}^{tZ} = \sum_{i=0}^{\infty} \frac{1}{i!} t^i Z^i,$$

with Z a real or complex matrix, from a Lie algebra to a Lie group [1, 2, 10, 18]. This property is of vital importance when solving ordinary differential equations (ODEs) on Lie groups with Lie-group methods that require exponentials [7].

Many of the new schemes are based on a splitting of the matrix Z into terms in $\mathfrak{g}$ that are easy to exponentiate exactly. Often, commutator terms are introduced to obtain higher order approximations.

The scope of this study is to analyze the error (local and global) of some of these splitting schemes for the approximation of the matrix exponential. The order conditions that we consider are based on a special *inverse BCH* formula derived in the context of Generalized Polar Decompositions (GPDs) [11, 18], having the property that if $Z = P + K$, where $\sigma(P) = -P$ and $\sigma(K) = K$, with $\sigma : \mathfrak{g} \to \mathfrak{g}$ a Lie-algebra involutive automorphism, then $\exp(tZ) = \exp(X(t)) \exp(Y(t))$ where the functions $X(t)$ and $Y(t)$ too share the feature that $\sigma(X(t)) = -X(t)$ and $\sigma(Y(t)) = Y(t)$. A typical example is the case when Z is split into its symmetric and skew-symmetric components. Then, $\exp(X(t))$ and $\exp(Y(t))$ are the factors of the polar decomposition of $\exp(tZ)$. Choosing different type of automorphisms it is possible to analyze many different splitting methods.

A local error analysis is not difficult to derive: having a BCH formula [14] at hand, the local error is essentially the first non-matching term in the expansion. However, a local error analysis might not always be accurate. It is typically observed that the error in exponential approximations behaves at first like the local truncation error, then it might have a transition phase, and then grow or decay exponentially. Global error estimates usually give much better estimates, especially in the transition and exponential phase [12, 9, 8].

This work is divided in two parts. In the first part (the present article), we will analyze local and global error for splitting of order 2,3 and 4, analysing also the splitting in m terms. The theory we present is rather general and is based on expansions with integral reminders (these reminders are Adjoint mapping of commutator terms). The global bounds are then tested against random matrices.

In part two [17], our discussion is specialized to the case of splitting in bordered matrices as proposed in [18]. It is shown that these bounds can be computed while computing the splitting of Z, hence they give a very good picture of the error of the approximations. Application to the numerical solution of ODEs on Lie groups is also described at length. Other issues related to exponential approximations are also discussed here, among them, bounds for splitting in stiff and non-stiff parts and operator bounds in the presence of unbounded operators.

2 Notation and background theory

Although we wish to keep Lie-group and Lie-algebra notation and knowledge to a minimum level, we expect the reader to be familiar with the basic concepts of a Lie group, denoted as G, and its Lie algebra, denoted by $\mathfrak{g}$. These fundamental notions can be found in [7].

It is useful to recall some basic operators. Assume that $A, B \in \mathfrak{g}$.

- The Ad operator: If $a \in G$, then Ad_a is a linear map from $\mathfrak{g} \to \mathfrak{g}$. It acts by conjugation, i.e. given $B \in \mathfrak{g}$, then $\mathrm{Ad}_a B = aBa^{-1} \in \mathfrak{g}$.
- The ad operator: The ad-operator is the derivative of Ad and reduces to the classical commutator: $\mathrm{ad}_A B = [A, B]$, with $A, B \in \mathfrak{g}$. Moreover,
$$\mathrm{Ad}_{\exp(A)} B = \exp(\mathrm{ad}_A) B = \sum_{i=0}^{\infty} \frac{1}{i!} \mathrm{ad}_A^i B.$$
- The dexp operator: It is the "right-trivialization" of the derivative of the exponential map, which means that
$$\frac{\mathrm{d}}{\mathrm{d}t} \exp(C(t)) = \mathrm{dexp}_C(C') \exp(C),$$
where $C : t \mapsto C(t) \in \mathfrak{g}$. The map $\mathrm{dexp}_A(\cdot) : \mathfrak{g} \to \mathfrak{g}$ is linear and, moreover,
$$\mathrm{dexp}_A(B) = \sum_{i=0}^{\infty} \frac{1}{(i+1)!} \mathrm{ad}_A^{i+1}(B) = \frac{\mathrm{e}^u - 1}{u}\Big|_{u=\mathrm{ad}_A}(B).$$

These operator and their relation ease significantly our notation and computations.

We refer the reader to [7] and references therein for a further reading.

3 Series expansions

Assume that
$$Z = P + K.$$
It is useful to recall the series expansions of the functions $X(t)$ and $Y(t)$ in the formulas
$$\mathrm{e}^{tZ} = \mathrm{e}^{X(t)} \mathrm{e}^{Y(t)}, \tag{3.1}$$
if we consider a polar-type splitting, or
$$\mathrm{e}^{tZ} = \mathrm{e}^{X(t)} \mathrm{e}^{Y(t)} \mathrm{e}^{X(t)} \tag{3.2}$$
for a symmetric polar-type splitting, as discussed in [18]. For (3.1), the first terms in the expansions of $X(t)$ and $Y(t)$ are
$$\begin{aligned} X &= Pt - \tfrac{1}{2}[P,K]t^2 - \tfrac{1}{6}[K,[P,K]]t^3 \\ &\quad + \Big(\tfrac{1}{24}[P,[P,[P,K]]] - \tfrac{1}{24}[K,[K,[P,K]]]\Big)t^4 \end{aligned} \tag{3.3}$$

$$+\left(\tfrac{7}{360}[K,[P,[P,[P,K]]]]-\tfrac{1}{120}[K,[K,[K,[P,K]]]]-\tfrac{1}{180}[[P,K],[P,[P,K]]]\right)t^5$$
$$+\mathcal{O}\left(t^6\right),$$

$$Y = Kt-\tfrac{1}{12}[P,[P,K]]t^3+\left(\tfrac{1}{120}[P,[P,[P,[P,K]]]]\right.$$
$$\left.+\tfrac{1}{720}[K,[K,[P,[P,K]]]]-\tfrac{1}{240}[[P,K],[K,[P,K]]]\right)t^5+\mathcal{O}\left(t^7\right). \tag{3.4}$$

For the symmetric polar-type splitting (3.2), one has

$$X(t) = \tfrac{1}{2}Pt+\tfrac{1}{24}[K,[P,K]]t^3-(\tfrac{1}{1440}[K,[P,[P,[P,K]]$$
$$+\tfrac{1}{240}[K,[K,[K,[P,K]]]]+\tfrac{1}{360}[[P,K],[P,[P,K]]])t^5+\cdots \tag{3.5}$$

$$Y(t) = Kt+\tfrac{1}{24}[P,[P,K]]t^3+(\tfrac{1}{1920}[P,[P,[P,[P,K]]]]$$
$$-\tfrac{13}{1440}[K,[K,[P,[P,K]]]]-\tfrac{1}{240}[[P,K],[K,[P,K]]])t^5+\cdots \tag{3.6}$$

and both $X(t)$ and $Y(t)$ expand in odd powers of t only.

Note that (3.3)–(3.6) can be thought as inverse BCH formulas for (3.1) and (3.2). However, they possess the following important property: assume that $Z\in\mathfrak{g}$ and that $\sigma:\mathfrak{g}\to\mathfrak{g}$ is an involutive automorphism (i.e. $\sigma\circ\sigma=\mathrm{id}$, the identity function, $\sigma\neq\mathrm{id}$, and $\sigma([A,B])=[\sigma(A),\sigma(B)]$). Assume, moreover, that $\sigma(P)=-P$ and $\sigma(K)=K$. Then, also the functions $X(t)$ and $Y(t)$ have the property that $\sigma(X(t))=-X(t)$ and $\sigma(Y(t))=Y(t)$.

4 Local truncation errors

We commence our local truncation error analysis recalling the simplest case of a first order splitting,

$$Z=P_1+P_2+\cdots+P_{m-1}+K_{m-1},$$

in tandem with the approximation

$$\mathrm{e}^{tZ}\approx\mathrm{e}^{tP_1}\mathrm{e}^{tP_2}\cdots\mathrm{e}^{tP_{m-1}}\mathrm{e}^{tK_{m-1}},$$

where m is the number of split terms. Set

$$L_{1,m}(t) = \mathrm{e}^{tZ}-\mathrm{e}^{tP_1}\cdots\mathrm{e}^{tP_{m-1}}\mathrm{e}^{tK_{m-1}}+\mathcal{O}\left(t^3\right), \tag{4.1}$$
$$E_{1,m}(t) = \mathrm{e}^{tZ}-\mathrm{e}^{tP_1}\cdots\mathrm{e}^{tP_{m-1}}\mathrm{e}^{tK_{m-1}}, \tag{4.2}$$

the local and global error of the first order splitting respectively. In what follows we assume that the exponential of each split term is computed exactly.

One has

$$\begin{aligned}E_{1,m}(t) &= \mathrm{e}^{tZ}-\mathrm{e}^{tP_1}\mathrm{e}^{tP_2+\cdots tP_{m-1}+tK_{m-1}}\\ &\quad+\mathrm{e}^{tP_1}\mathrm{e}^{tP_2+\cdots tP_{m-1}+tK_{m-1}}-\mathrm{e}^{tP_1}\mathrm{e}^{tP_2}\mathrm{e}^{tP_3+\cdots tP_{m-1}+tK_{m-1}}\\ &\quad+\cdots+\mathrm{e}^{tP_1}\cdots\mathrm{e}^{tP_{m-2}}\mathrm{e}^{tP_{m-1}+tK_{m-1}}-\mathrm{e}^{tP_1}\cdots\mathrm{e}^{tP_{m-1}}\mathrm{e}^{tK_{m-1}},\end{aligned}$$

therefore, passing to the norm and disregarding higher error terms and making repetitively use of the formula

$$\mathrm{e}^{tZ}-\mathrm{e}^{tP}\mathrm{e}^{tK}=\frac{1}{2}t^2[P,K]+\mathcal{O}\left(t^3\right),\qquad P+K=Z,$$

we derive the bound

$$\|L_{1,m}(t)\| \quad \le \quad \frac{1}{2}t^2\Big(\|[P_1, P_2+\cdots+K_{m-1}]\| + \|[P_2, P_3+\cdots+K_{m-1}]\| + \cdots + \|[P_{m-1}, K_{m-1}]\|\Big). \tag{4.3}$$

4.1 Local error for the polar-type order-2 splitting

We consider next the case when the expansions (3.3)-(3.4) are truncated to order two (notice that the Y term does not require any order correction). From (3.3)-(3.4) we deduce that

$$\mathrm{e}^{tZ} - \mathrm{e}^{tP-\frac{1}{2}t^2[P,K]}\mathrm{e}^{tK} = \frac{1}{6}t^3[K,[P,K]] + \frac{1}{12}t^3[P,[P,K]] + \mathcal{O}\big(t^4\big)\,, \quad P+K=Z. \tag{4.4}$$

Denote now $Z_0 = Z$. We set $K_1 = Z_0 - P_1$, $Z_1 = K_1$ and in general $K_i = Z_{i-1} - P_i, Z_i = K_i$, for $i = 1, 2, \ldots, m-1$. Observe that $P_1 + P_2 + \cdots + P_{m-1} + K_{m-1} = Z$. Set now $L_{2,m}(t)$ the leading error term of the splitting,

$$L_{2,m}(t) = \mathrm{e}^{tZ} - \mathrm{e}^{tP_1-\frac{1}{2}t^2[P_1,K_1]}\mathrm{e}^{tP_2-\frac{1}{2}t^2[P_2,K_2]}\cdots\mathrm{e}^{tP_{m-1}-\frac{1}{2}t^2[P_{m-1},K_{m-1}]}\mathrm{e}^{tK_{m-1}} + \mathcal{O}\big(t^4\big)\,. \tag{4.5}$$

and

$$E_{2,m}(t) = \mathrm{e}^{tZ} - \mathrm{e}^{tP_1-\frac{1}{2}t^2[P_1,K_1]}\mathrm{e}^{tP_2-\frac{1}{2}t^2[P_2,K_2]}\cdots\mathrm{e}^{tP_{m-1}-\frac{1}{2}t^2[P_{m-1},K_{m-1}]}\mathrm{e}^{tK_{m-1}} \tag{4.6}$$

the global error.

Using (4.4) and proceeding as in the case of the order-1 splitting above, we find

$$\|L_{2,m}(t)\| \quad \le \quad t^3\sum_{i=1}^{m-1}\Big(\frac{1}{6}\|[K_i,[P_i,K_i]]\| + \frac{1}{12}\|[P_i,[P_i,K_i]]\|\Big), \tag{4.7}$$

where $K_0 = Z_0 = Z$ and $P_0 = O$.

4.2 Local error for the polar-type order-3 splitting

Let the expansions (3.3)-(3.4) be truncated to order three. From (3.3)-(3.4) we have that

$$\mathrm{e}^{tZ} - \mathrm{e}^{tP-\frac{1}{2}t^2[P,K]-\frac{1}{6}t^3[K,[P,K]]}\mathrm{e}^{tK-\frac{1}{12}t^3[P,[P,K]]} = -\frac{t^4}{24}([P,[P,[P,K]]] - [K,[K,[P,K]]) + \mathcal{O}\big(t^5\big)\,, \tag{4.8}$$

with $P + K = Z$.

It is important to stress that this is the first case when also the Y-component requires order corrections. Now, let us recall how the splitting is computed: first of all, we compute

$$Z = P_1 + K_1,$$

projecting Z into the $\mathfrak{p}_1$ and $\mathfrak{k}_1$ subspaces. Then the order corrections are computed and we may set

$$Z_1 = K_1 - \frac{1}{12}t^2[P_1,[P_1,K_1]].$$

Similarly, Z_1 is projected into $\mathfrak{p}_2$ and $\mathfrak{k}_2$ to obtain $Z_1 = P_2 + K_2$, and so on, so that in general

$$\begin{array}{rcl} Z_i &=& K_i - \frac{1}{12}t^2[P_i,[P_i,K_i]] \\ Z_i &=& P_{i+1} + K_{i+1} \end{array} \qquad i = 1, \ldots, m-2.$$

Note that now $P_1 + \cdots P_{m-1} + K_{m-1}$ does not equal Z, but it is true that

$$P_1 + \cdots + P_{m-1} + K_{m-1} = Z + \mathcal{O}\big(t^2\big)$$

instead.

We consider

$$\begin{aligned} L_{3,m}(t) &= \mathrm{e}^{tZ} - \mathrm{e}^{tP_1 - \frac{1}{2}t^2[P_1,K_1] - \frac{1}{6}t^3[K_1,[P_1,K_1]]} \ldots \mathrm{e}^{tP_{m-1} - \frac{1}{2}t^2[P_{m-1},K_{m-1}] - \frac{1}{6}t^3[K_{m-1},[P_{m-1},K_{m-1}]]} \\ &\quad \times \mathrm{e}^{tK_{m-1} - \frac{1}{12}t^3[P_{m-1},[P_{m-1},K_{m-1}]]} + \mathcal{O}\big(t^5\big)\,. \end{aligned} \tag{4.9}$$

the local error, and

$$\begin{aligned} E_{3,m}(t) &= \mathrm{e}^{tZ} - \mathrm{e}^{tP_1 - \frac{1}{2}t^2[P_1,K_1] - \frac{1}{6}t^3[K_1,[P_1,K_1]]} \ldots \mathrm{e}^{tP_{m-1} - \frac{1}{2}t^2[P_{m-1},K_{m-1}] - \frac{1}{6}t^3[K_{m-1},[P_{m-1},K_{m-1}]]} \\ &\quad \times \mathrm{e}^{tK_{m-1} - \frac{1}{12}t^3[P_{m-1},[P_{m-1},K_{m-1}]]}. \end{aligned} \tag{4.10}$$

the global error of the splitting. Subtracting and adding terms as above, we obtain

$$\begin{aligned} E_{3,m}(t) &= \mathrm{e}^{tZ} - \mathrm{e}^{tP_1 - \frac{1}{2}t^2[P_1,K_1] - \frac{1}{6}t^3[K_1,[P_1,K_1]]}\mathrm{e}^{tZ_1} \\ &\quad + \mathrm{e}^{tP_1 - \frac{1}{2}t^2[P_1,K_1] - \frac{1}{6}t^3[K_1,[P_1,K_1]]}\mathrm{e}^{tZ_1} \\ &\quad - \mathrm{e}^{tP_1 - \frac{1}{2}t^2[P_1,K_1] - \frac{1}{6}t^3[K_1,[P_1,K_1]]}\mathrm{e}^{tP_2 - \frac{1}{2}t^2[P_2,K_2] - \frac{1}{6}t^3[K_2,[P_2,K_2]]}\mathrm{e}^{tZ_2} \\ &\quad + \mathrm{e}^{tP_1 - \frac{1}{2}t^2[P_1,K_1] - \frac{1}{6}t^3[K_1,[P_1,K_1]]}\mathrm{e}^{tP_2 - \frac{1}{2}t^2[P_2,K_2] - \frac{1}{6}t^3[K_2,[P_2,K_2]]}\mathrm{e}^{tZ_2} \\ &\quad + \cdots \\ &\quad + \mathrm{e}^{tP_1 - \frac{1}{2}t^2[P_1,K_1] - \frac{1}{6}t^3[K_1,[P_1,K_1]]} \ldots \mathrm{e}^{tP_{m-2} - \frac{1}{2}t^2[P_{m-2},K_{m-2}] - \frac{1}{6}t^3[K_{m-2},[P_{m-2},K_{m-2}]]}\mathrm{e}^{tZ_{m-2}} \\ &\quad - \mathrm{e}^{tP_1 - \frac{1}{2}t^2[P_1,K_1] - \frac{1}{6}t^3[K_1,[P_1,K_1]]} \times \cdots \\ &\quad \times \mathrm{e}^{tP_{m-1} - \frac{1}{2}t^2[P_{m-1},K_{m-1}] - \frac{1}{6}t^3[K_{m-1},[P_{m-1},K_{m-1}]]}\mathrm{e}^{tK_{m-1} - \frac{1}{12}t^3[P_{m-1},[P_{m-1},K_{m-1}]]}. \end{aligned}$$

Passing to the norm and making use of (4.8), we obtain the bound for the principal error term

$$\|L_{3,m}(t)\| \le \frac{t^4}{24}\sum_{i=1}^{m-1}\Big(\|[P_i,[P_i,[P_i,K_i]]]\| + \|[K_i,[K_i,[P_i,K_i]]]\|\Big) \tag{4.11}$$

where, as above, $K_0 = Z_0$ and $P_0 = O$.

4.3 Local error for the symmetric order-2 splitting

We consider next symmetric splitting based on the expansions (3.5)-(3.6). The order-2 truncation of (3.5)-(3.6) yields the familiar Strang splitting, with leading error term

$$\mathrm{e}^{tZ} - \mathrm{e}^{\frac{1}{2}tP}\mathrm{e}^{tK}\mathrm{e}^{\frac{1}{2}P} = \frac{t^3}{12}(\frac{1}{2}[P,[P,K]] + [K,[K,P]]) + \mathcal{O}\big(t^5\big)\,. \tag{4.12}$$

Set

$$L_{2,m,\mathrm{sym}}(t) = \mathrm{e}^{tZ} - \mathrm{e}^{\frac{1}{2}tP_1} \cdots \mathrm{e}^{\frac{1}{2}tP_{m-1}}\mathrm{e}^{tK_{m-1}}\mathrm{e}^{\frac{1}{2}tP_{m-1}} \cdots \mathrm{e}^{\frac{1}{2}tP_1} + \mathcal{O}\big(t^5\big)\,, \tag{4.13}$$

$$E_{2,\mathrm{sym}}(t) = \mathrm{e}^{tZ} - \mathrm{e}^{\frac{1}{2}tP_1} \cdots \mathrm{e}^{\frac{1}{2}tP_{m-1}}\mathrm{e}^{tK_{m-1}}\mathrm{e}^{\frac{1}{2}tP_{m-1}} \cdots \mathrm{e}^{\frac{1}{2}tP_1} \tag{4.14}$$

the local and global error terms respectively. Proceeding in the usual fashion,

$$\begin{aligned} E_{2,m,\mathrm{sym}}(t) &= \mathrm{e}^{tZ} - \mathrm{e}^{\frac{1}{2}tP_1}\mathrm{e}^{K_1}\mathrm{e}^{\frac{1}{2}tP_1} \\ &\quad + \mathrm{e}^{\frac{1}{2}tP_1}\mathrm{e}^{K_1}\mathrm{e}^{\frac{1}{2}tP_1} + \cdots \\ &\quad + \mathrm{e}^{\frac{1}{2}tP_1} \cdots \mathrm{e}^{\frac{1}{2}tP_{m-2}}\mathrm{e}^{tK_{m-2}}\mathrm{e}^{\frac{1}{2}tP_{m-2}} \cdots \mathrm{e}^{\frac{1}{2}tP_1} \\ &\quad - \mathrm{e}^{\frac{1}{2}tP_1} \cdots \mathrm{e}^{\frac{1}{2}tP_{m-1}}\mathrm{e}^{tK_{m-1}}\mathrm{e}^{\frac{1}{2}tP_{m-1}} \cdots \mathrm{e}^{\frac{1}{2}tP_1} \end{aligned}$$

and passing to the norm, in tandem with (4.12), we obtain

$$\|L_{2,m,\mathrm{sym}}(t)\| \leq \frac{t^3}{12}\sum_{i=1}^{m-1}\Big(\frac{1}{2}\|[P_i,[P_i,K_i]]\| + \|[K_i,[K_i,P_i]]\|\Big), \tag{4.15}$$

with $P_0 = K_0 = O$. Note that

$$P_1 + \cdots + P_{m-1} + K_{m-1} = Z.$$

4.4 Local error for the symmetric order-4 splitting

Assume next that (3.5)-(3.6) are truncated to include the $\mathcal{O}\big(t^4\big)$-terms, so that we obtain a splitting of order four. We observe that the Y-component needs order corrections, hence the relations

$$\begin{aligned} Z_0 = Z &= P_1 + K_1 \\ Z_i &= K_i + \frac{1}{24}t^2[P_i,[P_i,K_i]], \quad i = 1,2,\ldots \\ P_{i+1} + K_{i+1} &= Z_i. \end{aligned}$$

As before,

$$\begin{aligned} L_{4,m,\mathrm{sym}} &= \mathrm{e}^{tZ} - \mathrm{e}^{\frac{1}{2}tP_1+\frac{1}{24}t^3[K_1,[P_1,K_1]]}\cdots \mathrm{e}^{\frac{1}{2}tP_{m-1}+\frac{1}{24}t^3[K_{m-1},[P_{m-1},K_{m-1}]]} \\ &\quad \times \mathrm{e}^{tK_{m-1}+\frac{1}{24}t^3[P_{m-1},[P_{m-1},K_{m-11}]]}\cdots \mathrm{e}^{\frac{1}{2}tP_1+\frac{1}{24}t^3[K_1,[P_1,K_1]]} + \mathcal{O}\big(t^7\big)\,, \end{aligned} \tag{4.16}$$

$$\begin{aligned} E_{4,\mathrm{sym}} &= \mathrm{e}^{tZ} - \mathrm{e}^{\frac{1}{2}tP_1+\frac{1}{24}t^3[K_1,[P_1,K_1]]}\cdots \mathrm{e}^{\frac{1}{2}tP_{m-1}+\frac{1}{24}t^3[K_{m-1},[P_{m-1},K_{m-1}]]} \\ &\quad \times \mathrm{e}^{tK_{m-1}+\frac{1}{24}t^3[P_{m-1},[P_{m-1},K_{m-11}]]}\cdots \mathrm{e}^{\frac{1}{2}tP_1+\frac{1}{24}t^3[K_1,[P_1,K_1]]}. \end{aligned} \tag{4.17}$$

Now, if $Z_{i-1} = P_i + K_i = Z_{i-1}$, one has

$$\begin{aligned} \mathrm{e}^{tZ_{i-1}} &- \mathrm{e}^{\frac{1}{2}tP_i+\frac{1}{24}t^3[K_i,[P_i,K_i]]}\mathrm{e}^{tK_i+\frac{1}{24}t^3[P_i,[P_i,K_i]]}\mathrm{e}^{\frac{1}{2}tP_i+\frac{1}{24}t^3[K_i,[P_i,K_i]]} \\ &= t^5\Big(\frac{1}{720}[K_i,[P_i,[P_i,[P_i,K_i]]]] - \frac{1}{120}[K_i,[K_i,[K_i,[P_i,K_i]]]] \\ &\quad - \frac{1}{180}[[P_i,K_i],[P_i,[P_i,K_i]]] - \frac{1}{1920}[P_i,[P_i,[P_i,[P_i,K_i]]]] \\ &\quad + \frac{13}{1440}[K_i,[K_i,[P_i,[P_i,K_i]]]] + \frac{1}{240}[[P_i,K_i],[K_i,[P_i,K_i]]]\Big) + \mathcal{O}\big(t^7\big)\,, \end{aligned} \tag{4.18}$$

hence, to ease our notation, we denote

$$\begin{aligned} E^{[i]} &= \Big(\frac{1}{720}\|[K_i,[P_i,[P_i,[P_i,K_i]]]]\| + \frac{1}{120}\|[K_i,[K_i,[K_i,[P_i,K_i]]]]\| \\ &\quad + \frac{1}{180}\|[[P_i,K_i],[P_i,[P_i,K_i]]]\| + \frac{1}{1920}\|[P_i,[P_i,[P_i,[P_i,K_i]]]]\| \\ &\quad + \frac{13}{1440}\|[K_i,[K_i,[P_i,[P_i,K_i]]]]\| + \frac{1}{240}\|[[P_i,K_i],[K_i,[P_i,K_i]]]\|\Big). \end{aligned}$$

Returning to (4.16) and passing to the norm in the usual fashion, we obtain the bound

$$\|L_{4,m,\mathrm{sym}}\| \leq t^5\sum_{i=1}^{m-1} E^{[i]}. \tag{4.19}$$

Note that also in this case $P_1 + \cdots P_{m-1} + K_{m-1} = Z + \mathcal{O}\big(t^2\big)$, with a nonzero coefficient for the t^2-term.

5 Global error analysis

5.1 Preliminary results

In what follows, we will make extensive use of the 2-norm (denoted simply as $\|\cdot\|$). For vectors,

$$\|\boldsymbol{x}\| = \left(\sum_{i=1}^{n} |x_i|^2\right)^{1/2},$$

while, for matrices,

$$\|A\| = \max_{\|\boldsymbol{x}\|=1} \|A\boldsymbol{x}\|.$$

Recall that

$$\|A\| = \sqrt{\Sigma_1(A)}, \tag{5.1}$$

where $\Sigma_1(A)$ is the largest of *singular value* of the matrix A, i.e. the largest eigenvalue of AA^*, where $A^* = \bar{A}^T$ denotes the Hermitian adjoint of A [3, 5]. If A is normal, then

$$\|A\| = \max\{|\lambda| : \lambda \text{ eigenvalue of } A\}. \tag{5.2}$$

It is also useful to recall the definition of the *logarithmic norm* μ of a matrix,

$$\mu(A) = \max\left\{\mu : \mu \text{ eigenvalue of } \frac{A + A^*}{2}\right\}, \tag{5.3}$$

which is the derivative of $\|\mathrm{e}^{tA}\|$: Set $\nu(t) = \|\mathrm{e}^{tA}\|$. Then, by differentiation, it is easy verified that

$$\nu'(t) = \mu(A)\nu(t), \quad t > 0,$$

from which we deduce that $\nu(t) = \mathrm{e}^{t\mu(A)}$, for all $t \geq 0$ ($\nu(0) = 1$). Therefore, the growth or decay of $\|\mathrm{e}^{tA}\|$ depends on whether the sign of $\mu(A)$ is positive or negative.

The logarithmic norm obeys the relations

$$\begin{aligned}
\mu(A) &\leq \|A\|, \\
\mu(A + B) &\leq \mu(A) + \|B\|, \\
\|\mathrm{e}^{\alpha A}\| &\leq \mathrm{e}^{\alpha\mu(A)}, \\
\|\mathrm{e}^{\alpha A}\| &\geq \mathrm{e}^{-\alpha\mu(-A)},
\end{aligned} \tag{5.4}$$

with $\alpha \geq 0$, and it is very useful in the analysis of exponential approximations [13].

Another useful result regarding bounds with the logarithmic norm is the lemma below.

Lemma 5.1 *Let A be an square matrix. For every $t \geq 0$ it is true that*

$$\|\mathrm{e}^{tA} - \sum_{k=0}^{s} \frac{1}{k!}(tA)^k\| \leq \frac{\|A^{s+1}\|}{\mu(A)^{s+1}}\left(\mathrm{e}^{t\mu(A)} - \sum_{k=0}^{s} \frac{t^k}{k!}\mu(A)^k\right).$$

Proof. Set $S(t) = \mathrm{e}^{tA} - \sum_{k=0}^{s} \frac{1}{k!}(tA)^k$. One has that $S(0) = O$ and

$$\begin{aligned}
S' &= A\mathrm{e}^{tA} - \sum_{k=0}^{s-1} \frac{1}{k!} t^k A^{k+1} \\
&= A\mathrm{e}^{tA} - A\sum_{k=0}^{s-1} \frac{1}{k!} t^k A^k \\
&= AS + \frac{1}{s!} t^s A^{s+1}.
\end{aligned}$$

By the variation-of-constants theorem,

$$S(t) = \int_0^t \mathrm{e}^{(t-u)A}\frac{1}{s!}u^s A^{s+1}\,\mathrm{d}u.$$

We pass to the norm, and use the above mentioned properties of the lognorm,

$$\|S(t)\| \le \int_0^t \mathrm{e}^{(t-u)\mu(A)}\|A^{s+1}\|\frac{1}{s!}u^s\,\mathrm{d}u = \|A^{s+1}\|\mathrm{e}^{t\mu(A)}\int_0^t \mathrm{e}^{-u\mu(A)}\frac{1}{s!}u^s\,\mathrm{d}s. \tag{5.5}$$

We integrate by parts,

$$\int_0^t \mathrm{e}^{-u\mu(A)}\frac{1}{s!}u^s\,\mathrm{d}s = \int_0^t \frac{\mathrm{d}}{\mathrm{d}u}\left(-\frac{1}{\mu(A)}\frac{u^s}{s!}\mathrm{e}^{-u\mu(A)}\right)\,\mathrm{d}u + \int_0^t \frac{1}{\mu(A)}\frac{u^{s-1}}{(s-1)!}\mathrm{e}^{-u\mu(A)}\,\mathrm{d}u.$$

We recursively integrate by part the last term to obtain

$$\begin{aligned}\int_0^t \mathrm{e}^{-u\mu(A)}\frac{u^s}{s!}\,\mathrm{d}s &= \sum_{k=0}^{s}\int_0^t \frac{\mathrm{d}}{\mathrm{d}u}\left(-\frac{1}{\mu(A)^{s-k+1}}\frac{u^k}{k!}\mathrm{e}^{-u\mu(A)}\right)\,\mathrm{d}u\\ &= -\frac{1}{\mu(A)^{s+1}}\sum_{k=0}^{s}\int_0^t \frac{\mathrm{d}}{\mathrm{d}u}\left(\mu(A)^k\frac{u^k}{k!}\mathrm{e}^{-u\mu(A)}\right)\,\mathrm{d}u\\ &= -\frac{1}{\mu(A)^{s+1}}\left(\sum_{k=0}^{s}\frac{(\mu(A)t)^k}{k!}\mathrm{e}^{-t\mu(A)} - 1\right).\end{aligned}$$

Substitution in (5.5) yields the desired result. □

The bounds we have derived in §4 are bounds for the principal error term in the approximations and they are valid when $0 < t \ll 1$ is small. The real error of the exponential approximation, however, behaves like the local truncation error in the region of convergence and then, after a transitional phase, might grow or decay exponentially. Therefore, using the local error for error control can easily give completely wrong estimates and good global estimates should be used instead.

Sheng [12] derived global error bounds to the splitting of the exponential for some low-order exponential splitting. In his paper, he derived bounds for the order-1 splitting with principal error term (4.1), for the order-2 Strang splitting (4.13) and for the parallel splitting

$$\mathrm{e}^{t(A_1+\cdots+A_m)} = \frac{1}{2}(\mathrm{e}^{tA_1}\cdots\mathrm{e}^{tA_m} + \mathrm{e}^{tA_m}\cdots\mathrm{e}^{tA_1}). \tag{5.6}$$

The goal of this section is to derive similar bounds for the splitting discussed in §4.1–4.4. Before doing this, let us recall the results derived by Sheng.

Theorem 5.2 (Sheng '93) *Let $A_1 + \cdots + A_m = Z$. Then, for any $t > 0$ we have*

$$\|E_{1,m}(t)\| \le \frac{1}{2}t^2\sum_{i=1}^{m-1}\prod_{k=0}^{i-1}\mathrm{e}^{t\mu(A_k)}\|[A_i,\sum_{j=i+1}^{m}A_j]\|\max\{\mathrm{e}^{t\mu(\sum_{j=1}^m A_j)},\mathrm{e}^{t(\mu(A_i)+\mu(\sum_{j=i+1}^m A_j))}\}, \tag{5.7}$$

where $A_0 = O$.

One of our most important applications is the case when Z is skew-symmetric as well as the split terms $A_1,\ldots,A_m$. We immediately deduce the following result.

Corollary 5.2.1 *In the same assumptions of Theorem 5.2, let $A_i \in \mathfrak{so}(n)$, $i = 1, \dots, m$. Then, for all $t \geq 0$,*

$$\|E_1(t)\| \leq \min\{2, \frac{1}{2}t^2 \sum_{i=1}^{m-1} \|[A_i, \sum_{j=i+1}^{m} A_j]\|\}. \tag{5.8}$$

Proof. Note that when $X \in \mathfrak{so}(n)$, then $\mu(X) = 0$. Moreover, for skew-symmetric matrices have norm equal one, therefore,

$$\|\mathrm{e}^{tZ} - \mathrm{e}^{tA_1} \cdots \mathrm{e}^{tA_m}\| \leq \|\mathrm{e}^{tZ}\| + \|\mathrm{e}^{tA_1}\| \cdots \|\mathrm{e}^{tA_m}\| \leq 2,$$

for all t. □

The above corollary implies that, for skew-symmetric matrices, the error in the approximation behaves like the local truncation error until it reaches the maximum error (two). This is very relevant, since the local truncation error is much easier to compute than the global error. As we shall see in the sequel, this error behaviour holds (with small modifications) for the other splitting considered in the paper.

For the Strang splitting, we recall the result below.

Theorem 5.3 (Sheng '93) *Let $A_1 + \cdots + A_m = Z$. Then, for any $t > 0$ there exist parameters $\theta_1, \dots, \theta_m; 0 < \theta_i < t, i = 1, 2, \dots, m$ such that*

$$\begin{aligned}
\|E_{2,m,\mathrm{sym}}(t)\| \leq\ & \frac{1}{6}t^2 \sum_{i=1}^{m-1} \|\frac{1}{2}A_i + \sum_{j=i+1}^{m} A_j\| \, \|[A_i, \sum_{j=i+1}^{m} A_j\| \\
& \times \max\{\mathrm{e}^{t(\mu(\frac{1}{2}A_i)+\mu(\frac{1}{2}A_i+\sum_{j=1}^{m} A_j))}, \mathrm{e}^{t\mu(\sum_{j=i+1}^{m} A_j)}\}, \\
& \times \max\{\mathrm{e}^{\theta_i(\frac{1}{2}\mu(A_i)+\mu(\sum_{j=1}^{m} A_j))}, \mathrm{e}^{\theta_i\mu(\frac{1}{2}A_i+\sum_{j=i+1}^{m} A_j)}\} \\
& \times \exp\left(t \sum_{k=0}^{i-1} \mu(A_k)\right),
\end{aligned} \tag{5.9}$$

where $A_0 = O$.

Another global bound for the Strang splitting is given in [8]: the bound is derived in the more general case when $Z = A + B$, with A an unbounded operator. In part II, we shall see that also the bound obtained in this paper, with due modification, can be used to derive a similar result.

A corollary similar to 5.2.1 can be derived also in this case, and will be presented later in this paper.

To commence our investigations, we need some introductory results.

Lemma 5.4 *Let $n > 0$ be a given integer. The function*

$$f_n(u) = \begin{cases} \frac{\mathrm{e}^u(\sum_{i=0}^{n-1}(-1)^i a_i u^{n-i-1}) + (-1)^n a_n}{u^n} & u < 0, \\ \frac{1}{n} & u = 0, \\ \frac{(\sum_{i=0}^{n-1} a_i(-1)^i u^{n-i-1}) + (-1)^n a_n \mathrm{e}^{-u}}{u^n} & u > 0, \end{cases}$$

where

$$\begin{aligned} a_i &= \frac{(n-1)!}{(n-i-1)!}, \quad i = 0, 1, 2, \dots, n-1, \\ a_n &= (n-1)!, \end{aligned}$$

is continuous. Moreover, for all $-\infty < u < \infty$, it is true that

$$0 < f_n(u) \leq \frac{1}{n}.$$

Notice that the functions $f_n(u)$ are related to integrals of the type $\frac{1}{u^n}\int_0^u x^{n-1}\mathrm{e}^x\,\mathrm{d}x$. These will appear time and again in the sequel.

Lemma 5.5 *Consider the linear operator* $\mathrm{ad}_P = [P,\,\cdot\,]$ *acting on a matrix* A*. If* $\mu(\mathrm{ad}_P) \neq 0$*, it is true that*

$$\|\mathrm{dexp}_P A\| \leq \|A\|_F \frac{\mathrm{e}^{\mu(\mathrm{ad}_P)} - 1}{\mu(\mathrm{ad}_P)},$$

where the subscript 'F*' denotes the Frobenius norm on matrices. If* $\mu(\mathrm{ad}_P) = 0$*, then*

$$\|\mathrm{dexp}_P A\| \leq \|A\|_F.$$

Proof. We commence observing that $\mathrm{ad}_P A = (I \otimes P - P^T \otimes I)\mathrm{vec}A$, hence formally[1]

$$\mathrm{vec}(\mathrm{dexp}_P A) = B^{-1}(\mathrm{e}^B - I_{n\times n})\mathrm{vec}A,$$

where we have set $B = (I \otimes P - P^T \otimes I)$.

Observe that $\|X\| \leq \|X\|_F = \|\mathrm{vec}X\|$. Hence,

$$\|\mathrm{dexp}_P A\| \leq \|\mathrm{dexp}_P A\|_F \leq \|B^{-1}(\mathrm{e}^B - I_{n\times n})\mathrm{vec}A\| \leq \|A\|_F \times \|B^{-1}(\mathrm{e}^B - I_{n\times n})\|.$$

We focus next on $\nu = \|B^{-1}(\mathrm{e}^B - I_{n\times n})\|$. Set $S(t) = (tB)^{-1}(\mathrm{e}^{tB} - I_{n\times n}) = (tB)^{-1}T(t)$, where $T(t) = \mathrm{e}^{tB} - I_{n\times n}$. Clearly, $\nu = \|S(1)\|$. We commence noticing that $T(0) = 0$. Moreover, by differentiation, $T'(t) = B\mathrm{e}^{tB}$, hence,

$$T(t) = B\int_0^t \mathrm{e}^{\tau B}\,\mathrm{d}\tau.$$

Thus,

$$S(t) = \frac{1}{t}\int_0^t \mathrm{e}^{\tau B}\,\mathrm{d}\tau,$$

and passing to the norm $(t > 0, \mu(B) \neq 0)$,

$$\|S(t)\| \leq \frac{1}{t}\int_0^t \mathrm{e}^{\tau\mu(B)}\,\mathrm{d}\tau = \frac{\mathrm{e}^{t\mu(B)} - 1}{t\mu(B)}.$$

Recalling that $\mu(B) = \mu(\mathrm{ad}_P)$, the first assertion follows. The case $\mu(B) = 0$ also follows by considering the limit of the above formula for $\mu(B) \to 0$. □

We are now ready to present global bounds for higher-order methods based on the generalized polar decomposition. We commence considering a two-terms order-2 splitting.

5.2 Global bounds for polar-type order 2

Recall that the global error for the polar-type order 2 splitting is

$$E_2(t) = \mathrm{e}^{t(P+K)} - \mathrm{e}^{\Omega(t)}\mathrm{e}^{tK}, \qquad \Omega(t) = tP - \frac{t^2}{2}[P,K]. \tag{5.10}$$

[1] If B is not invertible, the formula should be intended as a series expansion. However, all the computations are formally true.

Theorem 5.6 *For all $t > 0$, the global error (5.10) is bound by*

$$\|E_2(t)\| \le \left(\frac{t^3}{3}\alpha + \frac{t^4}{4}\gamma(t) + \frac{t^5}{5}\delta(t) + \frac{t^6}{6}\eta(t) + \frac{t^7}{7}\theta(t)\right) \mathrm{e}^{\frac{1}{2}t^2\|[P,K]\|} \max\{\mathrm{e}^{t\mu(P+K)}, \mathrm{e}^{t(\mu(P)+\mu(K))}\},$$

where

$$\begin{aligned}
\alpha &= \frac{1}{4}\|[P,[P,K]]\| + \frac{1}{2}\|[K,[P,K]\|, \\
\gamma(t) &= \frac{1}{4}\|[P,[[P,K],K]\| + \|P\|^2 \frac{\mathrm{e}^{\nu(t)} - 1 - \nu(t) - \frac{1}{2}\nu(t)^2}{\nu(t)^3}(\frac{1}{2}\|[P,K]\|_F + \|P\|\|K\|_F) \\
\delta(t) &= \frac{1}{8}\|[[P,K],[[P,K],K]]\| \\
&\qquad + \|P\|\|[P,K]\| \frac{\mathrm{e}^{\nu(t)} - 1 - \nu(t) - \frac{1}{2}\nu(t)^2}{\nu(t)^3}(\frac{1}{2}\|[P,K]\|_F + \frac{3}{2}\|P\|\|K\|_F) \\
\eta(t) &= \|[P,K]\|^2 \frac{\mathrm{e}^{\nu(t)} - 1 - \nu(t) - \frac{1}{2}\nu(t)^2}{\nu(t)^3}(\frac{1}{8}\|[P,K]\|_F + \frac{3}{4}\|P\|\|K\|_F) \\
\theta(t) &= \frac{1}{8}\|[P,K]\|^3\|K\|_F \frac{\mathrm{e}^{\nu(t)} - 1 - \nu(t) - \frac{1}{2}\nu(t)^2}{\nu(t)^3},
\end{aligned}$$

and finally $\nu(t) = t\mu(P) + \frac{1}{2}t^2\|[P,K]\|$.

Proof. We differentiate $E_2(t)$ to obtain

$$\begin{aligned}
E_2' &= (P+K)\mathrm{e}^{t(P+K)} - \mathrm{dexp}_\Omega \Omega' \,\mathrm{e}^\Omega \mathrm{e}^{tK} - \mathrm{e}^\Omega K \mathrm{e}^{tK} \\
&= (P+K)E_2 + (P+K)\mathrm{e}^\Omega \mathrm{e}^{tK} - \mathrm{dexp}_\Omega \Omega' \,\mathrm{e}^\Omega \mathrm{e}^{tK} - \mathrm{e}^\Omega K \mathrm{e}^{tK} \\
&= (P+K)E_2 + (P - \mathrm{dexp}_\Omega \Omega')\mathrm{e}^\Omega \mathrm{e}^{tK} + [K, \mathrm{e}^\Omega]\mathrm{e}^{tK}
\end{aligned}$$

with initial condition $E_2(0) = O$. Applying the variation of constants theorem we obtain

$$E_2(t) = \int_0^t \mathrm{e}^{(t-\tau)(P+K)}\Big(S_1(\tau) + S_2(\tau)\Big)\mathrm{e}^{\Omega(\tau)}\mathrm{e}^{\tau K}\,\mathrm{d}\tau, \tag{5.11}$$

where we have denoted

$$S_1(\tau) = P - \mathrm{dexp}_{\Omega(\tau)}\Omega'(\tau), \quad S_2(\tau) = [K, \mathrm{e}^{\Omega(\tau)}]\mathrm{e}^{-\Omega(\tau}.$$

Passing to the norm,

$$\|E_2(\tau)\| \le \int_0^t \mathrm{e}^{(t-\tau)\mu(P+K)}\|S_1(\tau) + S_2(\tau)\|\mathrm{e}^{\mu(\Omega)}\mathrm{e}^{\tau\mu(K)}. \tag{5.12}$$

It is here that our analysis departs from that of Sheng: had Ω reduced to τP, the S_1-term would have disappeared and one could have found bounds to the remainder $S(\tau) = [K, \mathrm{e}^\Omega]$ by using the variation of constants theorem again. This is not our case and to obtain error bounds that locally behave like the local truncation error we need to perform a careful analysis of S_1 and S_2.

Let us commence with the S_1-term. We have $\Omega'(\tau) = P - \tau[P,K]$, and, because of the linearity of the dexp-operator,

$$\begin{aligned}
S_1(\tau) &= P - \mathrm{dexp}_\Omega \Omega' = P - \sum_{k=0}^\infty \frac{1}{(k+1)!}\mathrm{ad}_\Omega^k(P - \tau[P,K]) \\
&= P - P + \tau[P,K] - \sum_{k=1}^\infty \frac{1}{(k+1)!}\mathrm{ad}_\Omega^k(P - \frac{\tau}{2}[P,K] - \frac{\tau}{2}[P,K]) \\
&= \tau[P,K] - \frac{\tau}{2}\sum_{k=1}^\infty \frac{1}{(k+1)!}\mathrm{ad}_\Omega^k([P,K]),
\end{aligned}$$

given that $\mathrm{ad}_\Omega^k(P-\frac{1}{2}\tau[P,K])=1/\tau(\mathrm{ad}_\Omega^k\Omega)=O$ for $k=1,2,\ldots$. Furthermore,

$$\begin{aligned}S_{1(\tau)} &= \tau[P,K]+\frac{1}{2}([\tau P-\frac{\tau^2}{2}[P,K],P])-\frac{1}{2}\tau\sum_{k=2}^{\infty}\frac{1}{(k+1)!}\mathrm{ad}_\Omega^k([P,K])\\ &= \tau[P,K]+\frac{1}{4}\tau^2[P,[P,K]]-\frac{1}{2}\tau\sum_{k=2}^{\infty}\frac{1}{(k+1)!}\mathrm{ad}_\Omega^k([P,K]).\end{aligned}$$

We consider next $S_2(\tau)$. We have

$$\begin{aligned}S_2(\tau) &= [K,\mathrm{e}^{\Omega}]\mathrm{e}^{-\Omega}=(K-\mathrm{Ad}_{\exp\Omega}K)\\ &= =K-\exp(\mathrm{ad}_\Omega)K=K-\sum_{k=0}^{\infty}\frac{1}{k!}\mathrm{ad}_\Omega^kK\\ &= K-K-[\tau P-\frac{\tau^2}{2}[P,K],K]-\sum_{k=2}^{\infty}\frac{1}{k!}\mathrm{ad}_\Omega^kK\\ &= -\tau[P,K]+\frac{\tau^2}{2}[[P,K],K]-\sum_{k=2}^{\infty}\frac{1}{k!}\mathrm{ad}_\Omega^kK.\end{aligned}$$

We need to extract also the $k=2$ term in the above sum (since it contributes $\mathcal{O}(\tau^2)$): we obtain

$$\begin{aligned}S_2(\tau) &= -\tau[P,K]+\frac{\tau^2}{2}[[P,K],K]-\frac{1}{2}[\tau P-\frac{\tau^2}{2}[P,K],[\tau P-\frac{\tau^2}{2}[P,K],K]]-\sum_{k=3}^{\infty}\frac{1}{k!}\mathrm{ad}_\Omega^kK\\ &= -\tau[P,K]+\frac{\tau^2}{2}[[P,K],K]-\frac{\tau^2}{2}[P,[P,K]]\\ &\quad+\frac{\tau^3}{4}[P,[[P,K],K]]-\frac{\tau^4}{8}[[P,K],[[P,K],K]]-\sum_{k=3}^{\infty}\frac{1}{k!}\mathrm{ad}_\Omega^kK.\end{aligned}$$

Hence,

$$\begin{aligned}S_1(\tau)+S_2(\tau) &= -\tau^2\Big(\frac{1}{4}[P,[P,K]]+\frac{1}{2}[K,[P,K]]\Big)\\ &\quad+\frac{\tau^3}{4}[P,[[P,K],K]]-\frac{\tau^4}{8}[[P,K],[[P,K],K]]\\ &\quad-\frac{\tau}{2}\sum_{k=2}^{\infty}\frac{1}{(k+1)!}\mathrm{ad}_\Omega^k([P,K])-\sum_{k=3}^{\infty}\frac{1}{k!}\mathrm{ad}_\Omega^kK,\end{aligned}$$

and, passing to the norm,

$$\begin{aligned}\|S_1(\tau)+S_2(\tau)\| &\leq \alpha\tau^2+\gamma\tau^3+\delta\tau^4\\ &\quad+\frac{\tau}{2}\left\|\frac{\mathrm{e}^z-1-z-\frac{1}{2}z^2}{z}\Big|_{z=\mathrm{ad}_\Omega}[P,K]\right\|\\ &\quad+\|(\mathrm{e}^z-1-z-\frac{1}{2}z^2)|_{z=\mathrm{ad}_\Omega}K\|,\end{aligned}$$

where $\alpha=\frac{1}{4}\|[P,[P,K]]\|+\frac{1}{2}\|[K,[P,K]]\|$, and similarly γ and δ are the norms of the $\mathcal{O}(\tau^3)$ and $\mathcal{O}(\tau^4)$ terms above respectively. The two bounds

$$\begin{aligned}\left\|\frac{\mathrm{e}^z-1-z-\frac{1}{2}z^2}{z}\Big|_{z=\mathrm{ad}_\Omega}[P,K]\right\| &\leq \frac{\|\Omega\|^2}{\mu(\Omega)^2}\frac{\mathrm{e}^{\mu(\Omega)}-1-\mu(\Omega)-\frac{1}{2}\mu(\Omega)^2}{\mu(\Omega)}\|[P,K]\|_F\\ \|(\mathrm{e}^z-1-z)|_{z=\mathrm{ad}_\Omega}K\| &\leq \frac{\|\Omega\|^3}{\mu(\Omega)^3}(\mathrm{e}^{\mu(\Omega)}-1-\mu(\Omega)-\frac{1}{2}\mu(\Omega)^2)\|K\|_F\end{aligned}$$

are derived using an argument very similar to that in Lemma 5.5 and Lemma 5.1 respectively. Note that they the right-hand-sides are bound by

$$\frac{1}{6}\|\Omega\|^2\|[P,K]\|_F, \qquad \frac{1}{6}\|\Omega\|^3\|K\|_F$$

when $\mu(\Omega) = 0$ (they follow by taking the limit).

We substitute back into (5.12), to find ($\mu(\Omega) \neq 0$)

$$\begin{aligned} \|E_2(t)\| \quad \leq \quad & \mathrm{e}^{t\mu(P+K)} \int_0^t \mathrm{e}^{\mu(\Omega)+\tau\mu(K)-\tau\mu(P+K)} \Big(\alpha\tau^2 + \gamma\tau^3 + \delta\tau^4 \\ & + \frac{\tau\|\Omega\|^2}{2\mu(\Omega)^2} \frac{\mathrm{e}^{\mu(\Omega)} - 1 - \mu(\Omega) - \frac{1}{2}\mu(\Omega)^2}{\mu(\Omega)} \|[P,K]\|_F \\ & + \frac{\|\Omega\|^3}{\mu(\Omega)^3} (\mathrm{e}^{\mu(\Omega)} - 1 - \mu(\Omega) - \frac{1}{2}\mu(\Omega)^2)\|K\|_F \Big)\,\mathrm{d}\tau \end{aligned} \tag{5.13}$$

When $\mu(\Omega) = 0$ instead,

$$\|E_2(t)\| \leq \mathrm{e}^{t\mu(P+K)} \int_0^t \mathrm{e}^{\tau(\mu(K)-\mu(P+K))} \Big(\alpha\tau^2 + \gamma\tau^3 + \delta\tau^4 + \frac{\tau}{12}\|\Omega\|^2\|[PK]\|_F + \frac{1}{6}\|\Omega\|^3\|K\|_F\big)\,\mathrm{d}\tau.$$

Set $\beta = \mu(K) - \mu(P+K)$ and note that $\|\Omega\| \leq \tau\|P\| + \frac{\tau^2}{2}\|[P,K]\|$. Then

$$\|E_2(t)\| \leq \mathrm{e}^{t\mu(P+K)}(\alpha f_3(t\beta)t^3 + \tilde{\gamma} f_4(t\beta)t^4 + \tilde{\delta} f_5(t\beta)t^5 + \tilde{\eta} f_6(t\beta)t^6 + \tilde{\theta} f_7(t\beta)t^7),$$

where

$$\begin{aligned} \tilde{\alpha} &= \alpha, \\ \tilde{\gamma} &= \gamma + \frac{1}{12}\|P\|^2\|[P,K]\|_F + \frac{1}{6}\|P\|^3\|K\|_F, \\ \tilde{\delta} &= \delta + \frac{1}{12}\|P\|\|[P,K]\| \times \|[P,K]\|_F + \frac{1}{4}\|P\|^2\|[P,K]\|\|K\|_F, \\ \tilde{\eta} &= \frac{1}{8}\|P\|\|[P,K]\|^2\|K\|_F, \\ \tilde{\theta} &= \frac{1}{48}\|[P,K]\|^3\|K\|_F. \end{aligned}$$

Using the bounds for f_n given in Lemma 5.4,

$$\|E_2(t)\| \leq (\frac{t^3}{3}\tilde{\alpha} + \frac{t^4}{4}\tilde{\gamma} + \frac{t^5}{5}\tilde{\delta} + \frac{t^6}{6}\tilde{\eta} + \frac{t^7}{7}\tilde{\theta}) \max\{\mathrm{e}^{t\mu(P+K)}, \mathrm{e}^{t\mu(K)}\}. \tag{5.14}$$

Next, assume $\mu(\Omega) \neq 0$ for all t (in turn, for sufficiently small t this implies that $\mu(P) \neq 0$). Since the function $(\mathrm{e}^z - 1 - z - \frac{1}{2}z)/z^3$ is positive and strictly increasing for $z > 0$, we use the relation

$$\mu(A+B) \leq \mu(A) + \|B\|$$

to derive the bound

$$\frac{\mathrm{e}^{\mu(\Omega)} - 1 - \mu(\Omega) - \frac{1}{2}\mu(\Omega)^2}{\mu(\Omega)^3} \quad \leq \quad \frac{\mathrm{e}^{\nu} - 1 - \nu(t) - \frac{1}{2}\nu(t)^2}{\nu(t)^3}$$

where $\nu(t) = t\mu(P) + \frac{1}{2}t^2\|[P,K]\|$. We substitute in (5.13) to find

$$\begin{aligned}\|E_2(t)\| \quad \leq \quad & \mathrm{e}^{t\mu(P+K)+\frac{1}{2}t^2\|[P,K]\|}\left(\int_0^t \mathrm{e}^{\tau\mu(P)+\tau\mu(K)-\tau\mu(P+K)}(\alpha\tau^2+\gamma\tau^3+\delta\tau^4)\,\mathrm{d}\tau\right. && (5.15)\\ & + \frac{\mathrm{e}^{\nu(t)}-1-\nu(t)-\frac{1}{2}\nu(t)^2}{2\nu(t)^3}\|[P,K]\|_F \\ & \int_0^t \mathrm{e}^{\tau\mu(P)+\tau\mu(K)-\tau\mu(P+K)}\tau(\tau\|P\|+\frac{1}{2}\tau^2\|[P,K]\|)^2\,\mathrm{d}\tau \\ & + \frac{\mathrm{e}^{\nu(t)}-1-\nu(t)-\frac{1}{2}\nu(t)^2}{\nu(t)^3}\|K\|_F \\ & \left.\int_0^t \mathrm{e}^{\tau\mu(P)+\tau\mu(K)-\tau\mu(P+K)}(\tau\|P\|+\frac{1}{2}\tau^2\|[P,K]\|)^3\,\mathrm{d}\tau\right). && (5.16)\end{aligned}$$

As usual, set $\beta = \mu(P) + \mu(K) - \mu(P+K)$. We obtain:

$$\begin{aligned}\|E_2(t)\| \quad \leq \quad & \mathrm{e}^{t\mu(P+K)+\frac{1}{2}t^2\|[P,K]\|}\Big(t^3\alpha f_3(\beta t)+t^4\gamma f_4(\beta t)+t^5\delta f_5(\beta t) && (5.17)\\ & + \frac{\mathrm{e}^{\nu(t)}-1-\nu(t)-\frac{1}{2}\nu(t)^2}{2\nu(t)^3}\|[P,K]\|_F \\ & \times\Big(t^4\|P\|^2 f_4(t\beta)+\|P\|\|[P,K]\|t^5 f_5(t\beta)+\frac{1}{4}t^6\|[P,K]\|^2 f_6(t\beta)\Big) \\ & + \frac{\mathrm{e}^{\nu(t)}-1-\nu(t)-\frac{1}{2}\nu(t)^2}{\nu(t)^3}\|K\|_F \\ & \times\Big(t^4\|P\|^3 f_4(t\beta)+\frac{3}{2}\|P\|^2\|[P,K]\|t^5 f_5(t\beta) \\ & + \frac{3}{4}t^6\|P\|\|[P,K]\|^2 f_6(t\beta)+\frac{1}{8}t^7\|[P,K]\|^3 f_7(t\beta)\Big)\Big).\end{aligned}$$

Using the known bounds for the functions f_n, we obtain

$$\|E_2(t)\| \leq \Big(\frac{1}{3}\alpha(t)t^3+\frac{1}{4}\gamma(t)t^4+\frac{1}{5}t^5\delta(t)+\frac{1}{6}t^6\eta(t)+\frac{1}{7}t^7\theta(t)\Big)\mathrm{e}^{\frac{1}{2}t^2\|[P,K]\|}\max\{\mathrm{e}^{t\mu(P+K)},\mathrm{e}^{t(\mu(P)+\mu(K))}\},$$

where

$$\begin{aligned}\alpha(t) &= \alpha\\ \gamma(t) &= \gamma+\|P\|^2\frac{\mathrm{e}^{\nu(t)}-1-\nu(t)-\frac{1}{2}\nu(t)^2}{\nu(t)^3}(\frac{1}{2}\|[P,K]\|_F+\|P\|\|K\|_F)\\ \delta(t) &= \delta+\|P\|\|[P,K]\|\frac{\mathrm{e}^{\nu(t)}-1-\nu(t)-\frac{1}{2}\nu(t)^2}{\nu(t)^3}(\frac{1}{2}\|[P,K]\|_F+\frac{3}{2}\|P\|\|K\|_F)\\ \eta(t) &= \|[P,K]\|^2\frac{\mathrm{e}^{\nu(t)}-1-\nu(t)-\frac{1}{2}\nu(t)^2}{\nu(t)^3}(\frac{1}{8}\|[P,K]\|_F+\frac{3}{4}\|P\|\|K\|_F)\\ \theta(t) &= \frac{1}{8}\|[P,K]\|^3\|K\|_F\frac{\mathrm{e}^{\nu(t)}-1-\nu(t)-\frac{1}{2}\nu(t)^2}{\nu(t)^3}.\end{aligned}$$

(Observe the consistency of the $\mu(\Omega) = 0$ case as a limit of the general one). □

Note that, when t is small, all the exponential factors in (5.12) behave like $\mathcal{O}(1)$ terms, hence only contribution to the local error comes from the integration of $\|S_1(\tau)+S_2(\tau)\|$,

$$\begin{aligned}\int_0^t \|S_1(\tau)+S_2(\tau)\|\,\mathrm{d}\tau &= \int_0^t \tau^2\Big(\frac{1}{4}\|[P,[P,K]]\|+\frac{1}{2}\|[K,[P,K]]\|\Big)\,\mathrm{d}\tau+\mathcal{O}(t)^4\\ &= t^3\Big(\frac{1}{12}\|[P,[P,K]]\|+\frac{1}{6}\|[K,[P,K]]\|\Big)+\mathcal{O}\big(t^4\big)\,,\end{aligned}$$

in perfect agreement with (4.4).

Corollary 5.6.1 *Assume that $Z=P_1+\cdots+P_{m-1}+K_{m-1}$. Then, for all $t\geq 0$, it is true that*

$$\begin{aligned}\|E_{2,m}(t)\| \;\leq\; & \sum_{i=1}^{m-1}\Big(\frac{t^3}{3}\alpha_i+\frac{t^4}{4}\gamma_i(t)+\frac{t^5}{5}\delta_i(t)+\frac{t^6}{6}\eta_i(t)+\frac{t^7}{7}\theta_i(t)\Big)\\ &\times \mathrm{e}^{\sum_{k=0}^{i-1}(t\mu(P_k)+\frac{1}{2}t^2\|[P_k,K_k]\|)+\frac{1}{2}t^2\|[P_i,K_i]\|}\max\{\mathrm{e}^{t(\mu(P_i)+\mu(K_i))},\mathrm{e}^{t\mu(P_i+K_i)}\},\end{aligned}$$

where the P_i,K_i are the same as in Section 4.1, and $\alpha_i,\gamma_i(t),\ldots,\theta_i(t)$ are the same as in Theorem 5.6, previous replacement of P and K by P_i and K_i.

Proof. Observe that

$$\begin{aligned}E_{2,m}(t) \;=\; & \mathrm{e}^{tZ}-\mathrm{e}^{tP_1-\frac{1}{2}t^2[P_1,K_1]}\mathrm{e}^{tP_2+\cdots tP_{m-1}+tK_{m-1}}\\ &+\mathrm{e}^{tP_1-\frac{1}{2}t^2[P_1,K_1]}\mathrm{e}^{tP_2+\cdots tP_{m-1}+tK_{m-1}}\\ &-\mathrm{e}^{tP_1-\frac{1}{2}t^2[P_1,K_1]}\mathrm{e}^{tP_2-\frac{1}{2}t^2[P_2,K_2]}\mathrm{e}^{tP_3+\cdots tP_{m-1}+tK_{m-1}}\\ &+\cdots+\mathrm{e}^{tP_1-\frac{1}{2}t^2[P_1,K_1]}\cdots\mathrm{e}^{tP_{m-2}-\frac{1}{2}t^2[P_{m-2},K_{m-2}]}\mathrm{e}^{tP_{m-1}+tK_{m-1}}\\ &-\mathrm{e}^{tP_1-\frac{1}{2}t^2[P_1,K_1]}\cdots\mathrm{e}^{tP_{m-1}-\frac{1}{2}t^2[P_{m-1},K_{m-1}]}\mathrm{e}^{tK_{m-1}},\end{aligned}$$

hence, passing to the norm, and making repetitively use of the above theorem, the result follows. □

Corollary 5.6.2 *Assume that $P_1+\cdots+P_{m-1}+K_{m-1}=Z$ and $P_i,K_i\in\mathfrak{so}(n)$, $i=1,\ldots m-1$, where $K_i=P_{i+1}+\cdots+P_{m-1}+K_{m-1}$. Then, for all $t\geq 0$,*

$$\|E_2(t)\|\leq\min\Big\{2,\sum_{i=1}^{m-1}(\frac{t^3}{3}\tilde\alpha_i+\frac{t^4}{4}\tilde\gamma_i+\frac{t^5}{5}\tilde\delta_i+\frac{t^6}{6}\tilde\eta_i+\frac{t^7}{7}\tilde\theta_i)\Big\}\tag{5.18}$$

where the P_i,K_i are the same as in Section 4.1, and $\tilde\alpha_i=\alpha_i$, $\tilde\gamma_i=\gamma_i(0),\ldots,\tilde\theta_i=\theta_i(0)$ are evaluated as the limit as $t\to 0$ of the respective functions in Corollary 5.6.1.

Proof. Recall (5.14). We pass to the norm, bounding norms of exponentials by exponentials of logarithmic norms, and observe that, being all the matrices in question skew-symmetric, their logarithmic norm equals zero. The remaining part of the proof follows similarly. □

Although the previous bounds are sharp for t small, they might overestimate the error when t is large. Below we derive another bound following a slightly different principle. The new bound is less sharp for $t\ll 0$ but it is has usually a better behaviour for large t. We commence with some introductory results.

Lemma 5.7 *Assume that $A,B\in\mathfrak{g}$, α is a given scalar and that $m\geq 1$ is a given integer. Then, for all $\tau\in\mathbb{R}$ it is true that*

i) $[\mathrm{e}^{\alpha\tau^m A},B]=\mathrm{e}^{\alpha\tau^m A}\sum_{j=1}^{\infty}(-1)^{j+1}\frac{(\alpha\tau^m)^j}{j!}\mathrm{ad}_A^j(B)$

(left trivialization),

ii) $[\mathrm{e}^{\alpha\tau^m A}, B] = \sum_{j=1}^{\infty} \frac{(\alpha\tau^m)^j}{j!} \mathrm{ad}_A^j(B)\, \mathrm{e}^{\alpha\tau^m A}$
(right trivialization).

Moreover, for every index $n \geq 1$,

iii)
$$\begin{aligned}[\mathrm{e}^{\alpha\tau^m A}, B] = \mathrm{e}^{\alpha\tau^m A} \sum_{j=1}^{n-1} (-1)^{j+1} \frac{(\alpha\tau^m)^j}{j!} \mathrm{ad}_A^j(B) \\ - (-1)^n \alpha^n m^n \int_0^{\tau} \tau_1^{m-1} \int_0^{\tau_1} \tau_2^{m-1} \cdots \int_0^{\tau_{n-1}} \tau_n^{m-1} \mathrm{e}^{\alpha(\tau^m - \tau_n^m)A} \mathrm{ad}_A^n(B) \mathrm{e}^{\alpha\tau_n^m A}\, \mathrm{d}\tau_n \cdots \mathrm{d}\tau_1,\end{aligned}$$

(left trivialization with integral reminder),

iv)
$$\begin{aligned}[\mathrm{e}^{\alpha\tau^m A}, B] = \sum_{j=1}^{n-1} \frac{(\alpha\tau^m)^j}{j!} \mathrm{ad}_A^j(B) \mathrm{e}^{\alpha\tau^m A} \\ + \alpha^n m^n \int_0^{\tau} \tau_1^{m-1} \int_0^{\tau_1} \tau_2^{m-1} \cdots \int_0^{\tau_{n-1}} \tau_n^{m-1} \mathrm{e}^{\alpha\tau_n^m A} \mathrm{ad}_A^n(B) \mathrm{e}^{\alpha(\tau^m - \tau_n^m)A}\, \mathrm{d}\tau_n \cdots \mathrm{d}\tau_1\end{aligned}$$

(right trivialization with integral reminder).

Proof. We commence from *i)*. By direct computation,

$$\begin{aligned}[\mathrm{e}^{\alpha\tau^m A}, B] &= \mathrm{e}^{\alpha\tau^m A}(B - \mathrm{e}^{-\alpha\tau^m A} B \mathrm{e}^{\alpha\tau^m A}) = \mathrm{e}^{\alpha\tau^m A}\Big(B - \sum_{j=0}^{\infty} \frac{(-1)^j (\alpha\tau^m)^j}{j!} \mathrm{ad}_A^j B\Big) \\ &= \mathrm{e}^{\alpha\tau^m A} \sum_{j=1}^{\infty} \frac{(-1)^{j+1} (\alpha\tau^m)^j}{j!} \mathrm{ad}_A^j B.\end{aligned}$$

The procedure for *ii)* is the same, with instead $[\mathrm{e}^{\alpha\tau^m A}, B] = (\mathrm{e}^{\alpha\tau^m A} B \mathrm{e}^{-\alpha\tau^m A} - B)\mathrm{e}^{\alpha\tau^m A}$.

To conclude, we prove *iii)* (*iv)* follows by a similar computation). Consider *i)*, and split the sum after the first $n-1$ terms:

$$[\mathrm{e}^{\alpha\tau^m A}, B] = \mathrm{e}^{\alpha\tau^m A} \sum_{j=1}^{n-1} (-1)^{j+1} \frac{(\alpha\tau^m)^j}{j!} \mathrm{ad}_A^j(B) + \mathrm{e}^{\alpha\tau^m A} \sum_{j=n}^{\infty} (-1)^{j+1} \frac{(\alpha\tau^m)^j}{j!} \mathrm{ad}_A^j(B). \qquad (5.19)$$

We focus on the second term: by repeated differentiation and integration,

$$\begin{aligned}\sum_{j=n}^{\infty} (-1)^{j+1} \frac{(\alpha\tau^m)^j}{j!} \mathrm{ad}_A^j(B) &= \alpha m \sum_{j=n}^{\infty} (-1)^{j+1} \int_0^{\tau} \tau_1^{m-1} \frac{(\alpha\tau_1^m)^{j-1}}{(j-1)!} \mathrm{ad}_A^{j-n} \mathrm{ad}_A^n(B)\, \mathrm{d}\tau_1 \\ &= \alpha^2 m^2 \sum_{j=n}^{\infty} (-1)^{j+1} \int_0^{\tau} \tau_1^{m-1} \int_0^{\tau_1} \tau_2^{m-1} \frac{(\alpha\tau_2^m)^{j-2}}{(j-2)!} \mathrm{ad}_A^{j-n} \mathrm{ad}_A^n(B)\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1 \\ &= \cdots = \alpha^n m^n \sum_{j=n}^{\infty} (-1)^{j+1} \int_0^{\tau} \tau_1^{m-1} \int_0^{\tau_1} \tau_2^{m-1} \cdots \\ &\qquad \times \int_0^{\tau_{n-1}} \tau_n^{m-1} \frac{(\alpha\tau_n^m)^{j-n}}{(j-n)!} \mathrm{ad}_A^{j-n} \mathrm{ad}_A^n(B)\, \mathrm{d}\tau_n\, \mathrm{d}\tau_{n-1} \cdots \mathrm{d}\tau_1.\end{aligned}$$

Changing index of summation and then order of summation and integration,

$$\alpha^n m^n \sum_{j=n}^{\infty} (-1)^{j+1} \int_0^{\tau} \tau_1^{m-1} \int_0^{\tau_1} \tau_2^{m-1} \cdots \int_0^{\tau_{n-1}} \tau_n^{m-1} \frac{(\alpha\tau_n^m)^{j-n}}{(j-n)!} \mathrm{ad}_A^{j-n} \mathrm{ad}_A^n(B)\, \mathrm{d}\tau_n\, \mathrm{d}\tau_{n-1} \cdots \mathrm{d}\tau_1$$

$$
\begin{aligned}
&= (-1)^{n+1}\alpha^n m^n \sum_{j=0}^{\infty}(-1)^j \int_0^{\tau} \tau_1^{m-1}\int_0^{\tau_1} \tau_2^{m-1}\cdots\int_0^{\tau_{n-1}} \tau_n^{m-1}\frac{(\alpha\tau_n^m)^j}{j!}\mathrm{ad}_A^j\mathrm{ad}_A^n(B)\,\mathrm{d}\tau_n\,\mathrm{d}\tau_{n-1}\cdots\mathrm{d}\tau_1 \\
&= (-1)^{n+1}\alpha^n m^n \int_0^{\tau} \tau_1^{m-1}\int_0^{\tau_1} \tau_2^{m-1}\cdots\int_0^{\tau_{n-1}} \tau_n^{m-1}\mathrm{e}^{-\alpha\tau_n^m A}\mathrm{ad}_A^n B\mathrm{e}^{\alpha\tau_n^m A}\,\mathrm{d}\tau_n\,\mathrm{d}\tau_{n-1}\cdots\mathrm{d}\tau_1,
\end{aligned}
$$

hence the desired result follows by direct substitution in (5.19). □

Lemma 5.8 *[Taylor expansion of* $\mathrm{Ad}_{\exp(\alpha\tau^m A)}$ *with integral reminder]*
Let $A, B \in \mathfrak{g}$ and $m, n \geq 1$ be given integers. For all scalar α, it is true that

$$
\mathrm{e}^{\alpha\tau^m A}B\mathrm{e}^{-\alpha\tau^m A} = \sum_{j=0}^{n-1}\frac{(\alpha\tau^m)^j}{j!}\mathrm{ad}_A^j B + \alpha^n m^n \int_0^{\tau} \tau_1^{m-1}\int_0^{\tau_1} \tau_2^{m-1}\cdots\int_0^{\tau_{n-1}} \tau_n^{m-1}\mathrm{e}^{\alpha\tau_n^m A}\mathrm{ad}_A^n B\mathrm{e}^{-\alpha\tau_n^m A}\,\mathrm{d}\tau_n\cdots\mathrm{d}\tau_1.
$$

Proof. We know that $\mathrm{e}^{\alpha\tau A}B\mathrm{e}^{-\alpha\tau A} = \mathrm{Ad}_{\exp(\alpha\tau A)}B = ([\mathrm{e}^{\alpha\tau^m A}, B] + B])\mathrm{e}^{-\alpha\tau^m A}$. Hence the result follows by direct application of *iv)* of Lemma 5.7. □

In passing, we mention that Lemma 5.7-5.8 can also be proved by repetitively application of the variation of constants theorem.

Theorem 5.9 *Assume $Z = P + K$. Then, for all $t \geq 0$, it is true that*

$$
\|E_2(t)\| \leq t^3\mathrm{e}^{\frac{1}{2}t^2\|[P,K]\|}\Big(\gamma\mathrm{e}^{t(\mu(P)+\mu(K))} + \frac{1}{3}\alpha\max\{\mathrm{e}^{t(\mu(P)+\mu(K))}, \mathrm{e}^{t\mu(P+K)}\}\Big),
$$

where $\alpha = \frac{1}{2}\|[[K,P],K]\| + \|[[P,K],P]\|$ and $\gamma = \frac{1}{4}\|[[P,K],P]\|$.

Proof. We commence observing that

$$
\begin{aligned}
E_2(t) &= (\mathrm{e}^{t(P+K)} - \mathrm{e}^{-\frac{t^2}{2}[P,K]}\mathrm{e}^{tP}\mathrm{e}^{tK}) + (\mathrm{e}^{-\frac{t^2}{2}[P,K]}\mathrm{e}^{tP} - \mathrm{e}^{tP-\frac{t^2}{2}[P,K]})\mathrm{e}^{tK} \\
&= E_2^{[1]}(t) + E_2^{[2]}(t),
\end{aligned}
$$

thus, passing to the norm,

$$
\|E_2(t)\| \leq \|E_2^{[1]}(t)\| + \|E_2^{[2]}(t)\|.
$$

A bound for $\|E_2^{[2]}(t)\|$ comes as a direct consequence of Theorem 5.2,

$$
\|E_2^{[2]}(t)\| \leq \frac{t^3}{4}\|[P,[P,K]]\|\mathrm{e}^{t(\mu(P)+\mu(K))+\frac{t^2}{2}\|[P,K]\|},
$$

therefore, to complete the proof of our theorem, it is sufficient to derive a bound for $\|E_2^{[1]}(t)\|$. To this goal, we differentiate $E_2^{[1]}(t)$ to obtain

$$
\begin{aligned}
(E_2^{[1]})' &= \mathrm{e}^{t(P+K)}(P+K) + t\mathrm{e}^{-\frac{t^2}{2}[P,K]}[P,K]\mathrm{e}^{tP}\mathrm{e}^{tK} \\
&\quad - \mathrm{e}^{-\frac{t^2}{2}[P,K]}\mathrm{e}^{tP}P\mathrm{e}^{tK} - \mathrm{e}^{-\frac{t^2}{2}[P,K]}\mathrm{e}^{tP}\mathrm{e}^{tK}K \\
&= E_2^{[1]}(P+K) + \mathrm{e}^{-\frac{t^2}{2}[P,K]}\mathrm{e}^{tP}(\mathrm{e}^{-tP}t[P,K]\mathrm{e}^{tP}\mathrm{e}^{tK} + [\mathrm{e}^{tK}, P]),
\end{aligned}
$$

with initial condition $E_2^{[1]}(0) = O$. Applying the Variation of Constants Theorem,

$$
E_2^{[1]}(t) = \int_0^t \mathrm{e}^{-\frac{\tau^2}{2}[P,K]}\mathrm{e}^{\tau P}\Big(\tau S_1(\tau)\mathrm{e}^{\tau K} + S_2(\tau)\Big)\mathrm{e}^{(t-\tau)(P+K)}\,\mathrm{d}\tau, \tag{5.20}
$$

where we have set

$$\begin{aligned} S_1(\tau) &= \mathrm{e}^{-\tau P}[P,K]\mathrm{e}^{\tau P}, \\ S_2(\tau) &= [\mathrm{e}^{\tau K}, P]. \end{aligned}$$

We focus next on the function $S_1(\tau)$. Because of Lemma 5.8, with $\alpha = -1, n = 1$,

$$S_1(\tau) = [P,K] + \int_0^\tau \frac{\mathrm{d}}{\mathrm{d}s} S_1(s)\,\mathrm{d}s = [P,K] + \int_0^\tau \mathrm{e}^{-sP}[[P,K],P]\mathrm{e}^{sP}\,\mathrm{d}s. \tag{5.21}$$

For $S_2(\tau)$, we apply *iv)* of Lemma 5.7, with $\alpha = n = 1$, and obtain

$$S_2(\tau) = \tau[K,P]\mathrm{e}^{\tau K} + \int_0^\tau \int_0^s \mathrm{e}^{uK}[K,[K,P]]\mathrm{e}^{-uK}\,\mathrm{d}u\,\mathrm{d}s\mathrm{e}^{\tau K}. \tag{5.22}$$

Next, we substitute (5.22) and (5.21) into (5.20) to obtain

$$\begin{aligned} E_2^{[1]}(t) &= \int_0^t \mathrm{e}^{-\frac{\tau^2}{2}[P,K]}\Big(\tau \int_0^\tau \mathrm{e}^{(\tau-s)P}[[P,K],P]\mathrm{e}^{sP}\mathrm{e}^{\tau K}\,\mathrm{d}s \\ &\quad + \mathrm{e}^{\tau P}\int_0^\tau\int_0^s \mathrm{e}^{uK}[K,[K,P]]\mathrm{e}^{(\tau-u)K}\,\mathrm{d}u\,\mathrm{d}s\Big)\mathrm{e}^{(t-\tau)(P+K)}\,\mathrm{d}\tau, \end{aligned} \tag{5.23}$$

hence, passing to the norm and using (5.4),

$$\begin{aligned} \|E_2^{[1]}(t)\| &\le \int_0^t \mathrm{e}^{\frac{\tau^2}{2}\|[P,K]\|}\Big(\tau\mathrm{e}^{\tau(\mu(K)+\mu(P))}\|[[P,K],P]\|\int_0^\tau \mathrm{d}s \\ &\quad + \mathrm{e}^{\tau(\mu(K)+\mu(P))}\|[[K,P],K]\|\int_0^\tau\int_0^s \mathrm{d}u\,\mathrm{d}s\Big)\mathrm{e}^{(t-\tau)\mu(P+K)}\,\mathrm{d}\tau \\ &= \mathrm{e}^{t\mu(P+K)}\int_0^t \alpha\tau^2\mathrm{e}^{\tau(\mu(P)+\mu(K)-\mu(P+K))+\frac{\tau^2}{2}\|[P,K]\|}\,\mathrm{d}\tau, \end{aligned}$$

where

$$\alpha = \frac{1}{2}\|[[K,P],K]\| + \|[[P,K],P]\|.$$

Set $\beta = \mu(P) + \mu(K) - \mu(P+K)$. We have

$$\|E_2^{[1]}\| \le \mathrm{e}^{t\mu(P+K)+\frac{t^2}{2}\|[P,K]\|}\alpha\int_0^t \tau^2\mathrm{e}^{\tau\beta}\,\mathrm{d}\tau \le t^3\alpha\mathrm{e}^{t\mu(P+K)+\frac{t^2}{2}\|[P,K]\|}\frac{\mathrm{e}^{t\beta}(\beta^2t^2-2\beta t+2)-2}{t^3\beta^3}$$

and hence, by virtue of Lemma 5.4

$$\begin{aligned} \|E_2^{[1]}\| &\le \alpha t^3\frac{\mathrm{e}^{t(\mu(P)+\mu(K))+\frac{t^2}{2}\|[P,K]\|}(\beta^2t^2-2\beta t+2)-2\mathrm{e}^{t\mu(P+K)+\frac{t^2}{2}\|[P,K]\|}}{\beta^3t^3} \\ &\le t^3\alpha\begin{cases} \frac{1}{3}\mathrm{e}^{t\mu(P+K)+\frac{1}{2}t^2\|[P,K]\|} & \text{if } \beta<0 \\ \frac{1}{3}\mathrm{e}^{t(\mu(P)+\mu(K)+\frac{1}{2}t^2\|[P,K]\|} & \text{if } \beta\ge 0, \end{cases} \end{aligned}$$

from which,

$$\|E_2^{[1]}\| \le \frac{1}{3}t^3\alpha\max\{\mathrm{e}^{t(\mu(P)+\mu(K))+\frac{1}{2}t^2\|[P,K]\|}, \mathrm{e}^{t\mu(P+K)+\frac{1}{2}t^2\|[P,K]\|}\}.$$

This, in tandem with the bound derived for $E_2^{[2]}(t)$ completes the proof of the theorem. □

The bounds of Theorems 5.6-5.9 are compared in Figure 5.1 below. We have tested them for normalized 50×50 random matrices P and K with entries in $[0,1]$, and $t \in [10^{-6}, 10^2]$. The bound of Theorem 5.6

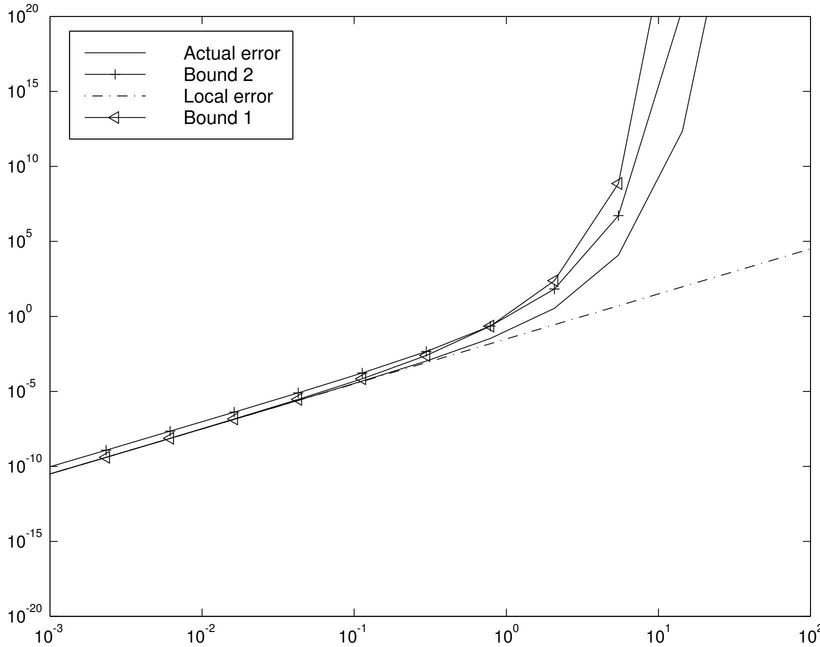

Figure 5.1: Error bounds by Theorem 5.6 (triangles joined by solid line), Theorem 5.9 (pluses joined by solid line), actual error (solid line) and local truncation error (dotted line) versus t. See text for details.

is plotted by triangles joined by a solid line, that of Theorem 5.9 by pluses joined by solid line. The actual error is computed using MATLAB's exponential function `expm`. The bound by Theorem 5.9 is sharper for large t due to the difficulty of deriving sharp bounds for the commutator series arising from the dexp expansion in Theorem 5.6.

Corollary 5.9.1 *Assume that $Z = P_1 + P_2 + \cdots + P_{m-1} + K_{m-1}$. Then, for all $t \geq 0$ it is true that*

$$\|E_{2,m}(t)\| \leq \frac{t^3}{3} \sum_{i=1}^{m-1} \prod_{k=0}^{i-1} \mathrm{e}^{t\mu(P_k)+\frac{1}{2}t^2\|[P_k,K_k]\|}(\gamma_i N_i(t) + \alpha_i M_i(t)),$$

where $P_0 = O, K_0 = Z$, and, for $i = 1, 2, \ldots, m-1$, $K_i = P_{i+1} + \cdots + P_{m-1} + K_{m-1}$, $\gamma_i = \frac{3}{4}\|[[P_i, K_i], P_i]\|$, $\alpha_i = \frac{4}{3}\gamma_i + \frac{1}{2}\|[[K_i, P_i], K_i]\|$, $N_i(t) = \exp\left(t(\mu(P_i) + \mu(K_i)) + \frac{1}{2}t^2\|[P_i, K_i]\|\right)$, and finally $M_i(t) = \max\{N_i(t), \exp\left(t\mu(P_i + K_i) + \frac{1}{2}t^2\|[P_i, K_i]\|\right)\}$.

Proof. The proof is similar to that of Corollary 5.6.1: applying repetitively Theorem 5.9, the desired result is easily verified. □

Corollary 5.9.2 *In the same assumptions of Corollary 5.6.1, let $P_1, \ldots, P_{m-1}, K_{m-1} \in \mathfrak{so}(n)$. Then, for all $t \geq 0$, it is true that*

$$\|E_2(t)\| \leq \min\left\{2, \frac{t^3}{3} \sum_{i=1}^{m-1} (\alpha_i + \gamma_i)\right\}, \tag{5.24}$$

where α_i and γ_i are the same as in Corollary 5.9.1

Proof. Similar to that of Corollary 5.6.2. □

5.3 Global bounds for the polar-type order 3 splitting

In what follows, we will employ the following convention to ease our notation: we will write $[A_1 A_2 \ldots, A_l]$ for $[A_1,[A_2,[\ldots,[A_{l-1},A_l]]]]$. Thus, $[PK]$ stands for $[P,K]$, $[PPK]$ for $[P,[P,K]]$, $[KKPK]$ for $[K,[K,[P,K]]]$, and so on. Other types of commutators are denoted in the usual manner.

Theorem 5.10 *Assume that $Z=P+K$. Then, for all $t\geq 0$, it is true that*

$$\begin{aligned} \|E_3(t)\| \quad &\leq \quad (\frac{1}{4}\tilde{\gamma}t^4+\frac{1}{5}\tilde{\delta}t^5)\mathrm{e}^{t(\mu(P)+\mu(K))+\frac{1}{2}t^2\|[PK]\|+\frac{t^3}{6}\|[KPK]\|+\frac{1}{12}t^3\|[PPK]\|} \\ &\quad + (\frac{1}{4}\tilde{\tilde{\gamma}}t^4+\frac{1}{5}\tilde{\tilde{\delta}}t^5)\mathrm{e}^{t\mu(P)+\frac{1}{2}t^2\|[PK]\|+\frac{1}{4}t^3\|[PPK]\|} \\ &\quad + (\frac{1}{4}\gamma t^4+\frac{1}{5}\delta t^5+\frac{1}{6}\eta t^6)\mathrm{e}^{\frac{1}{2}t^2\|[PK]\|+\frac{1}{6}t^3\|[KPK]\|+\frac{1}{3}t^3\|[PPK]\|} \\ &\qquad \times \max\{\mathrm{e}^{t(\mu(P)+\mu(K))},\mathrm{e}^{t\mu(P+K)}\}, \end{aligned} \tag{5.25}$$

where

$$\begin{aligned} \gamma &= \frac{1}{2}\|[KPPK]\|+\frac{5}{6}\|[PPPK]\|+\frac{1}{6}\|[KKPK]\|, \\ \delta &= \frac{1}{4}\|[[KPK],[PK]\|+\frac{1}{3}\|[[PPK],[PK]]\|, \\ \eta &= \frac{1}{6}\|[[KPK],[PPK]]\|, \\ \tilde{\gamma} &= \frac{1}{6}\|[KKPK]\|+\frac{1}{3}\|[KPPK]\|, \\ \tilde{\delta} &= \frac{5}{24}\|[[KPK],[PK]]\|, \\ \tilde{\tilde{\gamma}} &= \frac{1}{3}\|[PPPK]\|, \\ \tilde{\tilde{\delta}} &= \frac{5}{12}\|[[PK],[PPK]]\|. \end{aligned}$$

Proof. First, we observe that

$$\mathrm{e}^{tP-\frac{1}{2}t^2[PK]}=\mathrm{e}^{-\frac{1}{2}[PK]}\mathrm{e}^{tP}\mathrm{e}^{-\frac{1}{4}t^3[PPK]}+\mathcal{O}(t^4).$$

(The last exponential is necessary to keep the leading error term as an $\mathcal{O}(t^4)$-term). Making use of the above formula, we write $E_3(t)$ as

$$\begin{aligned} E_3(t) \quad &= \quad \mathrm{e}^{t(P+K)}-\mathrm{e}^{tP-\frac{1}{2}t^2[PK]-\frac{1}{6}t^3[KPK]}\mathrm{e}^{tK-\frac{1}{12}t^3[PPK]} \\ &= \quad \Big(\mathrm{e}^{t(P+K)}-\mathrm{e}^{-\frac{1}{6}t^3[KPK]}\mathrm{e}^{-\frac{1}{2}t^2[PK]}\mathrm{e}^{tP}\mathrm{e}^{-\frac{1}{3}t^3[PPK]}\mathrm{e}^{tK}\Big) \\ &\quad + \Big(\mathrm{e}^{-\frac{1}{6}t^3[KPK]}\mathrm{e}^{-\frac{1}{2}t^2[PK]}\mathrm{e}^{tP}\mathrm{e}^{-\frac{1}{3}t^3[PPK]}\mathrm{e}^{tK} \\ &\quad - \mathrm{e}^{-\frac{1}{6}t^3[KPK]}\mathrm{e}^{tP-\frac{1}{2}t^2[PK]}\mathrm{e}^{-\frac{1}{12}t^3[PPK]}\mathrm{e}^{tK}\Big) \\ &\quad + \Big(\mathrm{e}^{-\frac{1}{6}t^3[KPK]}\mathrm{e}^{tP-\frac{1}{2}t^2[PK]}\mathrm{e}^{-\frac{1}{12}t^3[PPK]}\mathrm{e}^{tK} \\ &\quad - \mathrm{e}^{-\frac{1}{6}t^3[KPK]}\mathrm{e}^{tP-\frac{1}{2}t^2[PK]}\mathrm{e}^{tK-\frac{1}{12}t^3[PPK]}\Big) \\ &\quad + \Big(\mathrm{e}^{-\frac{1}{6}t^3[KPK]}\mathrm{e}^{tP-\frac{1}{2}t^2[PK]}\mathrm{e}^{tK-\frac{1}{12}t^3[PPK]} \\ &\quad - \Big(\mathrm{e}^{tP-\frac{1}{2}t^2[PK]-\frac{1}{6}t^3[KPK]}\mathrm{e}^{tK-\frac{1}{12}t^3[PPK]}\Big) \\ &= \quad E_3^{[1]}(t)+E_3^{[2]}(t)+E_3^{[3]}(t)+E_3^{[4]}(t), \end{aligned}$$

The error terms $E_3^{[3]}$ and $E_3^{[4]}$ are of the form (5.7) and can be bound by means of Theorem 5.2,

$$\begin{aligned}\|E_3^{[3]}(t)\| &\le \frac{t^4}{24}\|[KPPK]\|\|\mathrm{e}^{-\frac{t^3}{6}[KPK]}\|\|\mathrm{e}^{tP-\frac{1}{2}t^2[PK]}\|\mathrm{e}^{t\mu(K)+\frac{1}{12}t^3\|[PPK]\|} &(5.26)\\ &\le \frac{t^4}{24}\|[KPPK]\|\mathrm{e}^{t(\mu(P)+\mu(K))+\frac{1}{2}t^2\|[PK]\|+\frac{t^3}{6}\|[KPK]\|+\frac{1}{12}t^3\|[PPK]\|}\\ \|E_4^{[4]}(t)\| &\le \frac{1}{2}\|[\frac{1}{6}t^3[KPK],tP-\frac{1}{2}t^2[PK]]\|\|\mathrm{e}^{tK-\frac{1}{12}t^3[KPK]}\|\mathrm{e}^{t\mu(P)+\frac{1}{2}t^2\|[PK]\|+\frac{1}{6}t^3\|[KPK]\|} &(5.27)\\ &\le (\frac{1}{12}t^4\|[KPPK]\|+\frac{1}{24}t^5\|[[KPK],[PK]]\|)\mathrm{e}^{t(\mu(P)+\mu(K))+\frac{1}{2}t^2\|[PK]\|+\frac{1}{6}t^3\|[KPK]\|+\frac{1}{12}t^3\|[PPK]\|}\end{aligned}$$

while $E_3^{[2]}$ is of similar to $E_2^{[1]}$ in Theorem 5.6 and can be bound by

$$\begin{aligned}\|E_3^{[2]}(t)\| &\le \frac{1}{3}\mathrm{e}^{t\mu(P)+\frac{1}{2}t^2\|[PK]\|+\frac{1}{4}t^3\|[PPK]\|}\Big(\frac{1}{2}\|[tP,[\frac{1}{2}t^2[PK],tP]]\|+\|[\frac{1}{2}t^2[PK],[\frac{1}{2}t^2[PK],tP]]\|\Big)\\ &= \frac{t^4}{12}\mathrm{e}^{t\mu(P)+\frac{1}{2}t^2\|[PK]\|+\frac{1}{4}t^3\|[PPK]\|}\Big(\|[PPPK]\|+t\|[[PK],[PPK]]\|\Big). &(5.28)\end{aligned}$$

Hence we only need to derive a bound for $E_3^{[1]}$. The 'algorithm' is essentially the same as for Theorem 5.6: we commence differentiating $E_3^{[1]}$ and after some algebraic manipulation we obtain

$$\begin{aligned}(E_3^{[1]})' &= E_3^{[1]}(P+K)+\mathrm{e}^{-\frac{1}{6}t^3[KPK]}\Big(\frac{1}{2}t^2[KPK]\mathrm{e}^{-\frac{1}{2}t^2[PK]}\mathrm{e}^{tP}\mathrm{e}^{-\frac{1}{3}t^3[PPK]}\mathrm{e}^{tK}\\ &\quad+t\mathrm{e}^{-\frac{1}{2}t^2[PK]}[PK]\mathrm{e}^{tP}\mathrm{e}^{-\frac{1}{3}t^3[PPK]}\mathrm{e}^{tK}\\ &\quad+\mathrm{e}^{-\frac{1}{2}t^2[PK]}\mathrm{e}^{tP}\mathrm{e}^{-\frac{1}{3}t^3[PPK]}[\mathrm{e}^{tK},P]\\ &\quad+\mathrm{e}^{-\frac{1}{2}t^2[PK]}\mathrm{e}^{tP}[\mathrm{e}^{-\frac{1}{3}t^3[PPK]},P]\mathrm{e}^{tK}\\ &\quad+t^2\mathrm{e}^{-\frac{1}{2}t^2[PK]}\mathrm{e}^{tP}\mathrm{e}^{-\frac{1}{3}t^3[PPK]}[PPK]\mathrm{e}^{tK}\Big)\end{aligned}$$

in tandem with $E_3^{[1]}(0)=O$. Integrating,

$$\begin{aligned}E_3^{[1]}(t) &= \int_0^t \mathrm{e}^{-\frac{1}{6}\tau^3[KPK]}\Big(\frac{1}{2}\tau^2[KPK]\mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}\mathrm{e}^{\tau K} &(5.29)\\ &\quad+\tau\mathrm{e}^{-\frac{1}{2}\tau^2[PK]}[PK]\mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}\mathrm{e}^{\tau K}\\ &\quad+\mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}[\mathrm{e}^{\tau K},P]\\ &\quad+\mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\mathrm{e}^{tP}[\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]},P]\mathrm{e}^{\tau K}\\ &\quad+\tau^2\mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}[PPK]\mathrm{e}^{\tau K}\Big)\mathrm{e}^{(t-\tau)(P+K)}\,\mathrm{d}\tau.\end{aligned}$$

We commence by considering the term $S_1(\tau)=[\mathrm{e}^{\tau K},P]$. Using *iv)* of Lemma 5.7, we find

$$S_1(\tau)=-\tau[PK]\mathrm{e}^{\tau K}-\frac{1}{2}\tau^2[KPK]\mathrm{e}^{\tau K}-\int_0^\tau\int_0^s\int_0^u \mathrm{e}^{wK}[KKPK]\mathrm{e}^{-wK}\,\mathrm{d}w\,\mathrm{d}u\,\mathrm{d}s\;\mathrm{e}^{\tau K}. \quad (5.30)$$

Substituting (5.30) back into (5.29) and collecting similar terms, we find

$$\begin{aligned}E_3^{[1]}(t) &= \int_0^t \mathrm{e}^{-\frac{1}{6}\tau^3[KPK]}\Big(\frac{1}{2}\tau^2[[KPK],\mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}]\mathrm{e}^{\tau K} &(5.31)\\ &\quad+\tau\mathrm{e}^{-\frac{1}{2}\tau^2[PK]}[[PK],\mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}]\mathrm{e}^{\tau K}\\ &\quad+\mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\mathrm{e}^{tP}[\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]},P]\mathrm{e}^{\tau K}\\ &\quad+\tau^2\mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}[PPK]\mathrm{e}^{\tau K}\\ &\quad-\mathrm{e}^{\frac{1}{2}\tau^2[PK]}\mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}\int_0^\tau\int_0^s\int_0^u \mathrm{e}^{(\tau-w)K}[KKPK]\mathrm{e}^{-wK}\,\mathrm{d}w\,\mathrm{d}u\,\mathrm{d}s\Big)\mathrm{e}^{(t-\tau)(P+K)}\,\mathrm{d}\tau.\end{aligned}$$

We focus next on

$$S_2(\tau) = [[PK], \mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}] = S_{2,1}(\tau) + S_{2,2}(\tau),$$

where

$$\begin{aligned} S_{2,1}(\tau) &= -\mathrm{e}^{\tau P}[\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}, [PK]], \\ S_{2,2}(\tau) &= -[\mathrm{e}^{\tau P}, [PK]]\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}. \end{aligned}$$

As above,

$$[\mathrm{e}^{\tau P}, [PK]] = \tau \mathrm{e}^{\tau P}[PPK] - \mathrm{e}^{\tau P}\int_0^\tau \int_0^s \mathrm{e}^{-uP}[PPPK]\mathrm{e}^{uP}\,\mathrm{d}u\,\mathrm{d}s,$$

hence

$$S_{2,2} = -\tau \mathrm{e}^{\tau P}[PPK]\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]} + \mathrm{e}^{\tau P}\int_0^\tau \int_0^s \mathrm{e}^{-uP}[PPPK]\mathrm{e}^{uP}\,\mathrm{d}u\,\mathrm{d}s\;\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}.$$

By Lemma 5.8, with $m = 3, n = 2$,

$$S_{2,1} = \mathrm{e}^{\tau P}\int_0^\tau s^2 \int_0^s \mathrm{e}^{-\frac{1}{3}(\tau^3 - s^3)[PPK]}[[PPK], [PK]]\mathrm{e}^{-\frac{1}{3}s^3[PPK]}\,\mathrm{d}s.$$

Similarly, set

$$S_3(\tau) = [[KPK], \mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}] = S_{3,1}(\tau) + S_{3,2}(\tau) + S_{3,3}(\tau),$$

where

$$\begin{aligned} S_{3,1}(\tau) &= [[KPK], \mathrm{e}^{-\frac{1}{2}\tau^2[PK]}]\mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}, \\ S_{3,2}(\tau) &= \mathrm{e}^{-\frac{1}{2}\tau^2[PK]}[[KPK], \mathrm{e}^{\tau P}]\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}, \\ S_{3,3}(\tau) &= \mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\mathrm{e}^{\tau P}[[KPK], \mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}]. \end{aligned}$$

One has

$$\begin{aligned} S_{3,1}(\tau) &= -\int_0^\tau s\mathrm{e}^{-\frac{1}{2}(\tau^2 - s^2)[PK]}[[KPK], [PK]]\mathrm{e}^{-\frac{1}{2}s^2[PK]}\,\mathrm{d}s\;\mathrm{e}^{\tau P}\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}, \\ S_{3,2}(\tau) &= -\mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\int_0^\tau \mathrm{e}^{(\tau - s)P}[PKPK]\mathrm{e}^{sP}\,\mathrm{d}s\;\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}, \\ S_{3,3}(\tau) &= -\mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\mathrm{e}^{\tau P}\int_0^\tau \mathrm{e}^{-\frac{1}{3}(\tau^3 - s^3)[PPK]}s^2[[KPK], [PPK]]\mathrm{e}^{-\frac{1}{3}s^3[PPK]}\,\mathrm{d}s, \end{aligned}$$

and

$$S_4(\tau) = [\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}, P] = \int_0^\tau \mathrm{e}^{-\frac{1}{3}(\tau^3 - s^3)[PPK]}s^2[PPPK]\mathrm{e}^{-\frac{1}{3}s^2[PPK]}\,\mathrm{d}s.$$

We substitute the expressions for $S_2(\tau), S_3(\tau)$ and $S_4(\tau)$ in (5.31) to find

$$\begin{aligned} E_3^{[1]} &= \int_0^t \mathrm{e}^{-\frac{1}{6}\tau^3[KPK]}\Big(\frac{1}{2}\tau^2(S_{3,1} + S_{3,2} + S_{3,3})\mathrm{e}^{\tau K} \\ &\quad + \mathrm{e}^{-\frac{1}{2}\tau^2[PK]}\mathrm{e}^{\tau P}(\tau^2[\mathrm{e}^{-\frac{1}{4}\tau^3[PPK]}, [PPK]]\mathrm{e}^{\tau K} + \tau(T_1(\tau) + T_2(\tau))\mathrm{e}^{\tau K} \\ &\quad + S_4(\tau)\mathrm{e}^{\tau K} - T_3(\tau)\Big)\mathrm{e}^{(t-\tau)(P+K)}\,\mathrm{d}\tau \end{aligned}$$

where

$$
\begin{aligned}
T_1(\tau) &= \int_0^\tau \int_0^s \mathrm{e}^{-uP}[PPPK]\mathrm{e}^{uP}\,\mathrm{d}u\,\mathrm{d}s\;\mathrm{e}^{-\frac{1}{3}\tau^3[PPK]},\\
T_2(\tau) &= \int_0^\tau \mathrm{e}^{-\frac{1}{3}(\tau^3-s^3)[PPK]}s^2[[PPK],[PK]]\mathrm{e}^{-\frac{1}{3}s^3[PPK]}\,\mathrm{d}s,
\end{aligned}
$$

and finally

$$
T_3(\tau) = \mathrm{e}^{-\frac{1}{3}\tau^3[PPK]}\int_0^\tau\int_0^s\int_0^u \mathrm{e}^{(\tau-w)K}[KKPK]\mathrm{e}^{-wK}\,\mathrm{d}w\,\mathrm{d}u\,\mathrm{d}s.
$$

Note however that

$$
[\mathrm{e}^{-\frac{1}{4}\tau^3[PPK]},[PPK]] = O,
$$

hence, passing to the norm,

$$
\begin{aligned}
\|E_3^{[1]}\| \le \int_0^t &\mathrm{e}^{(t-\tau)\mu(P+K)+\frac{1}{6}\tau^3\|[KPK]\|}\Big(\frac{1}{2}\tau^2(\|S_{3,1}\|+\|S_{3,2}\|+\|S_{3,3}\|)\mathrm{e}^{\tau\mu(K)}\\
&+\mathrm{e}^{\tau\mu(K)+\frac{1}{2}\tau^2\|[PK]\|}(\tau\|\mathrm{e}^{\tau P}T_1(\tau)\|+\mathrm{e}^{\tau\mu(P)}\|T_2(\tau)\|)\\
&+\|T_3(\tau)\|+\|S_4(\tau)\|\mathrm{e}^{\tau\mu(K)}\Big)\,\mathrm{d}\tau.
\end{aligned}
$$

We start bounding individual terms: for what $S_{3,1}$ is concerned, notice that, for $0\le s\le t$, it is true that

$$
\begin{aligned}
\|S_{3,1}(\tau)\| &\le \int_0^\tau \mathrm{e}^{\frac{1}{2}(t^2-s^2)\|[PK]\|}s\|[[KPK],[PK]\|\mathrm{e}^{\frac{1}{2}s^2\|[PK]\|}\mathrm{e}^{\tau\mu(P)}\mathrm{e}^{\frac{1}{3}\tau^3\|[PPK]\|}\\
&\le \|[[KPK],[PK]]\|\mathrm{e}^{\tau\mu(P)+\frac{1}{2}\tau^2\|[PK]\|+\frac{1}{3}\tau^3\|[PPK]\|}\int_0^\tau s\,\mathrm{d}s\\
&= \frac{1}{2}\tau^2\|[[KPK],[PK]]\|\mathrm{e}^{\tau\mu(P)+\frac{1}{2}\tau^2\|[PK]\|+\frac{1}{3}\tau^3\|[PPK]\|}.
\end{aligned}
$$

Furthermore,

$$
\begin{aligned}
\|S_{3,2}(\tau)\| &\le \mathrm{e}^{\frac{1}{2}\tau^2\|[PK]\|}\int_0^\tau \mathrm{e}^{(\tau-s)\mu(P)}\|[KPPK]\|\mathrm{e}^{s\mu(P)}\,\mathrm{d}s\mathrm{e}^{\frac{1}{3}\tau^3\|[PPK]\|}\\
&\le \|[KPPK]\|\mathrm{e}^{\tau\mu(P)+\frac{1}{2}\tau^2\|[PK]\|+\frac{1}{3}\tau^3\|[PPK]\|}\int_0^\tau \mathrm{d}s\\
&= \tau\|[KPPK]\|\mathrm{e}^{\tau\mu(P)+\frac{1}{2}\tau^2\|[PK]\|+\frac{1}{3}\tau^3\|[PPK]\|},\\
\|S_{3,3}(\tau)\| &\le \frac{1}{3}\tau^3\|[[KPK],[PPK]]\|\mathrm{e}^{\tau\mu(P)+\frac{1}{2}\tau^2\|[PK]\|+\frac{1}{3}\tau^3\|[PPK]\|}.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
\|S_4(\tau)\| &\le \frac{1}{3}\tau^3\|[PPPK]\|\mathrm{e}^{\frac{1}{3}\tau^3\|[PPK]\|},\\
\|\mathrm{e}^{\tau P}T_1(\tau)\| &\le \frac{1}{2}\tau^2\|[PPPK]\|\mathrm{e}^{\tau\mu(P)+\frac{1}{3}\tau^3\|[PPK]\|},\\
\|T_2(\tau)\| &\le \frac{1}{3}\tau^3\|[[PPK],[PK]]\|\mathrm{e}^{\frac{1}{3}\tau^3\|[PPK]\|},\\
\|T_3(\tau)\| &\le \frac{1}{6}\tau^3\|[KKPK]\|\mathrm{e}^{\tau\mu(P)+\frac{1}{3}\tau^3\|[PPK]\|},
\end{aligned}
$$

hence

$$
\|E_3^{[1]}\| \le \mathrm{e}^{t\mu(P+K)+\frac{1}{2}t^2\|[PK]\|+\frac{1}{6}t^3\|[KPK]\|+\frac{1}{3}t^3\|[PPK]\|}\int_0^t \mathrm{e}^{\tau\beta}\Big(\tau^3\gamma+\tau^4\delta+\tau^5\eta\Big)\,\mathrm{d}\tau, \tag{5.32}
$$

where

$$\begin{aligned}\gamma &= \frac{1}{2}\|[KPPK]\| + \frac{5}{6}\|[PPPK]\| + \frac{1}{6}\|[KKPK]\|, \\ \delta &= \frac{1}{4}\|[[KPK],[PK]\| + \frac{1}{3}\|[[PPK],[PK]]\|, \\ \eta &= \frac{1}{6}\|[[KPK],[PPK]]\|,\end{aligned}$$

and $\beta = \mu(P) + \mu(K) - \mu(P+K)$. Integrating (5.32), we derive

$$\|E_3^{[1]}\| \leq \mathrm{e}^{t\mu(P+K)+\frac{1}{2}t^2\|[PK]\|+\frac{1}{6}t^3\|[KPK]\|+\frac{1}{3}t^3\|[PPK]\|}\Big(\gamma f_4(\beta t)t^4 + \delta f_5(\beta t)t^5 + \eta f_6(\beta t)t^6\Big),$$

where the f_ns are the functions in Lemma 5.4. Applying the same lemma, we deduce that

$$\|E_3^{[1]}\| \leq (\frac{1}{4}t^4\gamma + \frac{1}{5}t^5\delta + \frac{1}{6}t^6\eta)\mathrm{e}^{\frac{1}{2}t^2\|[PK]\|+\frac{1}{6}t^3\|[KPK]\|+\frac{1}{3}t^3\|[PPK]\|}\max\{\mathrm{e}^{t(\mu(P)+\mu(K))}, \mathrm{e}^{t\mu(P+K)}\},$$

hence, putting together all the error contributions, the theorem follows. □

Corollary 5.10.1 *Set $Z = Z_0 = P_1 + K_1$, for $i = 1, 2, \ldots, m-2$, set $Z_i = K_i - \frac{1}{12}t^2[P_iP_iK_i]$ and $Z_i = P_{i+1} + K_{i+1}$. Moreover, set $P_0 = 0$ and $K_0 = Z$. Then, for all $t \geq 0$ it is true that*

$$\|E_{3,m}(t)\| \leq \sum_{i=1}^{m-1} \mathrm{e}^{\sum_{k=0}^{i-1}(t\mu(P_k)+\frac{1}{2}t^2\|[P_k,K_k]\|+\frac{1}{6}t^3\|[K_k,[P_k,K_k]]\|)}\|\mathcal{E}_{3,i}(t)\|,$$

where $\mathcal{E}_{3,i}(t)$ is given in (5.25) with Z, P and K replaced by Z_{i-1}, P_i and K_i respectively.

Proof. Recall the description of the splitting in Section 4.2. The procedure is similar to that of Corollary 5.9.1. □

Corollary 5.10.2 *With the same notation of Corollary 5.10.1, assume that for all $i = 0, 1, \ldots, m-1$, P_i and K_i are in $\mathfrak{so}(n)$. Then, for all $t \geq 0$, it is true that*

$$\|E_{3,m}(t)\| \leq \max\{2, \sum_{i=1}^{m-1}(\frac{1}{4}t^4(\gamma_i + \tilde{\gamma}_i + \tilde{\tilde{\gamma}}_i + \frac{1}{5}t^5(\delta_i + \tilde{\delta}_i + \tilde{\tilde{\delta}}_i) + \frac{1}{6}t^6\eta_i)\},$$

where $\gamma_i, \delta_i, \tilde{\gamma}_i, \tilde{\delta}_i, \tilde{\tilde{\gamma}}_i, \tilde{\tilde{\delta}}_i\eta_i$ are as in Theorem 5.10, with P and K replaced by P_i and K_i respectively.

Proof. As for Corollary 5.9.2. □

5.4 Global bounds for the Strang splitting

Next, we return to the error (4.12) for the Strang splitting.

Theorem 5.11 *For all $t \geq 0$ it is true that the error of the Strang splitting $E_{2,\mathrm{sym}}(t)$ is bounded by*

$$\|E_{2,\mathrm{sym}}(t)\| \leq \frac{t^3}{12}(\frac{1}{2}\|[P,[P,K]]\| + \|[K,[K,P]]\|)\max\{\mathrm{e}^{t\mu(P+K)}, \mathrm{e}^{t(\mu(P)+\mu(K))}\}.$$

Proof. As usual, we have $E_{2,\text{sym}}(0) = O$. Differentiating,

$$\begin{aligned}
(E_{2,\text{sym}}(t))' &= \mathrm{e}^{t(P+K)}(P+K) - \mathrm{e}^{\frac{1}{2}tP}\frac{P}{2}\mathrm{e}^{tK}\mathrm{e}^{\frac{1}{2}tP} - \mathrm{e}^{\frac{1}{2}tP}\mathrm{e}^{tK}\mathrm{e}^{\frac{1}{2}tP}\frac{P}{2} - \mathrm{e}^{\frac{1}{2}tP}\mathrm{e}^{tK}K\mathrm{e}^{\frac{1}{2}tP} \\
&= E_{2,\text{sym}}(t)(P+K) + \mathrm{e}^{\frac{1}{2}tP}\mathrm{e}^{tK}\mathrm{e}^{\frac{1}{2}tP}\left(\frac{P}{2}+\frac{P}{2}+K\right) - \mathrm{e}^{\frac{1}{2}tP}\frac{P}{2}\mathrm{e}^{tK}\mathrm{e}^{\frac{1}{2}tP} \\
&\quad - \mathrm{e}^{\frac{1}{2}tP}\mathrm{e}^{tK}\mathrm{e}^{\frac{1}{2}tP}\frac{P}{2} - \mathrm{e}^{\frac{1}{2}tP}\mathrm{e}^{tK}K\mathrm{e}^{\frac{1}{2}tP} \\
&= E_{2,\text{sym}}(t)(P+K) + \frac{1}{2}\mathrm{e}^{\frac{1}{2}tP}[\mathrm{e}^{tK}, P]\mathrm{e}^{\frac{1}{2}tP} + \mathrm{e}^{\frac{1}{2}tP}\mathrm{e}^{tK}[\mathrm{e}^{\frac{1}{2}tP}, K],
\end{aligned}$$

hence,

$$E_{2,\text{sym}}(t) = \int_0^t \left(\frac{1}{2}\mathrm{e}^{\frac{1}{2}\tau P}[\mathrm{e}^{\tau K}, P]\mathrm{e}^{\frac{1}{2}\tau P} + \mathrm{e}^{\frac{1}{2}\tau P}\mathrm{e}^{\tau K}[\mathrm{e}^{\frac{1}{2}\tau P}, K]\right)\mathrm{e}^{(t-\tau)(P+K)}\,\mathrm{d}\tau. \tag{5.33}$$

We focus first on the term

$$S_1(\tau) = [\mathrm{e}^{\frac{1}{2}\tau P}, K], \qquad S_1(0) = 0.$$

By *iv)* of Lemma 5.7,

$$S_1(\tau) = \frac{1}{2}\int_0^\tau \mathrm{e}^{\frac{1}{2}sP}[PK]\mathrm{e}^{-\frac{1}{2}sP}\,\mathrm{d}s\;\mathrm{e}^{\frac{1}{2}\tau P}.$$

Similarly, by *iii)*, $S_2(\tau) = [\mathrm{e}^{\tau K}, P] = \mathrm{e}^{\tau K}\int_0^\tau \mathrm{e}^{-sK}[KP]\mathrm{e}^{sK}\,\mathrm{d}s$. Substituting the two expressions in (5.33), we obtain

$$E_{2,\text{sym}}(t) = \frac{1}{2}\int_0^t \mathrm{e}^{\frac{1}{2}\tau P}\mathrm{e}^{\tau K}\left(\int_0^\tau (\mathrm{e}^{-sK}[KP]\mathrm{e}^{sK} + \mathrm{e}^{\frac{1}{2}sP}[PK]\mathrm{e}^{-\frac{1}{2}sP})\,\mathrm{d}s\right)\mathrm{e}^{\frac{1}{2}\tau P}\mathrm{e}^{(t-\tau)(P+K)}\,\mathrm{d}\tau.$$

By Lemma 5.8,

$$\begin{aligned}
\mathrm{e}^{-sK}[KP]\mathrm{e}^{sK} &= [KP] + \int_0^s \mathrm{e}^{-uK}[KPK]\mathrm{e}^{uK}\,\mathrm{d}u, \\
\mathrm{e}^{\frac{1}{2}sP}[PK]\mathrm{e}^{-\frac{1}{2}sP} &= [PK] + \frac{1}{2}\int_0^s \mathrm{e}^{\frac{1}{2}uP}[PPK]\mathrm{e}^{-\frac{1}{2}uP}\,\mathrm{d}u.
\end{aligned}$$

Substituting back in $E_{2,\text{sym}}(t)$,

$$\begin{aligned}
E_{2,\text{sym}}(t) &= \frac{1}{2}\int_0^t \mathrm{e}^{\frac{1}{2}\tau P}\left(\int_0^\tau\int_0^s \mathrm{e}^{(\tau-s)K}[KPK]\mathrm{e}^{sK}\mathrm{e}^{\frac{1}{2}\tau P}\,\mathrm{d}u\,\mathrm{d}s\right. \\
&\qquad \left. + \frac{1}{2}\mathrm{e}^{\tau K}\int_0^\tau\int_0^s \mathrm{e}^{\frac{1}{2}sP}[PPK]\mathrm{e}^{\frac{1}{2}(\tau-s)P}\,\mathrm{d}u\,\mathrm{d}s\right)\mathrm{e}^{(t-\tau)(P+K)}\,\mathrm{d}\tau.
\end{aligned}$$

Passing to the norm,

$$\begin{aligned}
\|E_{2,\text{sym}}(t)\| &\le \frac{1}{2}\int_0^t \mathrm{e}^{\frac{1}{2}\tau\mu(P)}\mathrm{e}^{\tau\mu(K)+\frac{1}{2}\tau\mu(P)} \\
&\qquad \times \left(\|[KPK]\|\int_0^\tau\int_0^s \mathrm{d}u\,\mathrm{d}s + \frac{1}{2}\|[PPK]\|\int_0^\tau\int_0^s \mathrm{d}u\,\mathrm{d}s\right)\mathrm{e}^{(t-\tau)\mu(P+K)}\,\mathrm{d}\tau \\
&= \frac{1}{4}(\delta + \frac{1}{2}\gamma)\mathrm{e}^{t\mu(P+K)}\int_0^t \tau^2\mathrm{e}^{\beta t}\,\mathrm{d}\tau \\
&= \frac{t^3}{4}(\delta + \frac{1}{2}\gamma)\mathrm{e}^{t\mu(P+K)}f_3(\beta t),
\end{aligned}$$

where $\beta = \mu(P) + \mu(K) - \mu(P+K)$, $\delta = \|[KPK]\|$, $\gamma = \|[PPK]\|$ and finally f_3 is the function in Lemma 5.4. Applying the same lemma,

$$\|E_{2,\mathrm{sym}}(t)\| \leq \frac{t^3}{12}(\delta + \frac{1}{2}\gamma) \max\{\mathrm{e}^{t(\mu(P)+\mu(K))}, \mathrm{e}^{t\mu(P+K)}\},$$

hence the desired result. □

Note that when $0 < t \ll 1$, then $\|E_{2,\mathrm{sym}}(t)\|$ behaves exactly like the local truncation error of the Strang splitting.

The result can be easily generalized to the case of a m-terms Strang splitting.

Corollary 5.11.1 *Assume that $P_1 + P_2 + \cdots + P_{m-1} + K_{m-1} = Z$. Then the error*

$$E_{2,\mathrm{sym},m} = \mathrm{e}^{tZ} - \mathrm{e}^{\frac{1}{2}tP_1} \cdots \mathrm{e}^{\frac{1}{2}tP_{m-1}} \mathrm{e}^{tK_{m-1}} \mathrm{e}^{\frac{1}{2}tP_{m-1}} \cdots \mathrm{e}^{\frac{1}{2}tP_1}$$

is bounded in norm by

$$\|E_{2,\mathrm{sym},m}\| \leq \frac{t^3}{12} \sum_{i=1}^{m-1} \prod_{k=0}^{m-1} \mathrm{e}^{t\mu(P_k)} (\delta_i + \frac{1}{2}\gamma_i) \max\{\mathrm{e}^{t(\mu(P_i)+\mu(K_i))}, \mathrm{e}^{t\mu(P_i+K_i)}\},$$

where $P_0 = O$, $K_0 = Z$, and, for $i = 1, 2, \ldots m-1$, $K_i = P_{i+1} + \cdots + P_{m-1} + K_{m-1}$, $\delta_i = \|[P_i, [P_i, K_i]]\|$, and finally $\gamma_i = \|[K_i, [P_i, K_i]]\|$.

Proof. As above, we write

$$\begin{aligned}
E_{2,\mathrm{sym},m} \quad = \quad & \mathrm{e}^{tZ} - \mathrm{e}^{\frac{1}{2}tP_1} \mathrm{e}^{t(P_2+\cdots+K_{m-1})} \mathrm{e}^{\frac{1}{2}tP_1} \\
& + \mathrm{e}^{\frac{1}{2}tP_1} \mathrm{e}^{t(P_2+\cdots+K_{m-1})} \mathrm{e}^{\frac{1}{2}tP_1} \\
& - \mathrm{e}^{\frac{1}{2}tP_1} \mathrm{e}^{\frac{1}{2}tP_2} \mathrm{e}^{t(P_3+\cdots+K_{m-1})} \mathrm{e}^{\frac{1}{2}tP_2} \mathrm{e}^{\frac{1}{2}tP_1} \\
& + \cdots + \mathrm{e}^{\frac{1}{2}tP_1} \cdots \mathrm{e}^{\frac{1}{2}tP_{m-2}} \mathrm{e}^{t(P_{m-1}+K_{m-1})} \mathrm{e}^{\frac{1}{2}tP_{m-2}} \cdots \mathrm{e}^{\frac{1}{2}tP_1} \\
& - \mathrm{e}^{\frac{1}{2}tP_1} \cdots \mathrm{e}^{\frac{1}{2}tP_{m-1}} \mathrm{e}^{tK_{m-1}} \mathrm{e}^{\frac{1}{2}tP_{m-1}} \cdots \mathrm{e}^{\frac{1}{2}tP_1},
\end{aligned}$$

hence the result follows immediately by coupling terms and applying repetitively Theorem 5.11. □

When Z is a skew-symmetric matrix, as well as $P_1, \ldots, P_{m-1}, K_{m-1}$, the error is governed by the local truncation error until the maximum error is reached:

Corollary 5.11.2 *In the same assumptions as above, let $P_1, \ldots, P_{m-1}, K_{m-1} \in \mathfrak{so}(n)$. Then, for all $t \geq 0$,*

$$\|E_{2,\mathrm{sym}}(t)\| \leq \min\Big\{2, \frac{t^3}{12} \sum_{i=1}^{m-1} (\delta_i + \frac{1}{2}\gamma_i)\Big\}, \tag{5.34}$$

where δ_i and γ_i are the same as in Corollary 5.11.1.

5.5 Global bounds for the order-4 symmetric splitting

Theorem 5.12 *For all $t > 0$ it is true that*

$$\begin{aligned}
\|E_{4,\mathrm{sym}}(t)\| \quad \leq \quad & \tfrac{1}{12}\Big(\tfrac{t^5}{96}\|[PPKPK]\| + \tfrac{t^5}{24}\|[KKPPK]\| \\
& + \tfrac{t^7}{596}\|[[KPK],[KPPK]]\| + \tfrac{t^7}{1152}\|[[PPK],[KPPK]]\|\Big) \\
& \quad \times \mathrm{e}^{t(\mu(P)+\mu(K)) + \frac{1}{24}t^3\|[PPK]\| + \frac{1}{12}t^3\|KPK\|} \\
& + \Big(\tfrac{1}{5}\gamma t^5 + \tfrac{1}{7}\delta t^7 + \tfrac{1}{8}t^8\eta + \tfrac{1}{10}t^{10}\theta\Big) \\
& \quad \times \mathrm{e}^{\frac{1}{24}t^3\|[PPK]\| + \frac{1}{12}t^3\|KPK\|} \max\{\mathrm{e}^{t\mu(P+K)}, \mathrm{e}^{t(\mu(P)+\mu(K))}\},
\end{aligned}$$

where

$$
\begin{array}{rcl}
\gamma &=& \frac{1}{384}(\|[PPPPK]\| + \|[KPPPK]\|) + \frac{1}{16}\|[KKPPK]\| + \frac{1}{24}\|[KKKPK]\| \\
&& \quad + \frac{3}{128}\|[[PK],[PPK]]\| + \frac{1}{48}\|[[PK],[KPK]]\|, \\
\delta &=& \frac{1}{2304}\|[[PPK],[PPPK]]\| + \frac{1}{512}\|[[PPK],[KPPK]]\| + \frac{1}{288}\|[[PPK],[KKPK]]\| \\
&& \quad + \frac{1}{9216}\|[[KPK],[PPPK]]\| + \frac{1}{288}\|[[KPK],[KPPK]]\| + \frac{1}{1152}\|[[KPK],[KKPK]]\|, \\
\eta &=& \frac{1}{4608}\|[K,[PPK,KPPK]]\|, \\
\theta &=& \frac{1}{221184}\|[PPK,[PPK,KPPK]]\|.
\end{array}
$$

Proof. We proceed as in Theorems 5.9-5.10 and, in order to obtain a correct leading error term, we split each of the three terms by Strang-type compositions:

$$
\begin{array}{rcl}
E_{4,\mathrm{sym}}(t) &=& \mathrm{e}^{t(P+K)} - \mathrm{e}^{\Omega/2}\mathrm{e}^{\Theta}\mathrm{e}^{\Omega/2} \\
&=& E_4^{[1]}(t) + E_4^{[2]}(t) + E_4^{[3]} + E_4^{[4]},
\end{array}
$$

(for ease of notation, we write E_4 instead of $E_{4,\mathrm{sym}}$, etc.), where

$$
\Omega = P + \frac{1}{12}t^2[KPK], \qquad \Theta = K + \frac{1}{24}t^2[PPK],
$$

and

$$
\begin{array}{rcl}
E_4^{[1]} &=& \mathrm{e}^{t(P+K)} - \mathrm{e}^{\frac14 tP}\mathrm{e}^{\frac{1}{24}t^3[KPK]}\mathrm{e}^{\frac14 tP}\mathrm{e}^{\frac{1}{48}t^3[PPK]}\mathrm{e}^{tK}\mathrm{e}^{\frac{1}{48}t^3[PPK]}\mathrm{e}^{\frac14 tP}\mathrm{e}^{\frac{1}{24}t^3[KPK]}\mathrm{e}^{\frac14 tP} \\
E_4^{[2]} &=& \mathrm{e}^{\frac14 tP}\mathrm{e}^{\frac{1}{24}t^3[KPK]}\mathrm{e}^{\frac14 tP}\mathrm{e}^{\frac{1}{48}t^3[PPK]}\mathrm{e}^{tK}\mathrm{e}^{\frac{1}{48}t^3[PPK]}\mathrm{e}^{\frac14 tP}\mathrm{e}^{\frac{1}{24}t^3[KPK]}\mathrm{e}^{\frac14 tP} \\
&& \quad - \mathrm{e}^{\Omega/2}\mathrm{e}^{\frac{1}{48}t^3[PPK]}\mathrm{e}^{tK}\mathrm{e}^{\frac{1}{48}t^3[PPK]}\mathrm{e}^{\frac14 tP}\mathrm{e}^{\frac{1}{24}t^3[KPK]}\mathrm{e}^{\frac14 tP} \\
E_4^{[3]} &=& \mathrm{e}^{\Omega/2}\mathrm{e}^{\frac{1}{48}t^3[PPK]}\mathrm{e}^{tK}\mathrm{e}^{\frac{1}{48}t^3[PPK]}\mathrm{e}^{\frac14 tP}\mathrm{e}^{\frac{1}{24}t^3[KPK]}\mathrm{e}^{\frac14 tP} - \mathrm{e}^{\Omega/2}\mathrm{e}^{\Theta}\mathrm{e}^{\frac14 tP}\mathrm{e}^{\frac{1}{24}t^3[KPK]}\mathrm{e}^{\frac14 tP} \\
E_4^{[4]} &=& \mathrm{e}^{\Omega/2}\mathrm{e}^{\Theta}\mathrm{e}^{\frac14 tP}\mathrm{e}^{\frac{1}{24}t^3[KPK]}\mathrm{e}^{\frac14 tP} - \mathrm{e}^{\Omega/2}\mathrm{e}^{\Theta}\mathrm{e}^{\Omega/2}.
\end{array}
$$

The error terms $E_4^{[i]}$, for $i = 2,3,4$, can be bound using Theorem 5.3,

$$
\begin{array}{rcl}
E_4^{[2]}, E_4^{[4]} &\le& \frac{1}{12}\Big(\frac{t^5}{192}\|[PPKPK]\| + \frac{t^7}{1152}\|[[KPK],[KPPK]]\|\Big) \\
&& \quad \times\, \mathrm{e}^{t(\mu(P)+\mu(K)) + \frac{1}{24}t^3\|[PPK]\| + \frac{1}{12}t^3\|KPK\|}, \\
E_4^{[3]} &\le& \frac{1}{12}\Big(\frac{t^5}{24}\|[KKPPK]\|\frac{t^7}{1152}\|[[PPK],[KPPK]]\|\Big) \\
&& \quad \times\, \mathrm{e}^{t(\mu(P)+\mu(K)) + \frac{1}{24}t^3\|[PPK]\| + \frac{1}{12}t^3\|KPK\|},
\end{array}
$$

therefore, we only need to analyze $E_4^{[1]}$. To commence our analysis, let us introduce some simplifying notation:

$$
\tilde{P}(t) := \mathrm{e}^{\frac14 tP}, \quad A(t) := \mathrm{e}^{\frac{1}{24}t^3[KPK]}, \quad B(t) := \mathrm{e}^{\frac{1}{48}t^3[PPK]}, \quad \tilde{K} := \mathrm{e}^{tK}.
$$

Notice that $[\tilde{P}, P] = [\tilde{K}, K] = O$.

Differentiating $E_4^{[1]}(t)$, we obtain:

$$
E_4^{[1]\prime}(t) = E_4^{[1]}(P+K) + F_1(t) + F_2(t) + F_3(t) + F_4(t),
$$

where

$$
\begin{aligned}
F_1(t) &= \frac{1}{4}\tilde{P}[A\tilde{P}B\tilde{K}B\tilde{P}A\tilde{P},P]+\frac{1}{4}\tilde{P}A\tilde{P}[B\tilde{K}B\tilde{P}A\tilde{P},P]\\
&\quad+\frac{1}{4}\tilde{P}A\tilde{P}B\tilde{K}B\tilde{P}[A\tilde{P},P]\\
F_2(t) &= \tilde{P}A\tilde{P}B\tilde{K}[B\tilde{P}A\tilde{P},K]\\
F_3(t) &= -\frac{1}{8}t^2\tilde{P}A[KPK]\tilde{P}B\tilde{K}B\tilde{P}A\tilde{P}-\frac{1}{8}t^2\tilde{P}A\tilde{P}B\tilde{K}B\tilde{P}[KPK]A\tilde{P}\\
F_4(t) &= -\frac{1}{16}t^2\tilde{P}A\tilde{P}B[PPK]\tilde{K}B\tilde{P}A\tilde{P}-\frac{1}{16}t^2\tilde{P}A\tilde{P}B\tilde{K}[PPK]B\tilde{P}A\tilde{P}.
\end{aligned}
$$

Then, by variation of constants,

$$
E_4^{[1]}(t)=\int_0^t (F_1(\tau)+F_2(\tau)+F_3(\tau)+F_4(\tau))\mathrm{e}^{(t-\tau)(P+K)}\,\mathrm{d}\tau. \tag{5.35}
$$

To proceed further, consider the first term of F_1, and notice that the commutator acts as a differential operator,

$$
\begin{aligned}
[A\tilde{P}B\tilde{K}B\tilde{P}A\tilde{P},P] &= [A,P]\tilde{P}B\tilde{K}B\tilde{P}A\tilde{P}+A\tilde{P}[B,P]\tilde{K}B\tilde{P}A\tilde{P}+A\tilde{P}B[\tilde{K},P]B\tilde{P}A\tilde{P}\\
&\quad+A\tilde{P}B\tilde{K}[B,P]\tilde{P}A\tilde{P}+A\tilde{P}B\tilde{K}B\tilde{P}[A,P]\tilde{P},
\end{aligned}
$$

(recall that P and $\tilde{P}$ commute). The same type of expansion is applied to the other three terms, hence

$$
\begin{aligned}
F_1(\tau) &= \frac{1}{4}\tilde{P}[A,P]\tilde{P}B\tilde{K}B\tilde{P}A\tilde{P}+\frac{1}{2}\tilde{P}A\tilde{P}[B,P]\tilde{K}B\tilde{P}A\tilde{P}+\frac{1}{2}\tilde{P}A\tilde{P}B[\tilde{K},P]B\tilde{P}A\tilde{P}\\
&\quad+\frac{1}{2}\tilde{P}A\tilde{P}B\tilde{K}[B,P]\tilde{P}A\tilde{P}+\frac{3}{4}\tilde{P}A\tilde{P}B\tilde{K}B\tilde{P}[A,P]\tilde{P}.
\end{aligned}
$$

By a similar token,

$$
\begin{aligned}
F_2(\tau) &= \tilde{P}A\tilde{P}B\tilde{K}[B,K]\tilde{P}A\tilde{P}+\tilde{P}A\tilde{P}B\tilde{K}B[\tilde{P},K]A\tilde{P}\\
&\quad+\tilde{P}A\tilde{P}B\tilde{K}B\tilde{P}[A,K]\tilde{P}+\tilde{P}A\tilde{P}B\tilde{K}B\tilde{P}A[\tilde{P},K]
\end{aligned}
$$

We commence the expansions from the lowest order terms, $[\tilde{K},P]$ and $[\tilde{P},K]$. By Lemma 5.7,

$$
\begin{aligned}
[\tilde{K},P] &= \tilde{K}\Big(\tau[K,P]+\frac{1}{2}\tau^2[KPK]-\frac{1}{6}\tau^3[KKPK]\Big)\\
&\quad+\int_0^\tau\cdots\int_0^{\tau_3}\mathrm{e}^{(\tau-\tau_4)K}[KKKPK]\mathrm{e}^{\tau_4 K}\,\mathrm{d}\tau_4\cdots\mathrm{d}\tau_1\\
[\tilde{P},K] &= \Big(\frac{1}{4}\tau[P,K]+\frac{\tau^2}{32}[PPK]+\frac{\tau^3}{384}[PPPK]\Big)\tilde{P}\\
&\quad+\frac{1}{4^4}\int_0^\tau\cdots\int_0^{\tau_3}\mathrm{e}^{\frac{1}{4}\tau_4 P}[PPPPK]\mathrm{e}^{\frac{1}{4}(\tau-\tau_4)P}\,\mathrm{d}\tau_4\cdots\mathrm{d}\tau_1.
\end{aligned}
$$

We split the term $\tau\mathrm{e}^{\tau K}[K,P]=\frac{1}{2}\tau\mathrm{e}^{\tau K}[K,P]+\frac{1}{2}\tau\mathrm{e}^{\tau K}[K,P]$ and we couple each of these terms with one of the same type in $F_2(\tau)$. We have

$$
\begin{aligned}
&-\frac{\tau}{4}(\tilde{P}A\tilde{P}B\tilde{K}[P,K]B\tilde{P}A\tilde{P}+\tilde{P}A\tilde{P}B\tilde{K}[P,K]B\tilde{P}A\tilde{P}\\
&\quad-\tilde{P}A\tilde{P}B\tilde{K}B[P,K]\tilde{P}A\tilde{P}-\tilde{P}A\tilde{P}B\tilde{K}B\tilde{P}A[P,K]\tilde{P})\\
&=\frac{\tau}{4}(\tilde{P}A\tilde{P}B\tilde{K}[B,[P,K]]\tilde{P}A\tilde{P}+\tilde{P}A\tilde{P}B\tilde{K}[B\tilde{P}A,[P,K]]\tilde{P}).
\end{aligned}
$$

Observe that $[B\tilde{P}A, [P, K]] = [B, [P, K]]\tilde{P}A + B[\tilde{P}, [P, K]]A + B\tilde{P}[A, [P, K]]$. The commutators of $[P, K]$ with A and B yield higher order terms, while

$$[\tilde{P}, [P, K]] = \frac{1}{4}\tau[PPK]\tilde{P} + \frac{1}{16}\int_0^\tau \int_0^{\tau_1} \mathrm{e}^{\frac{1}{4}\tau_1 P}[PPPK]\mathrm{e}^{\frac{1}{4}(\tau-\tau_1)P}\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1.$$

The first term (pre- and post-multiplied by the appropriate factors) is coupled with the second term of $F_4(\tau)$, and this results into

$$\frac{1}{16}\tau^2\tilde{P}A\tilde{P}B\tilde{K}[B, [PPK]]\tilde{P}A\tilde{P} = O,$$

since B and $[PPK]$ commute. Next, we split the first term of $F_4(\tau)$ into two parts and we couple each of them with the $[PPK]$-terms arising in the expansion of $[\tilde{P}, K]$,

$$\begin{aligned}
&\frac{\tau^2}{32}\tilde{P}A\tilde{P}B(-[PPK]\tilde{K}B\tilde{P}A - [PPK]\tilde{K}B\tilde{P}A + \tilde{K}B[PPK]\tilde{P}A + \tilde{K}B\tilde{P}A[PPK])\tilde{P}\\
= \;&\frac{\tau^2}{32}\tilde{P}A\tilde{P}B([\tilde{K}B, [PPK]] + [\tilde{K}B\tilde{P}A, [PPK]])\tilde{P}\\
= \;&\frac{\tau^2}{32}\tilde{P}A\tilde{P}B(2[\tilde{K}, [PPK]]B\tilde{P}A + \tilde{K}B[\tilde{P}, [PPK]]A + \tilde{K}B\tilde{P}[A, [PPK]])\tilde{P}.
\end{aligned}$$

Thus, the terms of the type $[P, K]$ and $[PPK]$ are annihilated. Next, we turn over terms containing $[KPK]$: these arise in the expansion of $[\tilde{K}, P]$ and in $F_3(\tau)$. Splitting and combining as above, we obtain

$$\begin{aligned}
&\frac{\tau^2}{8}\tilde{P}A([\tilde{P}B\tilde{K}, [KPK]]B\tilde{P} + \tilde{P}B\tilde{K}[[KPK], B\tilde{P}])A\tilde{P}\\
= \;&\frac{\tau^2}{8}\tilde{P}A([\tilde{P}, [KPK]]B\tilde{K}B\tilde{P} + \tilde{P}[B, [KPK]]\tilde{K}B\tilde{P} + \tilde{P}B[\tilde{K}, [KPK]]\tilde{P}\\
&\quad + \tilde{P}B\tilde{K}[[KPK], B]\tilde{P} + \tilde{P}B\tilde{K}B[[KPK], \tilde{P}])A\tilde{P}.
\end{aligned}$$

This takes care of all the terms of order up to 3. Putting together all the pieces of the puzzle, we get the expression

$$\begin{aligned}
E_4^{[1]}(t) \;=\; &\int_0^t \Big(\frac{1}{4}\tilde{P}[A, P]\tilde{P}B\tilde{K}B\tilde{P}A\tilde{P} + \frac{1}{2}\tilde{P}A\tilde{P}[B, P]\tilde{K}B\tilde{P}A\tilde{P}\\
&+ \frac{1}{2}\tilde{P}A\tilde{P}B\Big(-\frac{\tau^3}{6}\tilde{K}[KKPK] + \int_0^\tau\cdots\int_0^{\tau_3} \mathrm{e}^{(\tau-\tau_4)K}[KKKPK]\mathrm{e}^{\tau_4 K}\,\mathrm{d}\tau_3\cdots\mathrm{d}\tau_1\Big)B\tilde{P}A\tilde{P}\\
&+ \frac{1}{2}\tilde{P}A\tilde{P}B\tilde{K}[B, P]\tilde{P}A\tilde{P} + \frac{3}{4}\tilde{P}A\tilde{P}B\tilde{K}B\tilde{P}[A, P]\tilde{P}\\
&+ \tilde{P}A\tilde{P}B\tilde{K}B\tilde{P}[A, K]\tilde{P} + \tilde{P}A\tilde{P}B\tilde{K}[B, K]\tilde{P}A\tilde{P}\\
&+ \frac{\tau^3}{384}\Big(\tilde{P}A\tilde{P}B\tilde{K}B[PPPK]\tilde{P}A\tilde{P} + \tilde{P}A\tilde{P}B\tilde{K}B\tilde{P}A[PPPK]\tilde{P}\Big)\\
&+ \frac{1}{256}\tilde{P}A\tilde{P}B\tilde{K}B\int_0^\tau\cdots\int_0^{\tau_3} \mathrm{e}^{\frac{1}{4}\tau_4 P}[PPPPK]\mathrm{e}^{\frac{1}{4}(\tau-\tau_4)P}\,\mathrm{d}\tau_4\cdots\mathrm{d}\tau_1\;A\tilde{P}\\
&+ \frac{1}{256}\tilde{P}A\tilde{P}B\tilde{K}B\tilde{P}A\int_0^\tau\cdots\int_0^{\tau_3} \mathrm{e}^{\frac{1}{4}\tau_4 P}[PPPPK]\mathrm{e}^{\frac{1}{4}(\tau-\tau_4)P}\,\mathrm{d}\tau_4\cdots\mathrm{d}\tau_1\\
&+ \frac{\tau}{64}\tilde{P}A\tilde{P}B\tilde{K}B\int_0^\tau\int_0^{\tau_1} \mathrm{e}^{\frac{1}{4}\tau_2 P}[PPPK]\mathrm{e}^{\frac{1}{4}(\tau-\tau_2)P}\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\;A\tilde{P}\\
&+ \frac{\tau}{4}\Big(2\tilde{P}A\tilde{P}B\tilde{K}[B, [PK]]\tilde{P}A\tilde{P} + \tilde{P}A\tilde{P}B\tilde{K}B\tilde{P}[A, [PK]]\tilde{P}\Big)
\end{aligned}$$

$$
\begin{aligned}
&+\frac{\tau^2}{32}\tilde{P}A\tilde{P}B\Big(2[\tilde{K},[PPK]]B\tilde{P}A+\tilde{K}B[\tilde{P},[PPK]]A+\tilde{K}B\tilde{P}[A,[PPK]]\Big)\tilde{P}\\
&+\frac{\tau^2}{8}\tilde{P}A\Big([\tilde{P},[KPK]]B\tilde{K}B\tilde{P}+\tilde{P}[B,[KPK]]\tilde{K}B\tilde{P}+\tilde{P}B[\tilde{K},[KPK]]B\tilde{P}\\
&\quad+\tilde{P}B\tilde{K}[[KPK],B]\tilde{P}+\tilde{P}B\tilde{K}B[[KPK],\tilde{P}]\Big)A\tilde{P}\Bigg)\,\mathrm{e}^{(t-\tau)(P+K)}\,\mathrm{d}\tau
\end{aligned}
$$

for $E_4^{[1]}$. However, we know that symmetric-type splitting possess an error that expands in odd powers of t and this means that also the order-4 terms annihilate. These arise in commutators of A, B with P, K, as well as in commutators of $[KPK], [PPK]$ with $\tilde{P}, \tilde{K}$. A long and tedious computation shows that this is indeed the case, and that the expression for $\|E_4^{[1]}\|$ is bounded by

$$
\|E_4(t)^{[1]}\| \le \Big(t^5\gamma f_5(\beta t)+t^7\delta f_7(\beta t)+t^8\eta f_8(\beta t)+t^{10}\theta f_{10}(\beta t)\Big)\mathrm{e}^{t\mu(P+K)+\frac{1}{24}t^3\|[PPK]\|+\frac{1}{12}t^3\|[KPK]\|}, \tag{5.36}
$$

where, as usual, $\beta=\mu(P)+\mu(K)-\mu(P+K)$, and, moreover,

$$
\begin{aligned}
\gamma &= \frac{1}{384}(\|[PPPPK]\|+\|[KPPPK]\|)+\frac{1}{16}\|[KKPPK]\|+\frac{1}{24}\|[KKKPK]\|\\
&\quad+\frac{3}{128}\|[[PK],[PPK]]\|+\frac{1}{48}\|[[PK],[KPK]]\|,\\
\delta &= \frac{1}{2304}\|[[PPK],[PPPK]]\|+\frac{1}{512}\|[[PPK],[KPPK]]\|+\frac{1}{288}\|[[PPK],[KKPK]]\|\\
&\quad+\frac{1}{9216}\|[[KPK],[PPPK]]\|+\frac{1}{288}\|[[KPK],[KPPK]]\|+\frac{1}{1152}\|[[KPK],[KKPK]]\|,\\
\eta &= \frac{1}{4608}\|[K,[PPK,KPPK]]\|,\\
\theta &= \frac{1}{221184}\|[PPK,[PPK,KPPK]]\|.
\end{aligned}
$$

Using the known bounds for the functions f_n, the desired result follows. □

It is sensible to belive that, continuing the expansion of $E_4^{[1]}$, the coefficient term $(\frac{1}{5}t^5\gamma+\frac{1}{7}t^7\delta+\frac{1}{8}t^8\eta+\frac{1}{10}t^{10}\theta)$ reduces to odd powers of t only.

Corollary 5.12.1 *Set $Z=Z_0=P_1+K_1$, for $i=1,2,\ldots,m-2$, set $Z_i=K_i+\frac{1}{24}t^2[P_i,[P_iK_i]]$ and $Z_i=P_{i+1}+K_{i+1}$. Moreover, set $P_0=0$ and $K_0=Z$. Then, for all $t\ge 0$ it is true that*

$$
\|E_{4,\mathrm{sym},m}(t)\| \le \sum_{i=1}^{m-1}\mathrm{e}^{\sum_{k=0}^{i-1}(t\mu(P_k)+\frac{1}{24}t^3\|[K_k,[P_k,K_k]]\|)}\|\mathcal{E}_{4,i}(t)\|,
$$

where $\mathcal{E}_{4,i}(t)$ is given in Theorem 5.12 with Z, P and K replaced by Z_{i-1}, P_i and K_i respectively.

Proof. Set $\Omega_i=tP_i+\frac{t^3}{12}[K_i,[P_i,K_i]]$ and $\Theta_i=Z_i=K_i+\frac{t^3}{24}[P_i,[P_iK_i]]$. Then,

$$
\begin{aligned}
E_{4,m} &= \mathrm{e}^{tZ}-\mathrm{e}^{\Omega_1/2}\cdots\mathrm{e}^{\Omega_{m-1}/2}\mathrm{e}^{Z_{m-1}}\mathrm{e}^{\Omega_{m-1}/2}\cdots\mathrm{e}^{\Omega_1/2}\\
&= \mathrm{e}^{tZ}-\mathrm{e}^{\Omega_1/2}\mathrm{e}^{Z_1}\mathrm{e}^{\Omega_1/2}\\
&\quad-\Big(\mathrm{e}^{\Omega_1/2}\mathrm{e}^{Z_1}\mathrm{e}^{\Omega_1/2}-\mathrm{e}^{\Omega_1/2}\mathrm{e}^{\Omega_2/2}\mathrm{e}^{Z_2}\mathrm{e}^{\Omega_2/2}\mathrm{e}^{\Omega_1/2}\Big)\\
&\quad\cdots\\
&\quad-\Big(\mathrm{e}^{\Omega_1/2}\cdots\mathrm{e}^{\Omega_{i-2}/2}\mathrm{e}^{Z_{i-2}}\mathrm{e}^{\Omega_{i-2}/2}\cdots\mathrm{e}^{\Omega_1/2}-\mathrm{e}^{\Omega_1/2}\cdots\mathrm{e}^{\Omega_{i-1}/2}\mathrm{e}^{Z_{i-1}}\mathrm{e}^{\Omega_{i-1}/2}\cdots\mathrm{e}^{\Omega_1/2}\Big).
\end{aligned}
$$

Using the above theorem and the triangle inequality, the result follows immediately. □

Corollary 5.12.2 *With the same notation of Corollary 5.12.1, assume that for all $i = 0, 1, \dots, m-1$, P_i and K_i are in $\mathfrak{so}(n)$. Then, for all $t \geq 0$, it is true that*

$$\|E_{4,m}(t)\| \leq \min\{2, \sum_{i=1}^{m-1} (\frac{1}{5}t^5\gamma_i + \frac{1}{7}t^7\delta_i + \frac{1}{8}t^8\eta_i + \frac{1}{10}t^{10}\theta_i)\},$$

where $\gamma_i, \delta_i, \eta_i$ and θ_i are as in Theorem 5.12, with P and K replaced by P_i and K_i respectively.

6 Numerical experiments

In this section we present some numerical experiments to test the bounds for the splitting derived above. All the experiments are performed in MATLAB.

Applications to the numerical solution of ODEs on Lie-group will be illustrated at length in part II [17].

6.1 Example 1: randomly generated matrices

We consider the case when $Z = P + K$ is the sum of two randomly generated 50×50 matrices P and K with entries in $[0, 1]$, normalized so that $\|P\| = \|K\| = 1$. Figure 6.2 displays the bounds (solid line) derived in this paper for $E_2(t)$ (by Theorem 5.9), $E_3(t)$, and $E_{2,\mathrm{sym}}(t)$, $E_{4,\mathrm{sym}}(t)$. The error is sampled for logarithmically-spaced values of $t \in [10^{-6}, 10]$. The diamonds joined by a dashed line indicate the real error of the splitting methods, whereby the exact exponentials are computed using the MATLAB routine `expm`. Notice that the error in the flat region is of the order of machine accuracy (10^{-14}). A close-up to the interval $[10^{-6}, 0]$ is displayed in Figure 6.3 and it reveals that the bounds are quite sharp in the region of convergence of the formulas. The bound for $E_3(t)$ is the less sharp.

The same bounds are tested in the case when P and K possess eigenvalues with negative real parts.[2] We scale the above matrices to $P - \lambda I$, $K - \lambda I$ with $\lambda = 10$. Also in this case, our bounds mimic very well the behaviour of the actual numerical error (see Figure 6.4).

Note that when P, K have all eigenvalues with negative real parts, then $\lim_{t\to\infty} \mathrm{e}^{t(P+K)} = O$. The same behaviour is observed for order-one splitting a.k.a. Theorem 5.2 and for order-two splitting a.k.a. the Strang splitting (4.12) and parallel splitting (5.6) [12]. It is well known that higher-order approximation methods that require commutators can be cause of instability. The condition $\mathrm{tr}[P, K] = 0$ indicates that $[P, K]$ is likely to have eigenvalues with positive real part. Thus, the approximation for $\mathrm{e}^{t(P+K)}$ starts converging to the zero matrix due to the dominance of P and K, but, after some time, the commutator terms take over and cause the approximation to explode exponentially. This behaviour is displayed very well in Figure 6.4 for $E_3(t)$ and $E_{4,\mathrm{sym}}(t)$, while the exponential growth happens at a latter time for $E_2(t)$. For this reason, it is clear that schemes with commutators are not desirable for this kind of problems and other algorithms, like Padé approximants, low-order splitting techniques with positive stepsizes, Krylov methods etc. are very popular instead [15, 4, 6, 16].

We are especially interested in testing the m-terms bound, since such a splitting originally motivated our study. We generate $Z = P + K$ where P, K are 50×50 random matrices with entries in $[0, 1]$. Then, Z is scaled to have unit norm. We split $Z = P_1 + \cdots + P_{m-1} + K_{m-1}$ (plus higher order terms for splitting of order $3, 4$), in bordered matrices, consisting of one row and one column, as proposed in [18]. Figure 6.5 indicates that our bounds give a good estimate of the real error and that the global behaviour is well captured.

A second test case is again that of matrices having eigenvalues with negative real part. We scale the matrix Z above to $Z - \lambda I$, with $\lambda = 20$. Also in this case, our bounds capture the global behaviour of the error. The theoretical estimates are not far off the actual error of the approximations. One can observe that the bound for the order-3 method does not predict any decay for increasing t — or, we might say, it

[2] We stress that we do not recommend the use of splitting that require commutators in this particular example for stability's sake. However, we mean that negative definite matrices constitute a good test for the accuracy of our bounds.

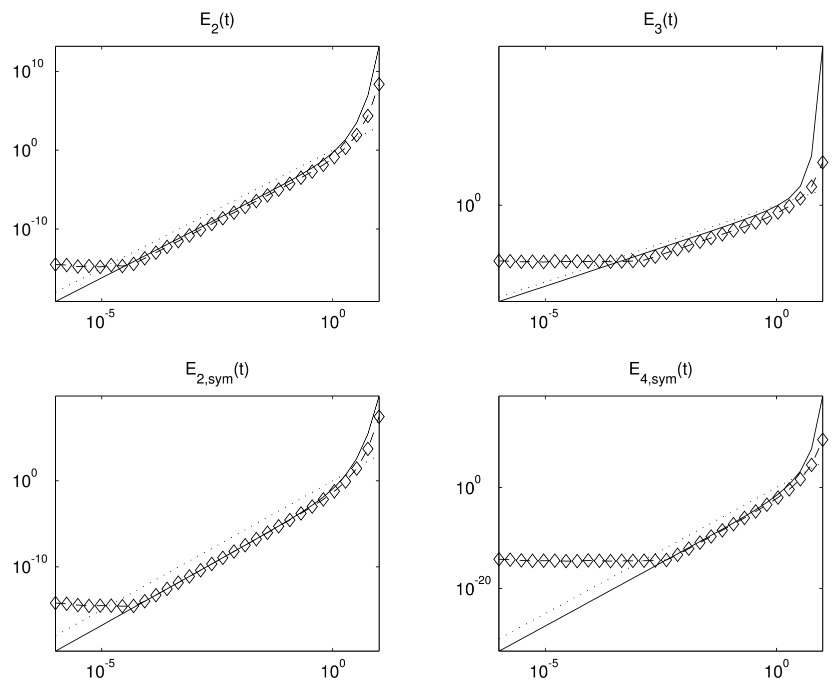

Figure 6.2: Error bounds (solid lines) and real errors (diamonds joined by dashed lines) versus t for E_2 (by Theorem 5.9), E_3, and the symmetric splitting $E_{2,\mathrm{sym}}$, $E_{4,\mathrm{sym}}$ for random 50×50 matrices P, K. The dotted lines indicate the slope of the local error term.

overshoots the exponential growth of the error (that happens slightly later in time). The exponential growth happens also for the symmetric order-4 method slightly later in time. Unfortunately, the computations become so sensitive that it is difficult to perform numerical experiments where these phenomena are easily displayed.

6.2 Example 2: exponential of skew-symmetric matrices

We consider the case when $Z \in \mathfrak{so}(n)$ and $Z = P+K$ where also $P, K \in \mathfrak{so}(n)$, but otherwise normalized random matrices.

This example is special because, given that $\exp(tZ)$ and $\exp(tP)$ and $\exp(tK)$ are orthogonal, one always has that the global error is bounded

$$E(t) \leq \|\mathrm{e}^{tZ}\| + \|\mathrm{e}^{tP}\|\|\mathrm{e}^{tK}\| = 2 \tag{6.1}$$

as a consequence of the triangle inequality. (The assertion is obviously true also for higher order of approximants and for a m-term splitting).

In all these cases, it is observed that the error in the splitting behaves essentially like the local truncation error until it reaches the trivial bound (6.1). From that point onward, it remains constant (see Figure 6.7). The same type of behaviour is observed in the case of an m-terms splitting.

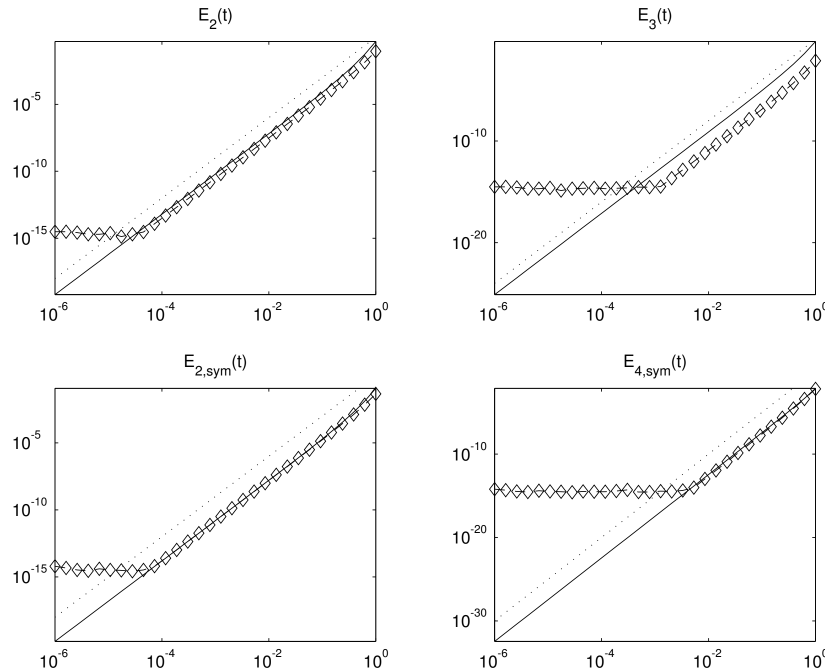

Figure 6.3: Close-up of the error bounds (solid lines) and real errors (diamonds joined by dashed lines) displayed in Figure 6.2. The lines are very close, indicating that the bounds are sharp in the region of convergence.

6.3 Example 3: exponential of matrices in $\mathfrak{so}(p,q)$

Our last test is for matrices in $\mathfrak{so}(p,q)$, i.e. matrices Z such that $Z = -JZ^TJ$, where J is

$$J = \begin{pmatrix} -1 & 0 & & & \\ 0 & -1 & & & \\ & \ddots & \ddots & \ddots & \\ & & & 1 & 0 \\ & & & 0 & 1 \end{pmatrix}$$

(the (-1) occur p times while the $(+1)$ occur q times). We test the two-terms bounds for a normalized random 50×50 matrix Z. The matrices P, K are obtained setting (in MATLAB) `P = [0, Z(1,2:end); Z(2:end,1), zeros(49)]` and $K = Z - P$. The two examples are different in the way P and K capture the essence of Z. In the first example, the matrix Z is skew-symmetric in the $Z(2:50, 2:50)$ block, and symmetric in the first row-column, while in the second example, the skew-symmetric part is the main 49×49 block, while the last row-column are symmetric. In this latter case, due P and K are almost skew-symmetric, and the error grows slower than in the first case, where P is symmetric and K is skew-symmetric (except for the $(1,1)$-entry). Also the bounds appear to sense the difference (to a certain extent).

7 Conclusions

In this paper we have analyzed the error of various splitting for the matrix exponential. These splitting methods possess the property that if $Z \in \mathfrak{g}$, a matrix Lie algebra, then the approximation for $\exp(tZ)$

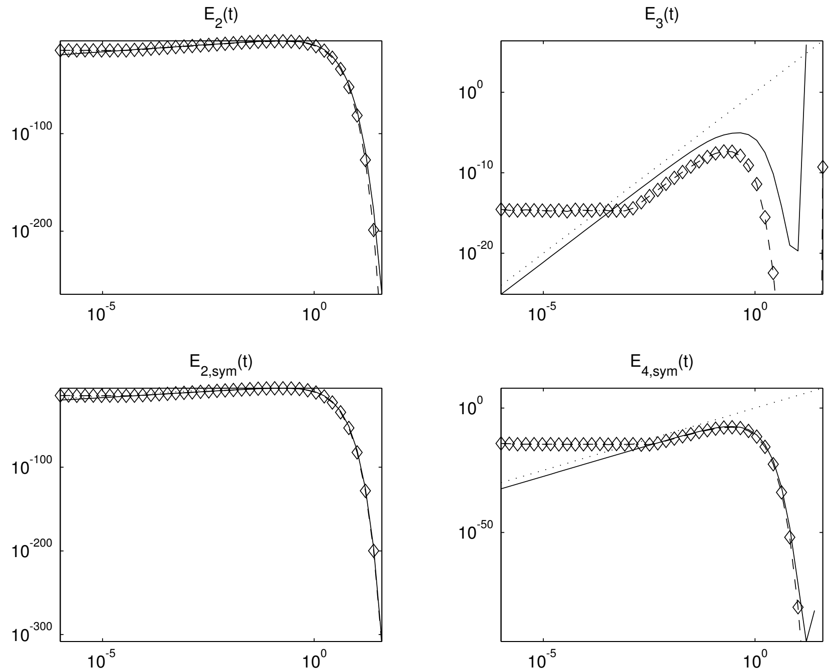

Figure 6.4: Error bounds (solid lines) and real errors (diamonds joined by dashed lines) versus t for E_2 (by Theorem 5.9), E_3, and the symmetric splitting $E_{2,\mathrm{sym}}$, $E_{4,\mathrm{sym}}$. The matrices P, K of Figure 6.2 are scaled to $P - \lambda I$, $K - \lambda I$ with $\lambda = 10$. The dotted lines indicate the slope of the local error term. The solid line cease when overflow is reached.

resides in G, the Lie group of $\mathfrak{g}$.

Particular attention has been devoted to the case when the order conditions arise from Generalized Polar Decompositions [18], but the analysis is valid also in the case when the split terms do not necessarily mirror the splitting of $\mathfrak{g}$ into fixed and anti-fixed set of an automorphism σ.

We have derived both local and global bounds. The global bounds have been derived splitting the exponentials into factors that are easier to treat individually. Using trivializations with integral reminders of commutators, we have derived bounds that are consistent with the order of the methods and are expressed in terms of commutators and exponentials of logarithmic norms.

The bounds have been tested in several numerical experiments for random matrices within certain classes. The numerical experiments indicate that the bounds capture well the behaviour of the actual error of the underlying splitting methods.

In the second part of this work [17] we shall see how the bounds can be specialized to the case of bordered matrices and how they can be performed throughout the splitting of the matrix Z. The fact that we can estimate the error in the approximation of the exponential while performing the splitting of Z is very relevant in applications since this type of forward error estimates are usually quite sharp. We will also discuss in detail the application to the numerical solution of ODEs on Lie groups. We also intend to extend our analysis in the case when Z is an operator. This latter case is of particular interest in the numerical solution of PDEs of evolution.

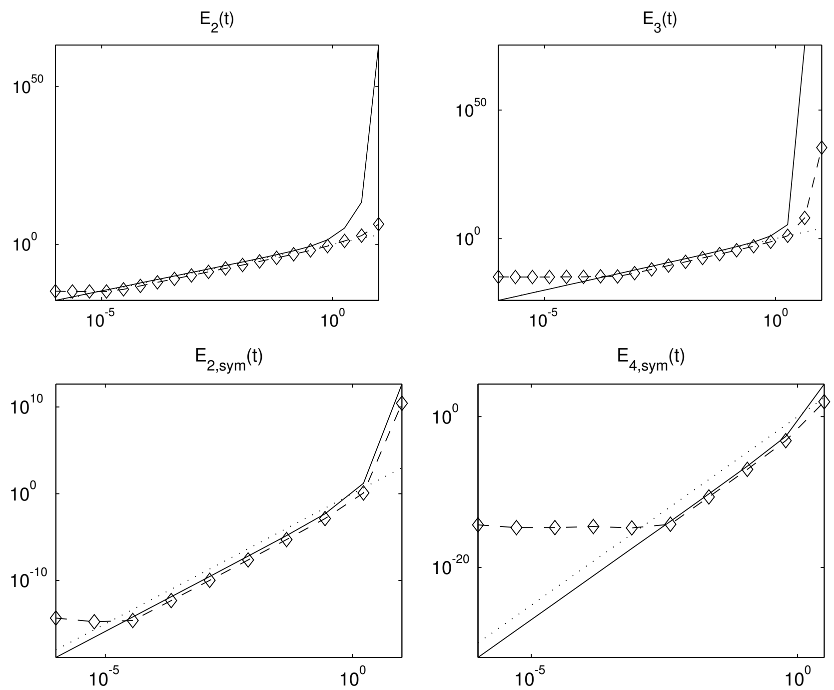

Figure 6.5: Error bounds (solid lines) and real errors (diamond joined by dashed lines) versus t for $E_{2,m}, E_{3,m}, E_{2,\mathrm{sym},m}$, and $E_{4,\mathrm{sym},m}$, where $m = 50$ for Z, a 50×50 normalized random matrix with entries in $[0, 1]$. The split terms are obtained by means GPDs in bordered matrices (see text for more details).

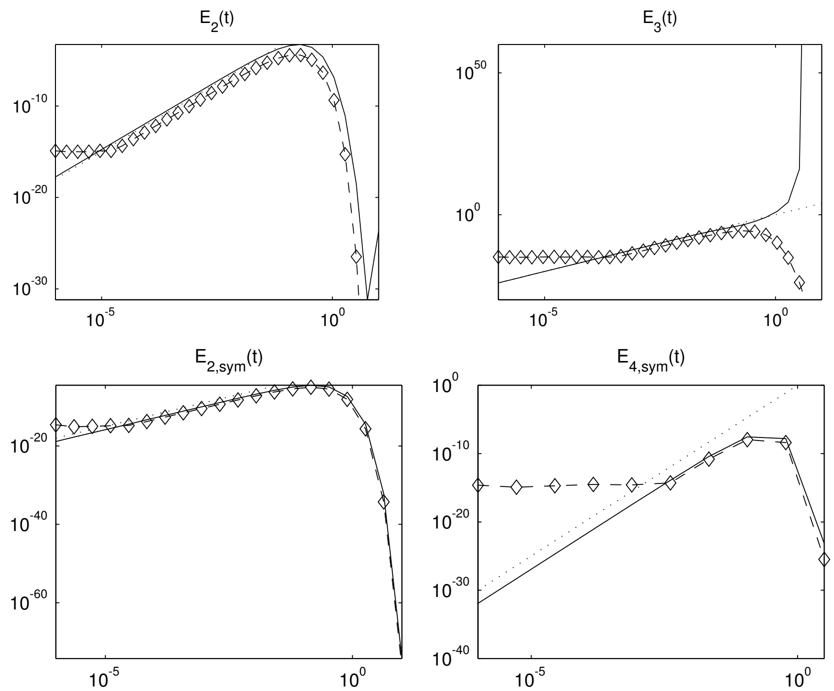

Figure 6.6: Error bounds (solid lines) and real errors (diamond joined by dashed lines) versus t for $E_{2,m}, E_{3,m}, E_{2,\mathrm{sym},m}$, and $E_{4,\mathrm{sym},m}$ for $Z - \lambda I$, $\lambda = 20$.

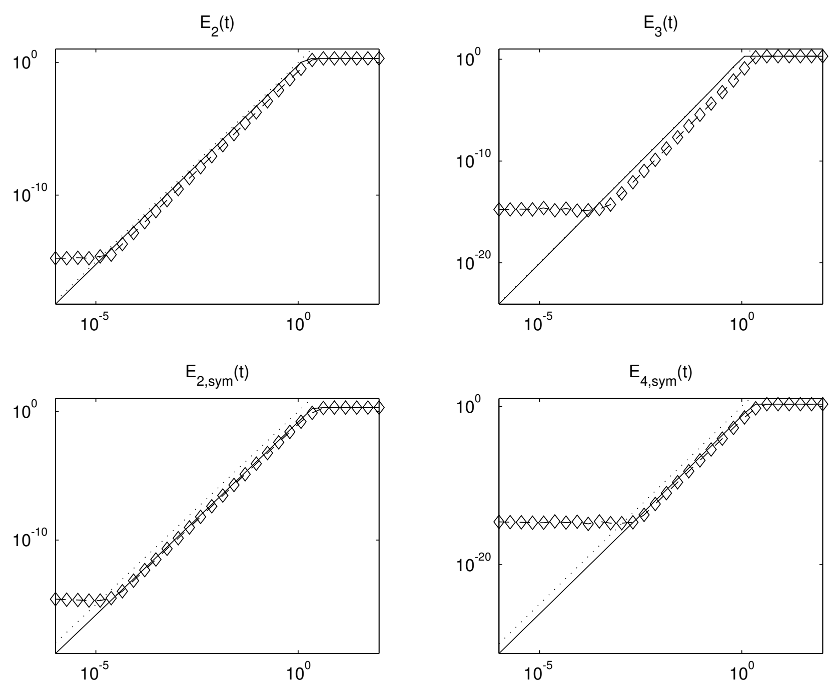

Figure 6.7: Estimated (solid line) and real errors (diamonds joined by dashed line) for 50×50 skew-symmetric matrices P, K versus $t \in [10^{-6}, 10^{2}]$.

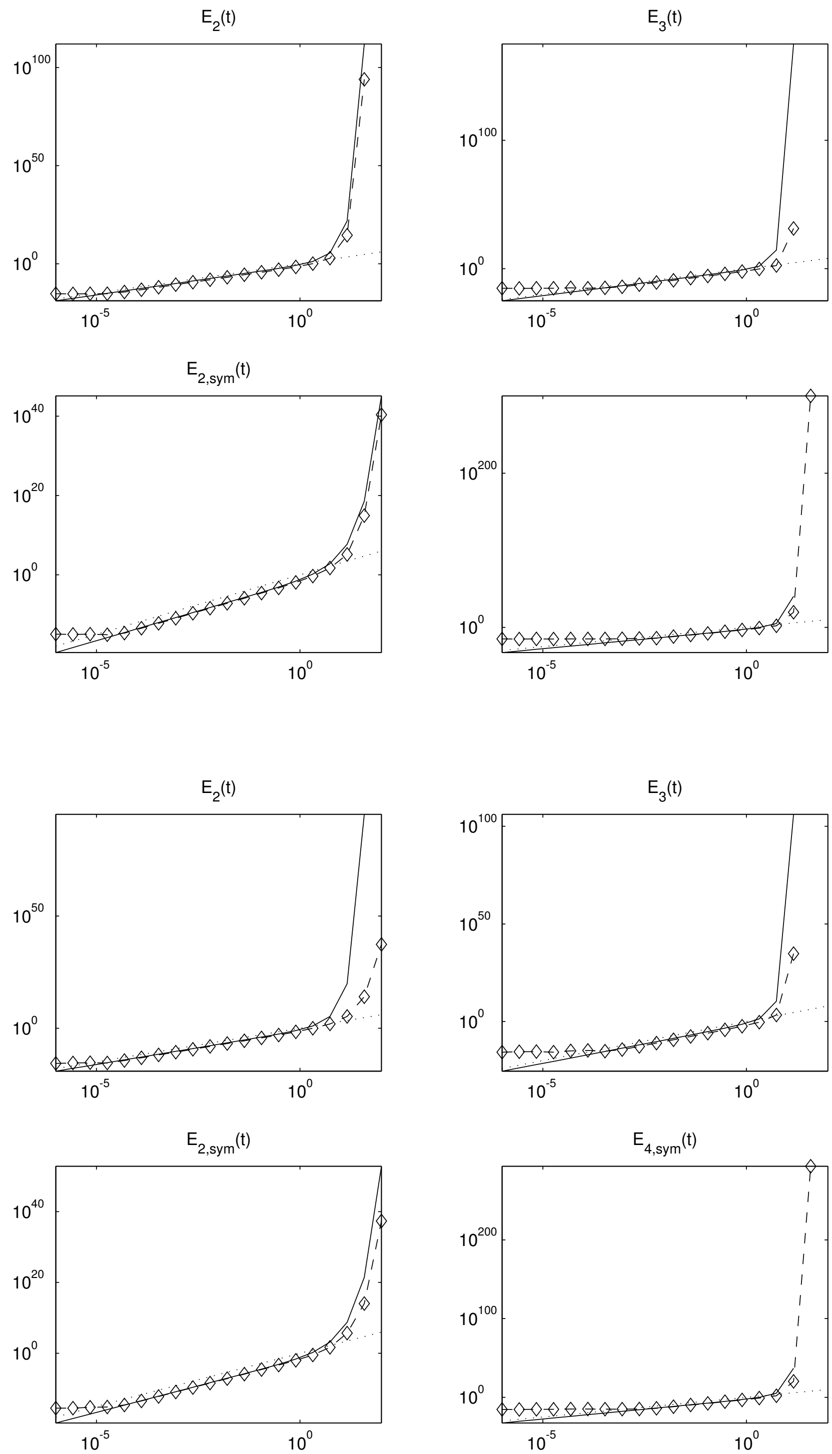

Figure 6.8: Estimated and actual errors for $Z \in \mathfrak{so}(-1, 49)$ (top) and $Z \in \mathfrak{so}(49, -1)$ (bottom). The symbols are as usual.

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