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On the solution of linear differential equations in Lie groups

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Abstract

The subject matter of this paper is the solution of the linear differential equation $y' = a(t)y$, $y(0) = y_0$, where $y_0 \in G$, $a(\,\cdot\,) : \mathbb{R}^+ \to \mathfrak{g}$ and $\mathfrak{g}$ is a Lie algebra of the Lie group G. By building upon an earlier work of Wilhelm Magnus [16], we represent the solution as an infinite series whose terms are indexed by binary trees. This relationship between the infinite series and binary trees leads both to a convergence proof and to a constructive computational algorithm. This numerical method requires the evaluation of a large number of multivariate integrals but this can be accomplished in a tractable manner by using quadrature schemes in a novel manner and by exploiting the structure of the Lie algebra.

1 Introduction

The theme underlying this paper is the solution of the differential equation

$$y' = a(t)y, \quad t \geq 0, \qquad y(0) = y_0 \in G, \tag{1.1}$$

where G is a Lie group, $a \in \mathrm{Lip}[\mathbb{R}^+ \to \mathfrak{g}]$ for every $t \geq 0$ and $\mathfrak{g}$ is the Lie algebra of G. It is well-known that the solution of (1.1) stays on G for all $t \geq 0$. The retention of this important structural feature of the differential equation under discretization of y is at the centre of our discussion.

We briefly recall that a *Lie group* G is a differentiable manifold, equipped with a group structure which is continuous with respect to the underlying topology of the manifold. The *Lie algebra* $\mathfrak{g}$ of G, its tangent space at identity, is a linear space closed under an binary operation $[\,\cdot\,,\cdot\,] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$. This binary operation (colloquially termed 'commutation' or 'a Lie bracket') is linear in each component, antisymmetric:

$$[a, b] = -[b, a], \qquad a, b \in \mathfrak{g},$$

and subject to the *Jacobi identity*

$$[a, [b, c]] + [b, [c, a]] + [c, [a, b]] = 0. \tag{1.2}$$

[1]The work of the second author was supported by UK Engineering and Physical Sciences Research Council and by Norwegian Research Council.

A crucial feature of $\mathfrak{g}$ is that it can be mapped to G by the *exponential map:* Given $b \in \mathfrak{g}$ and $t \in \mathbb{R}^+$, $\exp(tb) \in G$ is the flow generated by the *infinitesimal generator* b [19].

An important special case is when G is a subset of $\mathrm{GL}(\mathbb{C}, n)$ the *general linear group* of all complex nonsingular $n \times n$ matrices. It is then called a *matrix Lie group* and important special cases are $\mathrm{SL}(\mathbb{C}, n)$, the *special linear group* of complex matrices with a unit determinant, $\mathrm{U}(\mathbb{C}, n)$, the *unitary group* of complex unitary matrices, $\mathrm{O}(\mathbb{R}, n)$, the *orthogonal group* of real orthogonal matrices and the *special unitary* and *special orthogonal groups,* $\mathrm{SU}(\mathbb{C}, n) = \mathrm{U}(\mathbb{C}, n) \cap \mathrm{SL}(\mathbb{C}, n)$ and $\mathrm{SO}(\mathbb{R}, n) = \mathrm{O}(\mathbb{R}, n) \cap \mathrm{SL}(\mathbb{C}, n)$ respectively. The corresponding Lie algebras are well-known [19]. In the case of matrix Lie groups, the exponential operator is just

$$\exp(tb) = \sum_{k=0}^{\infty} \frac{1}{k!}(tb)^k,$$

where $[a, b] = ab - ba$ is the usual commutator of two matrices.

We assume in the sequel that G is a matrix Lie group, whereby (1.1) becomes a matricial *ordinary differential system.* This restriction is more in the nature of conceptualisation than essence, since all our theory remains intact for general Lie groups. In particular, this is the case when $\mathfrak{g}$ consists of differential operators. However, the latter lead to a range of computational problems that are outside the realm of this paper and might well be the subject of a future article.

The retention of a Lie group structure is often an imperative in numerical discretization, since it represents invariants that are satisfied by the original differential equations. Important examples, ubiquitous in applications, include the conservation of orthogonality, volume and symplecticity [14]. Arguably, even more important are invariants that correspond to differential systems on *homogeneous manifolds* (manifolds that are invariant when subjected to a transitive group action). As long as it is known how to discretize in a Lie group, it is possible also to discretize flows on homogeneous manifolds [17, 18].

There are two points of departure for this paper. Firstly, in an important paper [16], Wilhelm Magnus derived "the continuous analogue of the Baker–Hausdorff formula", an expansion,

$$\begin{aligned}\sigma(t) = {}& \int_0^t a(\kappa)\mathrm{d}\kappa + \tfrac{1}{2}\int_0^t \left[a(\kappa), \int_0^\kappa a(\xi)\mathrm{d}\xi\right] \mathrm{d}\kappa \\ & + \tfrac{1}{4}\int_0^t \left[a(\kappa), \int_0^\kappa \left[a(\xi), \int_0^\xi a(\eta)\mathrm{d}\eta\right] \mathrm{d}\xi\right] \mathrm{d}\kappa \\ & + \tfrac{1}{12}\int_0^t \left[\left[a(\kappa), \int_0^\kappa a(\xi)\mathrm{d}\xi\right], \int_0^\kappa a(\eta)\mathrm{d}\eta\right] \mathrm{d}\kappa + \cdots,\end{aligned} \tag{1.3}$$

such that

$$y(t) = \exp[\sigma(t)]y_0, \qquad t \geq 0. \tag{1.4}$$

Magnus neither proves convergence (to quote from [16, Theorem III], "if certain unspecified conditions of convergence are satisfied, ...") nor derives the general form of the expansion (1.3). Both tasks – and more – will be accomplished in the sequel. However, his conceptual contribution, building upon an earlier work of Feynman, Friedrichs and Zassenhaus (cf. [16] for detailed references), is crucial and it motivates our name, *Magnus series,* for the general form of the expansion (1.3). We note in passing that all the operations in (1.3) (integration, commutation and linear combination) respect the Lie algebra. Therefore, by virtue of (1.4), the solution $y(t)$ lies in the Lie group for every $t \geq 0$. This has been already observed by Magnus.

Our second point of departure is the method of *iterated commutators,* which has been originally published by the first author [12]. (Elements of this approach, in a non-numerical setting, have been introduced earlier by Fer [9].) We let $y_0 = y$ and $a_0 = a$ and set

$$a_{m+1}(t) := \sum_{k=1}^{\infty} \frac{k}{(k+1)!} \mathrm{ad}^k \left(a_m(t), \int_0^t a_m(\kappa)\mathrm{d}\kappa \right), \qquad m \in \mathbb{Z}^+, \tag{1.5}$$

where

$$\mathrm{ad}^k(p,q) := \begin{cases} p, & k = 0, \\ [\mathrm{ad}^{k-1}(p,q), q], & k \in \mathbb{N}. \end{cases} \tag{1.6}$$

It is proved in [12] that

$$a_m(t) = \mathcal{O}\left(t^{2^{m+1}-2}\right), \qquad t \to 0,$$

therefore

$$y_{[m]}(t) := \exp\left[\int_0^t a_0(\kappa)\mathrm{d}\kappa\right] \exp\left[\int_0^t a_1(\kappa)\mathrm{d}\kappa\right] \cdots \exp\left[\int_0^t a_m(\kappa)\mathrm{d}\kappa\right] y_0$$

approximates the solution y of (1.1) to order $2^{m+1} - 2$. Judiciously truncating the expansion (1.5) and replacing integrals by quadrature formulae, this becomes the basis for an effective numerical method.

Note that, according to (1.5), if a_m lies in a Lie algebra, then so does a_{m+1}. Therefore $y_{[m]}$ remains in the Lie group. It is fair to mention that the purpose of [12] was the numerical calculation of the fundamental solution of a linear system of ordinary differential equations and Lie groups are not even mentioned in that publication. The connection between iterated commutators and Lie-group theory was noted by Casas [5] and Zanna [23]. It is interesting to mention the origins of the method of iterated commutators in the classical technique of *Lie reduction* [24].

The plan of this paper is as follows. In section 2 we introduce the method of Magnus series and demonstrate that, by indexing the terms in the expansion with a subset of binary trees, it is possible to derive explicit recurrence relations, as well as a convergence proof.

An implementation of Magnus series to a computational end entails an approximate quadrature of possibly large number of multivariate integrals. This is already demonstrated by the expansion (1.3). As is well known, multivariate quadrature is computationally intensive [7], hence presenting a major obstacle toward any numerical application of our theoretical construct. Fortunately, it is possible to reduce the cost of computation very significantly indeed by paying attention to the special form of integrands and domains of integration. As a matter of fact, the cost in function evaluations reduces to that of a single, univariate quadrature! Section 3 is concerned with numerical quadrature of multivariate integrals within the context of Magnus series.

Another important saving in a numerical implementation of Magnus series is the reduction in the number of commutators, which, in tandem with function evaluations and exponentiation, is the main contributor to the computational cost of the algorithm. The number of commutators can be overwhelmingly reduced by two devices. Firstly, subjected to our quadrature formulae, different integrals require the evaluation of the same commutators. This can be completely described by exploiting our graph-theoretical interpretation of expansion coefficients. Secondly, the Jacobi identity (1.2) allows the replacement of certain terms within quadrature formulae by linear combinations of other terms. This procedure can be quantified exactly by combinatorial theory [20]. A helpful way to rephrase our results is by observing that our quadrature formulae project the solution into a relatively low-dimensional subspace of the Lie algebra. The reduction in the number of commutators is the theme of Section 4.

We have already mentioned the method of iterated commutators, which provides an alternative representation of the solution of (1.1) in a Lie group. In a sense, Magnus series and iterated commutators stand for diametrically opposed approaches: the first represents the solution as a single exponential with a 'complicated' argument and the second yields $y(t)$ as an infinite product of exponentials with simple arguments. In Section 5 we demonstrate that these approaches can be combined.

Finally, we devote Section 6 to a number of numerical examples that demonstrate that our approach works and that, indeed, it offers an avenue toward competitive computational methods. Detailed complexity analysis of different combinations of Magnus series and iterated commutators will be published elsewhere by the present authors.

Section 6 is also concerned with concluding remarks and a brief discussion of the ramifications of Magnus series and of the advantages and obstacles in their numerical implementation.

We wish to conclude this introductory section by acknowledging very helpful discussions with a number of colleagues. Particular thanks are due to Brad Baxter, Hermann Brunner, Yunkang Liu, Per-Christian Moan, Robert Mclachlan, Hans Munthe-Kaas, Malcolm Sabin and Antonella Zanna.

2 Magnus series and binary trees

We wish to represent the solution of (1.1) in the form (1.4). To this end we note the following classical theorems of Hausdorff. Although their proofs are neither new nor particularly complicated, we include them for the sake of completeness. For simplicity's sake, the proof of Theorem 1 is given for the case of a matrix Lie group, whereby $\exp\sigma$ becomes the standard exponential function.

Theorem 1 [11] *The function σ is the solution of the differential equation*

$$\sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{(\ell+1)!} \mathrm{ad}^\ell(\sigma', \sigma) = a, \quad t \geq 0, \qquad \sigma(0) = 0. \tag{2.1}$$

Proof Letting (1.4) in (1.1), we deduce at once that

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{e}^{\sigma(t)}\right) \mathrm{e}^{-\sigma(t)} = a, \qquad t \geq 0,$$

and $\sigma(0) = 0$. But, expanding into series and changing the order of summation,

$$\begin{aligned}\left(\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{e}^{\sigma(t)}\right) \mathrm{e}^{-\sigma(t)} &= \left(\sum_{k=1}^{\infty} \frac{1}{k!} \sum_{j=1}^{k} \sigma^{j-1} \sigma' \sigma^{k-j}\right) \times \left[\sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{\ell!} \sigma^\ell\right] \\ &= \sum_{\ell=1}^{\infty} \frac{(-1)^\ell}{\ell!} \sum_{j=1}^{\ell} \left[\sum_{k=j}^{\ell} (-1)^k \binom{\ell}{k}\right] \sigma^{j-1} \sigma' \sigma^{\ell-j}.\end{aligned}$$

It is trivial to prove by induction that

$$\sum_{k=j}^{\ell} (-1)^k \binom{\ell}{k} = (-1)^j \binom{\ell-1}{j-1}, \qquad 1 \leq j \leq \ell,$$

therefore

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{e}^{\sigma(t)}\right) \mathrm{e}^{-\sigma(t)} = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{(\ell+1)!} \sum_{j=0}^{\ell} (-1)^j \binom{\ell}{j} \sigma^j \sigma' \sigma^{\ell-j}.$$

The proof is complete since an easy induction affirms the identity

$$\mathrm{ad}^\ell(p, q) = \sum_{j=0}^{\ell} (-1)^j \binom{\ell}{j} p^j q p^{\ell-j}, \qquad p, q \in \mathfrak{g}, \quad \ell \in \mathbb{Z}^+.$$

□

Theorem 2 [11] *Let $d_0 \neq 0$ and*

$$d(z) = \sum_{\ell=0}^{\infty} d_\ell z^\ell, \qquad z \in \mathbb{C},$$

be a given function, analytic in a proper neighbourhood of the origin. Then there exists $t^* > 0$ such that the solution of the equation

$$\sum_{\ell=0}^{\infty} d_\ell \mathrm{ad}^\ell(\sigma', \sigma) = a, \quad 0 \leq t \leq t^*, \qquad \sigma(0) = 0, \tag{2.2}$$

is the same as that of

$$\sigma' = \sum_{m=0}^{\infty} f_m \mathrm{ad}^m(a,\sigma), \quad 0 \le t \le t^*, \qquad \sigma(0) = 0, \tag{2.3}$$

where

$$f(z) := \sum_{m=0}^{\infty} f_m z^m = \frac{1}{d(z)}, \qquad z \in \mathbb{C}.$$

Proof Let σ be the solution of (2.3). We wish to demonstrate that it is also the solution of (2.2). It is a trivial consequence of (1.6) that

$$\mathrm{ad}^{\ell-m}(\mathrm{ad}^m(p,q)) = \mathrm{ad}^{\ell}(p,q), \qquad 0 \le m \le \ell,$$

hence it follows by substituting σ' on the left-hand side of (2.2) that

$$\begin{aligned} \sum_{\ell=0}^{\infty} d_\ell \mathrm{ad}^\ell(\sigma',\sigma) &= \sum_{\ell=0}^{\infty} d_\ell \mathrm{ad}^\ell \left(\sum_{m=0}^{\infty} f_m \mathrm{ad}^m(a,\sigma), \sigma \right) \\ &= \sum_{m=0}^{\infty} \sum_{\ell=k}^{\infty} d_{\ell-m} f_m \mathrm{ad}^{\ell-m}(\mathrm{ad}^m(a,\sigma),\sigma) \\ &= \sum_{\ell=0}^{\infty} \left(\sum_{m=0}^{\ell} f_m d_{\ell-m} \right) \mathrm{ad}^\ell(a,\sigma). \end{aligned}$$

Since f is the reciprocal of d, it is true that

$$\sum_{m=0}^{\ell} f_m d_{\ell-m} = \begin{cases} 1, & \ell = 0, \\ 0, & \ell \in \mathbb{N}, \end{cases}$$

consequently

$$\sum_{\ell=0}^{\infty} d_\ell \mathrm{ad}^\ell(\sigma',\sigma) = a$$

and we recover (2.2). □

In the case of (2.1), we have

$$d(z) = \frac{1 - \mathrm{e}^{-z}}{z}.$$

Mindful of the identity

$$\frac{z}{\mathrm{e}^z - 1} = \sum_{m=0}^{\infty} \frac{B_m}{m!} z^m,$$

where $\{B_m\}_{m \in \mathbb{Z}^+}$ are *Bernoulli numbers* [1, p. 804], we deduce that

$$f(z) = \frac{z}{1 - \mathrm{e}^{-z}} = \frac{z}{\mathrm{e}^z - 1} + z,$$

therefore

$$f(z)=\sum_{m=0}^{\infty}\frac{B_m}{m!}z^m+z=1+\tfrac{1}{2}z+\tfrac{1}{12}z^2-\tfrac{1}{720}z^4+\tfrac{1}{30240}z^6-\tfrac{1}{1209600}z^8+\cdots. \tag{2.4}$$

Note that $B_{2m+1}=0$ for $m\in\mathbb{N}$.

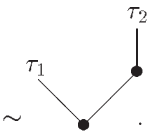
In the sequel we address ourselves to expansions of the general equation (2.3). Whenever necessary, the coefficients $\{f_m\}_{m\in\mathbb{Z}^+}$ may be substituted in line with (2.4) but, as a rule, the more general treatment leads to a more transparent and uncluttered exposition. We note in passing that, as long as $a(t)\in\mathfrak{g}$, $t\geq 0$, it is true that $\sigma(t)\in\mathfrak{g}$, $t\geq 0$. Perhaps the easiest proof follows readily from (2.3) by applying the method of proof of the Picard–Lindölef theorem and noting that the Lie algebra $\mathfrak{g}$ is closed with respect to the operations of integration, commutation and linear combination.

Let us examine the Magnus series (1.3). Following its inner logic, we search for a general expansion of the *Lie-algebraic differential equation* (2.3) in terms that are formed by multiple integrations and commutations. Let $\mathscr{E}$ be the set of the derivatives of all the terms in the expansion. We propose the following two *composition rules* which recursively define $\mathscr{E}$:

1. $a(t)\in\mathscr{E}$;
2. If $p(t),q(t)\in\mathscr{E}$ then $[p(t),\int_0^t q(\kappa)\mathrm{d}\kappa]\in\mathscr{E}$.

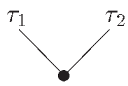
It is an easy exercise to verify that the first few terms in (1.3) are recovered with our two composition rules. More general analysis, however, is greatly assisted by identifying the terms in $\mathscr{E}$ with a subset of planar binary trees. We refer to [10] for basic concepts of graph theory.

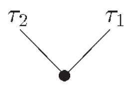
We associate the function a with the trivial tree of order one, consisting of a single vertex. Moreover, given that $p(t),q(t)\in\mathscr{E}$ are associated with the planar binary trees τ_1,τ_2 respectively (a relationship that we express as $p\sim\tau_1$, $q\sim\tau_2$), we associate

$[p(t),\int_0^t q(\kappa)\mathrm{d}\kappa]\sim$  .

In other words, integration corresponds to appending a new root to a tree (thereby increasing its order by one), while commutation corresponds to joining two trees with a single root.

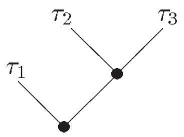
Note that the antisymmetry of the commutator implies that



$+$


$=0,$

while the Jacobi identity (1.2) can be recast in a graph-theoretic form as



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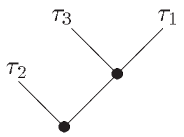

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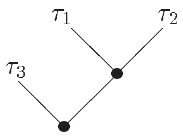
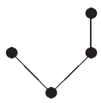
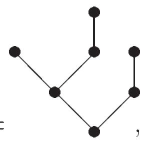
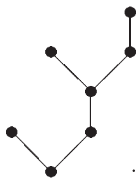


$=0.$ (2.5)

Although of no immediate interest in this section, the Jacobi identity is critical to successful implementation of the computational procedure of this paper. Its significance will become clear in Section 4.

The terms in (1.3) can be readily associated with binary trees and this helps in visualising this relationship. It is helpful, as a notational convention and in line with the definition of $\mathscr{E}$, to consider σ', i.e. to 'strip' the outer integral in each term, since this somewhat simplifies the notation. Thus,

$a \sim \omega_0 =$ $\qquad [a, \int_0^t a] \sim \omega_1 =$  ,

$[[a, \int_0^t a], \int_0^t a] \sim \omega_2 =$  , $\qquad [a, \int_0^t [a, \int_0^\kappa a]] \sim \omega_3 =$  .

Note that, while ω_2 follows from a combination of ω_1 with ω_0, ω_3 is obtained by combining ω_0 with ω_1. Anticipating notation in the sequel. we denote this in the form

$$\omega_2 = \mathscr{R}(\omega_1, \omega_0), \qquad \omega_3 = \mathscr{R}(\omega_0, \omega_1).$$

Of course, such combinations are *not* commutative.

In general, we seek an expansion of the form

$$\sigma(t) = \sum_{k=1}^{\infty} \sum_{\tau \in \mathscr{T}_k} \alpha_\tau \int_0^t H_\tau(\kappa) \mathrm{d}\kappa, \tag{2.6}$$

where $\mathscr{T}_k$ is the set of all binary trees of order k (that is, with k vertices) which correspond to terms H_τ that can be obtained by means of our two composition rules. Thus, for example, $\mathscr{T}_1 = \{\omega_0\}$, $\mathscr{T}_4 = \{\omega_1\}$, $\mathscr{T}_7 = \{\omega_2, \omega_3\}$ and $\mathscr{T}_m = \emptyset$ for $m = 2, 3, 5, 6$. The coefficients α_τ depend solely on the sequence $\{f_\ell\}_{\ell \in \mathbb{Z}^+}$. As a tribute to Wilhelm Magnus, whose pioneering work [16] inspired our analysis, we henceforth call (2.6) the *Magnus series* of σ. Note that $H_\tau(t) \in \mathfrak{g}$ for all $\tau \in \mathscr{T}_k$, $k \in \mathbb{Z}^+$, implies $\sigma(t) \in \mathfrak{g}$, therefore $\exp[\sigma(t)] \in G$, provided that (2.6) converges.

Let

$$U_m = \mathrm{ad}^m \left(a, \sum_{k=1}^{\infty} \sum_{\tau \in \mathscr{T}_k} \alpha_\tau \int_0^t H_\tau \right), \qquad m \in \mathbb{Z}^+,$$

therefore, according to (2.3),

$$\sigma' = \sum_{m=0}^{\infty} f_m U_m. \tag{2.7}$$

It follows at once from (1.6) that for every $m \in \mathbb{N}$

$$U_m = \left[\mathrm{ad}^{m-1} \left(a, \sum_{k=1}^{\infty} \sum_{\tau \in \mathscr{T}_k} \alpha_\tau \int_0^t H_\tau \right), \sum_{k=1}^{\infty} \sum_{\tau \in \mathscr{T}_k} \alpha_\tau \int_0^t H_\tau \right]$$

$$= \left[U_{m-1}, \sum_{k=1}^{\infty} \sum_{\tau \in \mathscr{T}_k} \alpha_\tau \int_0^t H_\tau \right]$$

$$= \sum_{k=1}^{\infty} \sum_{\tau \in \mathscr{T}_k} \alpha_\tau [U_{m-1}, \textstyle\int_0^t H_\tau]. \tag{2.8}$$

Because of the second composition rule, it follows at once by induction that for every H_τ there exists terms $H_{\tau_1}, H_{\tau_2}, \ldots, H_{\tau_r}$, say, such that

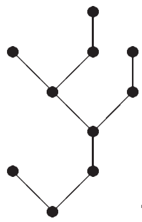
$$H_\tau := R(\tau_1, \tau_2, \ldots, \tau_r) = [\cdots[[a, \textstyle\int H_{\tau_1}], \int H_{\tau_2}], \ldots, \int H_{\tau_r}]. \tag{2.9}$$

Proposition 3 *For every $m \in \mathbb{N}$ it is true that*

$$U_m = \sum_{k_1=1}^{\infty} \sum_{k_2=1}^{\infty} \cdots \sum_{k_m=1}^{\infty} \sum_{\tau_1 \in \mathscr{T}_1} \sum_{\tau_2 \in \mathscr{T}_2} \cdots \sum_{\tau_m \in \mathscr{T}_m} \alpha_{\tau_1} \alpha_{\tau_2} \cdots \alpha_{\tau_m} R(\tau_1, \tau_2, \ldots, \tau_m) \tag{2.10}$$

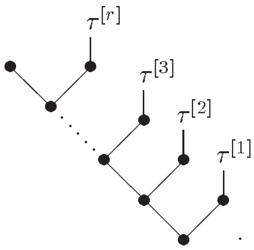
Proof By induction on (2.8). □

We denote the binary tree corresponding to $R(\tau_1, \tau_2, \ldots, \tau_r)$ by $\mathscr{R}(\tau_1, \tau_2, \ldots, \tau_r)$. This representation is not unique, e.g.



$$\sim \mathscr{R}(\omega_1, \omega_0) = \mathscr{R}(\omega_2).$$

To ensure uniqueness we choose $\tau_1, \tau_2, \ldots, \tau_r$ as follows. Every binary tree τ which can be obtained from our composition rules can be uniquely written in the form



Then $\tau = \mathscr{R}(\tau^{[r]}, \tau^{[r-1]}, \ldots, \tau^{[1]})$ and this is the representation that we adopt in the sequel. In particular, in the last example we obtain $\mathscr{R}(\omega_2)$.

Proposition 4 *Given any $r \in \mathbb{N}$ and $\tau_k \in \mathscr{T}_{m_k}$, $k = 1, 2, \ldots, r$, it is true that*

$$\operatorname{ord} \mathscr{R}(\tau_1, \tau_2, \ldots, \tau_r) = \sum_{k=1}^{r} m_k + 2r + 1, \tag{2.11}$$

where $\operatorname{ord} \tau$ *is the order (i.e., the number of vertices) of the tree τ.*

Proof It follows from the definition of $\mathscr{R}$ that

$$\operatorname{ord}\mathscr{R}(\tau_1,\tau_2,\ldots,\tau_r)=\operatorname{ord}\mathscr{R}(\tau_1,\tau_2,\ldots,\tau_{r-1})+m_r+2.$$

The proof of (2.11) follows from this identity by straightforward induction. □

Corollary $\mathscr{T}_k=\emptyset$ *whenever* $k\neq 1 \bmod 3$.

Proof We prove by induction that all the trees allowed by our composition rules have order 1 mod 3. Clearly, $\operatorname{ord}\omega_0=1$. Assuming that $m_k=3\ell_k+1$, $k=1,2,\ldots,r$, we deduce from (2.11) that

$$\operatorname{ord}\mathscr{R}(\tau_1,\tau_2,\ldots,\tau_r)=3\left(\sum_{k=1}^{r}\ell_k+1\right)+1.$$

Hence our assertion is true. □

Substitution of (2.10) in (2.7) and comparison of terms corresponding to order-k trees yield

$$\sum_{\tau\in\mathscr{T}_k}\alpha_\tau H_\tau=\sum_{\ell=1}^{\lfloor (k-1)/2\rfloor} f_\ell \sum_{\substack{n_1,n_2,\ldots,n_\ell\in\mathbb{N}\\ n_1+\cdots+n_\ell=n-2\ell-1}}\;\sum_{\substack{\tau_i\in\mathscr{T}_i\\ i=1,2,\ldots,\ell}}\alpha_{\tau_1}\alpha_{\tau_2}\cdots\alpha_{\tau_\ell}R(\tau_1,\tau_2,\ldots,\tau_\ell)$$

for every $k\in\mathbb{N}$. This identity simplifies by virtue of the corollary to Proposition 4, since we need to consider only trees of order 1 mod 3,

$$\sum_{\tau\in\mathscr{T}_{3m+1}}\alpha_\tau H_\tau=\sum_{\ell=1}^{\lfloor 3m/2\rfloor} f_\ell \sum_{\substack{n_1,n_2,\ldots,n_\ell\in\mathbb{Z}^+\\ n_1+\cdots+n_\ell=m-\ell}}\;\sum_{\substack{\tau_i\in\mathscr{T}_{3n_i+1}\\ i=1,2,\ldots,\ell}}\alpha_{\tau_1}\alpha_{\tau_2}\cdots\alpha_{\tau_\ell}R(\tau_1,\tau_2,\ldots,\tau_\ell). \tag{2.12}$$

Comparing the left- and the right-hand sides of (2.12), we deduce that

$$\begin{aligned}\mathscr{T}_{3m+1}=\{\mathscr{R}(\tau_1,\tau_2,\ldots,\tau_\ell)\,:\,\tau_i\in\mathscr{T}_{3n_i+1},\ i=1,2,\ldots,\ell,\\ n_1+n_2+\cdots+n_\ell+\ell=m,\ \ell=1,2,\ldots,\lfloor\tfrac{3m}{2}\rfloor\}.\end{aligned} \tag{2.13}$$

Another consequence of (2.12) is that the coefficients α_τ can be evaluated recursively,

$$\begin{aligned}\alpha_{\omega_0}&=f_0,\\ \alpha_{\mathscr{R}(\tau_1,\ldots,\tau_\ell)}&=f_\ell\prod_{i=1}^{\ell}\alpha_{\tau_i}.\end{aligned} \tag{2.14}$$

Table 1 displays all the expansion terms, trees and coefficients of order up to ten.

Assisted by Table 1, we present the first few terms of the Magnus expansion for the equation (2.3):

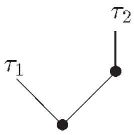
$$\sigma(t)=f_0\int_0^t a(\kappa)\,\mathrm{d}\kappa+f_0f_1\int_0^t\!\!\int_0^\kappa [a(\kappa),a(\xi)]\,\mathrm{d}\xi\,\mathrm{d}\kappa$$

$$
\begin{aligned}
&+ f_0^2 f_2 \int_0^t \int_0^\kappa \int_0^\kappa [[a(\kappa), a(\xi)], a(\eta)] \, \mathrm{d}\eta \, \mathrm{d}\xi \, \mathrm{d}\kappa \\
&+ f_0 f_1^2 \int_0^t \int_0^\kappa \int_0^\xi [a(\kappa), [a(\xi), a(\eta)]] \, \mathrm{d}\eta \, \mathrm{d}\xi \, \mathrm{d}\kappa \\
&+ f_0^2 f_1 f_2 \int_0^t \int_0^\kappa \int_0^\xi \int_0^\xi [a(\kappa), [[a(\xi), a(\eta)], a(\rho)]] \, \mathrm{d}\rho \, \mathrm{d}\eta \, \mathrm{d}\xi \, \mathrm{d}\kappa \\
&+ f_0 f_1^3 \int_0^t \int_0^\kappa \int_0^\xi \int_0^\eta [a(\kappa), [a(\xi), [a(\eta), a(\rho)]]] \, \mathrm{d}\rho \, \mathrm{d}\eta \, \mathrm{d}\xi \, \mathrm{d}\kappa \qquad (2.15) \\
&+ f_0^2 f_1 f_2 \int_0^t \int_0^\kappa \int_0^\xi \int_0^\kappa [[a(\kappa), [a(\xi), a(\eta)]], a(\rho)] \, \mathrm{d}\rho \, \mathrm{d}\eta \, \mathrm{d}\xi \, \mathrm{d}\kappa \\
&+ f_0^2 f_1 f_2 \int_0^t \int_0^\kappa \int_0^\kappa \int_0^\eta [[a(\kappa), a(\xi)], [a(\eta), a(\rho)]] \, \mathrm{d}\rho \, \mathrm{d}\eta \, \mathrm{d}\xi \, \mathrm{d}\kappa \\
&+ f_0^3 f_3 \int_0^t \int_0^\kappa \int_0^\kappa \int_0^\kappa [[[a(\kappa), a(\xi)], a(\eta)], a(\rho)] \, \mathrm{d}\rho \, \mathrm{d}\eta \, \mathrm{d}\xi \, \mathrm{d}\kappa + \cdots
\end{aligned}
$$

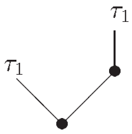
The original expansion (1.3) of Magnus [16] is readily recovered by using the values of $\{f_m\}$ from (2.4).

The order of magnitude of the elements in (2.4) is of interest, in particular whenever we wish to approximate y by truncating the series. Let us suppose that $a(t) = \mathcal{O}(t^\lambda)$, where $\lambda \in \mathbb{Z}^+$. Insofar as the present discussion is concerned, the reader might just as well assume that $\lambda = 0$ but the more general case will be useful in Section 5. We define the function β_τ as the least integer such that $H_\tau(t) = \mathcal{O}(t^{\beta_\tau})$, where H_τ is an expansion term corresponding to the tree τ. Therefore

1. $\beta_{\omega_0} = \lambda$;
2. $\beta_\tau \geq \beta_{\tau_1} + \beta_{\tau_2} + 1$, where

$\tau =$  (2.16)

3. $\beta_\tau \geq 2\beta_{\tau_1} + 2$, where

$\tau =$  (2.17)

In other words, $\tau_1 = \tau_2$ in (2.16) results in a larger exponent.

While 1 and 2 are trivial, the proof of 3 follows at once by letting $H_\tau = pt^{\beta_\tau} + \mathcal{O}(t^{\beta_\tau + 1})$, whereby

$$
[H_\tau, \textstyle\int H_\tau] = \left[pt^{\beta_\tau} + \mathcal{O}(t^{\beta_\tau+1}), \frac{1}{\beta_\tau + 1} pt^{\beta_\tau+1} + \mathcal{O}(t^{\beta_\tau+2}) \right] = \mathcal{O}(t^{2\beta_\tau+2}).
$$

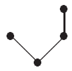
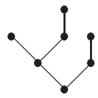
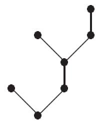
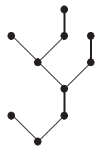
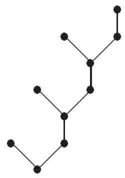
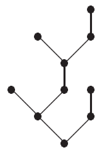
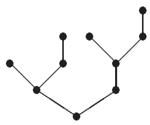
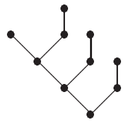
Order	Name	Expression	Tree	Representation	Coefficient
1	ω_0	a	$\bullet$	–	f_0
4	ω_1	$[a, \int a]$		$\mathscr{R}(\omega_0)$	$f_0 f_1$
7	ω_2	$[[a, \int a], \int a]$		$\mathscr{R}(\omega_0, \omega_0)$	$f_0^2 f_2$
	ω_3	$[a, \int [a, \int a]]$		$\mathscr{R}(\omega_1)$	$f_0 f_1^2$
10	ω_4	$[a, \int [[a, \int a], \int a]]$		$\mathscr{R}(\omega_2)$	$f_0^2 f_1 f_2$
	ω_5	$[a, \int [a, \int [a, \int a]]]$		$\mathscr{R}(\omega_3)$	$f_0 f_1^3$
	ω_6	$[[a, \int [a, \int a]], \int a]$		$\mathscr{R}(\omega_1, \omega_0)$	$f_0^2 f_1 f_2$
	ω_7	$[[a, \int a], \int [a, \int a]]$		$\mathscr{R}(\omega_0, \omega_1)$	$f_0^2 f_1 f_2$
	ω_8	$[[[a, \int a], \int a], \int a]$		$\mathscr{R}(\omega_0, \omega_0, \omega_0)$	$f_0^3 f_3$

Table 1: Expansion terms H_τ corresponding to trees τ of order ≤ 10, their representations $\mathcal{G}$ and coefficients α_τ.

Proposition 5 *For every $\tau \in \mathscr{T}_{3k+1}$, $k \in \mathbb{N}$, it is true that*

$$\beta_\tau \geq (k+1)(\lambda+1). \tag{2.18}$$

Proof By induction. We commence by observing that, according to 3, $\beta_{\omega_1} \geq 2(\lambda+1)$, consistently with (2.18). Next, suppose that $\tau \in \mathscr{T}_{3k+1}$, $k \geq 2$, is derived from τ_1 and τ_2 in line with (2.16). Then $\tau_1 \in \mathscr{T}_{3\ell+1}$, $\tau_2 \in \mathscr{T}_{3(k-\ell-1)+1}$ for some $\ell \in \{0, 1, \ldots, k-1\}$. Note that it is impossible for *both* $\tau_1 = \omega_0$ and $\tau_2 = \omega_0$.

If $\tau_2 = \omega_0$ then $\ell = k-1$ and, by induction, $\beta_{\tau_1} \geq (\ell+1)(\lambda+1)$. Therefore, according to 1 and 2,

$$\beta_\tau \geq \lambda + k(\lambda+1) + 1 = (k+1)(\lambda+1).$$

An identical argument affirms (2.18) when $\tau_1 = \omega_0$. Finally, if $\tau_1, \tau_2 \neq \omega_0$ then $\ell \in \{1, 2, \ldots, k-2\}$. Hence, by induction and 2,

$$\beta_{\tau_1} \geq (\ell+1)(\lambda+1), \quad \beta_{\tau_2} \geq (k-\ell)(\lambda+1) \qquad \Rightarrow \qquad \beta_\tau \geq (k+1)(\lambda+1)+1,$$

actually in excess of the lower bound (2.18). □

It is often possible to obtain better estimates than (2.18). Thus, for example, $\beta_{\omega_7} \geq 4\lambda+6$, because of 3, while $\tau_1 = \omega_1$, $\tau_2 = \omega_3$, composed with (2.16), yields $k=4$ and $\beta_\tau \geq 5\lambda+6$. However, the lower bound (2.18) is the best possible insofar as the totality of all the nontrivial trees is concerned.

The following theorem, critical to truncating Magnus series as a means to approximate the solution of (1.1), follows at once from our analysis.

Theorem 6 *Let $a(t) = \mathcal{O}(t^\lambda)$, $p \in \mathbb{N}$ and set*

$$\sigma_p(t) := \sum_{k=0}^{p-1} \sum_{\tau \in \mathscr{T}_{3k+1}} \alpha_\tau \int_0^t H_\tau(\kappa) \mathrm{d}\kappa. \tag{2.19}$$

Then $\sigma_p(t) = \sigma(t) + \mathcal{O}(t^{(p+1)(\lambda+1)+1})$, therefore $\exp \sigma_p(t) = y(t) + \mathcal{O}(t^{(p+1)(\lambda+1)+1})$.

Needless to say, as things stand, (2.15) is a purely formal construct, since we have not proved yet that a Magnus expansion converges. This is our next task.

Let us assume that $\mathfrak{g}$ is equipped with a norm $\|\cdot\|$ (as long as G is a matrix Lie group, $\|\cdot\|$ might be taken, for example, as the standard matrix Euclidean norm) and that there exist $\rho, t^* > 0$ such that

$$\|a(t)\| \leq \rho t^\lambda, \qquad 0 \leq t \leq t^*.$$

Proposition 7 *For every $\tau \in \mathscr{T}_{3k+1}$ it is true that*

$$\|H_\tau(t)\| \leq \rho t^\lambda \left(\frac{2\rho t^{\lambda+1}}{\lambda+1}\right)^k. \tag{2.20}$$

Proof By induction. The bound (2.20) is certainly true for $k=0$. Suppose that $k \in \mathbb{N}$ and that τ has been obtained from $\tau_1 \in \mathscr{T}_{3\ell+1}$ and $\tau_2 \in \mathscr{T}_{3(k-\ell-1)+1}$ by means of the composition rule (2.16). Then, by the induction assumption,

$$\begin{aligned}\|H_\tau(t)\| &= \|[H_{\tau_1}(t), \textstyle\int_0^t H_{\tau_2}(\kappa)\mathrm{d}\kappa]\| \le 2\|H_{\tau_1}(t)\| \displaystyle\int_0^t \|H_{\tau_2}(\kappa)\|\mathrm{d}\kappa \\ &\le 2\rho t^\lambda \left(\frac{2\rho t^{\lambda+1}}{\lambda+1}\right)^\ell \times \frac{\rho t^{\lambda+1}}{(k-\ell)(\lambda+1)} \left(\frac{2\rho t^{\lambda+1}}{\lambda+1}\right)^{k-\ell-1} \\ &\le \rho t^\lambda \left(\frac{2\rho t^{\lambda+1}}{\lambda+1}\right)^k,\end{aligned}$$

because $\ell \in \{0,1,\ldots,k-1\}$. □

Substituting (2.20) into the Magnus series, we deduce from the triangle inequality that

$$\begin{aligned}\|\sigma(t)\| &\le \tfrac{1}{2}\sum_{k=0}^\infty \frac{\theta_k}{k+1}\left(\frac{2\rho t^{\lambda+1}}{\lambda+1}\right)^{k+1} \\ &= \tfrac{1}{2}\int_0^{2\rho t^{\lambda+1}/(\lambda+1)} \Theta(z)\mathrm{d}z, \qquad 0 \le t \le t^*,\end{aligned} \tag{2.21}$$

where θ_k is the number of terms in the set $\mathscr{T}_{3k+1}$, $k \in \mathbb{Z}^+$ and Θ is the generating function of the sequence $\{\theta_k\}_{k\in\mathbb{Z}^+}$,

$$\Theta(z) = \sum_{k=0}^\infty \theta_k z^k.$$

Counting the members of $\mathscr{T}_{3k+1}$ is a trivial exercise in graph theory. Yet, we include it here for the sake of completeness. Every element of $\mathscr{T}_{3k+1}$ is obtained uniquely from (2.16), where $\tau_1 \in \mathscr{T}_{3\ell+1}$ and $\tau_2 \in \mathscr{T}_{3(k-\ell-1)+1}$ for some $\ell \in \{0,1,\ldots,k-1\}$. Likewise, for every such ℓ, τ_1 and τ_2, the composition (2.16) produces an element of $\mathscr{T}_{3k+1}$. Therefore

$$\theta_k = \sum_{\ell=0}^{k-1}\theta_\ell\theta_{k-\ell-1}, \qquad k \in \mathbb{N}.$$

Since $\theta_0 = 1$, we deduce that

$$\Theta(z) = \sum_{k=0}^\infty \theta_k z^k = 1 + \sum_{k=1}^\infty\sum_{\ell=0}^{k-1}\theta_\ell\theta_{k-\ell-1}z^k = 1 + z[\Theta(z)]^2.$$

Therefore $\Theta(z)$ is a solution of the quadratic equation

$$z[\Theta(z)]^2 - \Theta(z) + 1 = 0$$

and analyticity at the origin implies that

$$\Theta(z) = \frac{1-\sqrt{1-4z}}{2z} = \sum_{k=0}^\infty \frac{(2k)!}{k!(k+1)!}z^k. \tag{2.22}$$

We deduce not just the explicit value of θ_k, $k \in \mathbb{Z}^+$, but also that Θ is analytic for all $|z| \leq \frac{1}{4}$.

Theorem 8 *The Magnus series converges for all*

$$0 \leq t \leq \min \left\{ t^*, \left(\frac{\lambda+1}{8\rho} \right)^{1/(\lambda+1)} \right\}.$$

Moreover, within this range of t the solution of (1.1) *obeys the inequality*

$$\|y(t)\| \leq \|y_0\| \exp \left[\frac{1}{2} \int_0^{8\rho t^{\lambda+1}/(\lambda+1)} \frac{1-\sqrt{1-z}}{z} \mathrm{d}z \right].$$

Proof Follows at once from our analysis and the upper bound (2.21). □

3 Numerical quadrature of multivariate integrals

The first step in the implementation of a Magnus expansion as a numerical procedure is a truncation of the series. In line with Theorem 6, if all terms corresponding to $\mathscr{T}_k$, $k \geq p$ are truncated, the outcome is a pth-order method (we substitute $\lambda = 0$ in (2.19)). Next, all the integrals are replaced by quadratures of a sufficiently high order and, finally, we need to evaluate an exponential of an element in the Lie algebra $\mathfrak{g}$.

On the face of it, the most computationally-expensive step is the replacement of integrals by quadrature formulae.[2] Multivariate numerical integration is typically very expensive [7] and we need to approximate a significant number of integrals, e.g. four integrals for order $p = 4$ and nine for order $p = 5$. Naively, each integral might be approximated by Gaussian quadrature optimized with respect to the (multivariate) domain of integration, for example

$$\int_0^h a(\kappa)\mathrm{d}\kappa = h \sum_{j=1}^{\nu_1} b_j a(c_j h),$$

$$\int_0^h \int_0^\kappa [a(\kappa), a(\xi)]\mathrm{d}\xi \, \mathrm{d}\kappa = h^2 \sum_{j=1}^{\nu_2} \tilde{b}_j [a(\tilde{c}_{j,1} h), a(\tilde{c}_{j,2} h)],$$

where $\{c_j : j = 1, 2, \ldots, \nu_1\}$ are Gaussian points in $[0,1]$, $\{(\tilde{c}_{j,1}, \tilde{c}_{j,2} : j = 1, 2, \ldots, \nu_2\}$ are Gaussian points in the triangle with vertices at $\{(0,0), (1,0), (0,1)\}$, while b_j and $\tilde{b}_j$ are appropriate weights. In that case, stipulating that both quadratures are of the same order of accuracy requires $\nu_2 = \mathcal{O}(\nu_1^2)$. Further integrals, across simplices of increasingly higher dimension, require even more function evaluations. Fortunately, the naive approach is completely unnecessary and, as we demonstrate in this section, the evaluation of *all* the necessary quadratures to order p can be accomplished in just $\lfloor (p+1)/2 \rfloor$ function evaluations.

[2] We do not address ourselves in this paper to the evaluation of the exponential function.

Given $\tau \in \mathscr{T}_{3m+1}$, we can write the integral of H_τ in the form

$$\begin{aligned} I(h) &:= \int_0^h H_\tau(t)\mathrm{d}t \\ &= \int_0^h \int_0^{\kappa_{i_0}} \int_0^{\kappa_{i_1}} \cdots \int_0^{\kappa_{i_{m-1}}} \mathscr{L}(a(\kappa_0), a(\kappa_1), \ldots, a(\kappa_m))\mathrm{d}\kappa_m\,\mathrm{d}\kappa_{m-1}\cdots\mathrm{d}\kappa_0, \end{aligned} \tag{3.1}$$

where

$$i_j \in \{0, 1, \ldots, j\}, \qquad j = 0, 1, \ldots, m-1$$

and

$$\mathscr{L}: \overbrace{\mathfrak{g} \times \mathfrak{g} \times \cdots \times \mathfrak{g}}^{m+1 \text{ times}} \to \mathfrak{g}$$

is a multilinear form. For example, (2.15) demonstrates that

$\tau = \omega_0$:	$\mathscr{L}(x_0) = x_0$;	
$\tau = \omega_1$:	$\mathscr{L}(x_0, x_1) = [x_0, x_1]$,	$i_0 = 0$;
$\tau = \omega_2$:	$\mathscr{L}(x_0, x_1, x_2) = [[x_0, x_1], x_2]$,	$i_0 = 0,\ i_1 = 0$;
$\tau = \omega_3$:	$\mathscr{L}(x_0, x_1, x_2) = [x_0, [x_1, x_2]]$,	$i_0 = 0,\ i_1 = 1$.

Let $c_1, c_2, \ldots, c_\nu$ be ν distinct points in the interval $[0, 1]$, where $\nu \in \mathbb{N}$ is given. We wish to approximate $\int_0^h H_\tau(t)\mathrm{d}t$ by the quadrature formula

$$I(h) \approx Q(h) := h^{m+1} \sum_{\boldsymbol{\ell} \in \Lambda_m^\nu} b_{\boldsymbol{\ell}} \mathscr{L}(a(c_{\ell_0}h), a(c_{\ell_1}h), \ldots, a(c_{\ell_m}h)), \tag{3.2}$$

where Λ_m^ν is the set of all the combinations $\boldsymbol{\ell} = (\ell_0, \ell_1, \ldots, \ell_m)$ of $(m+1)$-tuples of integers from the set $\{1, 2, \ldots, \nu\}$ and the weights $b_{\boldsymbol{\ell}}$ are given. Note that the implementation of (3.2) requires the evaluation of the function a at just ν points. Moreover, as long as we can use the same nodes $\boldsymbol{c} = (c_1, c_2, \ldots, c_\nu)$ for *all* the integrals, the entire evaluation of σ_p requires just ν function evaluations!

Let $u_j \in \mathbb{P}_{\nu-1}$ be the jth cardinal polynomial of Lagrange interpolation at the points $c_1, c_2, \ldots, c_\nu$,

$$u_j(t) = \prod_{\substack{i=1 \\ i \neq j}}^{\nu} \frac{t - c_i}{c_j - c_i}, \qquad j = 1, 2, \ldots, \nu.$$

We approximate a by its *Lagrange interpolation polynomial*

$$a(t) \approx \hat{a}(t) = \sum_{j=1}^{\nu} a(c_j h) u_j\left(\frac{t}{h}\right),$$

hence $\hat{a}(c_k h) = a(c_k h)$, $k = 1, 2, \ldots, \nu$, and define the weights $b_{\boldsymbol{\ell}}$ through the explicit formula

$$b_{\boldsymbol{\ell}} = \int_0^1 \int_0^{\kappa_{i_0}} \int_0^{\kappa_{i_1}} \cdots \int_0^{\kappa_{i_{m-1}}} \prod_{i=1}^{\nu} u_{\ell_i}(\kappa_i)\mathrm{d}\kappa_m\,\mathrm{d}\kappa_{m-1}\cdots\mathrm{d}\kappa_0, \qquad \boldsymbol{\ell} \in \Lambda_m^\nu. \tag{3.3}$$

Because of the multilinearity of $\mathscr{L}$, we have

$$\begin{aligned}
&\mathscr{L}(\hat{a}(\kappa_0), \hat{a}(\kappa_1), \ldots, \hat{a}(\kappa_m)) \\
&= \mathscr{L}\left(\sum_{\ell_0=1}^{\nu} u_{\ell_0}\left(\frac{\kappa_0}{h}\right) a(c_{\ell_0}h), \sum_{\ell_1=1}^{\nu} u_{\ell_1}\left(\frac{\kappa_1}{h}\right) a(c_{\ell_1}h), \ldots, \sum_{\ell_m=1}^{\nu} u_{\ell_m}\left(\frac{\kappa_m}{h}\right) a(c_{\ell_m}h)\right) \\
&= \sum_{\ell_0=1}^{\nu}\sum_{\ell_1=1}^{\nu}\cdots\sum_{\ell_m=1}^{\nu}\prod_{i=0}^{\nu} u_{\ell_i}\left(\frac{\kappa_i}{h}\right)\mathscr{L}(a(c_{\ell_0}h), a(c_{\ell_1}h), \ldots, a(c_{\ell_m}h)).
\end{aligned}$$

Therefore, with the above definition of $b_{\boldsymbol{\ell}}$,

$$Q(h) = \int_0^h \int_0^{\kappa_{i_0}} \int_0^{\kappa_{i_1}} \cdots \int_0^{\kappa_{i_{m-1}}} \mathscr{L}(\hat{a}(\kappa_0), \hat{a}(\kappa_1), \ldots, \hat{a}(\kappa_m)) \mathrm{d}\kappa_m \, \mathrm{d}\kappa_{m-1} \cdots \mathrm{d}\kappa_0. \quad (3.4)$$

The identity (3.4) provides both the *raison d'etre* for the definition (3.3) and a convenient means for an order analysis of the quadrature formula $Q(h)$.

Let

$$\mathscr{S} = \mathscr{S}_{\boldsymbol{i}} := \{(\kappa_0, \kappa_1, \ldots, \kappa_m) \in \mathbb{R}^{m+1} \ : \ 0 \le \kappa_j \le \kappa_{i_{j-1}}, \ j = 1, 2, \ldots, m\},$$

so that $h\mathscr{S}$ is the domain of integration in (3.1), and

$$\mathrm{d}\boldsymbol{\kappa} = \mathrm{d}\kappa_m \, \mathrm{d}\kappa_{m-1} \cdots \mathrm{d}\kappa_0,$$

therefore

$$\begin{aligned}
I(h) &= \int_{h\mathscr{S}} \mathscr{L}(a(\kappa_0), a(\kappa_1), \ldots, a(\kappa_m)) \mathrm{d}\boldsymbol{\kappa}, \\
Q(h) &= \int_{h\mathscr{S}} \mathscr{L}(\hat{a}(\kappa_0), \hat{a}(\kappa_1), \ldots, \hat{a}(\kappa_m)) \mathrm{d}\boldsymbol{\kappa}.
\end{aligned}$$

Given that

$$a(t) = \sum_{k=0}^{\infty} a_k t^{k+\lambda},$$

where $\lambda \in \mathbb{Z}^+$, and letting

$$\mathscr{L}_{\boldsymbol{k}} := \mathscr{L}(a_{k_0}, a_{k_1}, \ldots, a_{k_m}),$$

we thus deduce that

$$\begin{aligned}
I(h) &= \int_{h\mathscr{S}} \sum_{k_0=0}^{\infty}\sum_{k_1=0}^{\infty}\cdots\sum_{k_m=0}^{\infty} \mathscr{L}_{\boldsymbol{k}} \kappa_0^{k_0+\lambda} \kappa_1^{k_0+\lambda} \cdots \kappa_m^{k_m+\lambda} \mathrm{d}\boldsymbol{\kappa} \\
&= h^{(m+1)(\lambda+1)} \sum_{k_0=0}^{\infty}\sum_{k_1=0}^{\infty}\cdots\sum_{k_m=0}^{\infty} h^{k_0+k_1+\cdots+k_m} \mathscr{L}_{\boldsymbol{k}} \int_{\mathscr{S}} \kappa_0^{k_0+\lambda} \kappa_1^{k_0+\lambda} \cdots \kappa_m^{k_m+\lambda} \mathrm{d}\boldsymbol{\kappa} \\
&= h^{(m+1)(\lambda+1)} \sum_{k_0=0}^{\infty}\sum_{k_1=0}^{\infty}\cdots\sum_{k_m=0}^{\infty} h^{k_0+k_1+\cdots+k_m} \gamma_{\boldsymbol{k}} \mathscr{L}_{\boldsymbol{k}},
\end{aligned}$$

where

$$\gamma_{\boldsymbol{k}} = \int_{\mathscr{S}} \kappa_0^{k_0+\lambda} \kappa_1^{k_0+\lambda} \cdots \kappa_m^{k_m+\lambda} \mathrm{d}\boldsymbol{\kappa}, \qquad \boldsymbol{k} \in (\mathbb{Z}^+)^{m+1}. \tag{3.5}$$

Likewise, it follows from (3.2) that

$$\begin{aligned} Q(h) &= h^{m+1} \sum_{\boldsymbol{\ell} \in \Lambda_m^\nu} b_{\boldsymbol{\ell}} \sum_{k_0=0}^{\infty} \sum_{k_1=0}^{\infty} \cdots \sum_{k_m=0}^{\infty} \mathscr{L}_{\boldsymbol{k}} c_{\ell_0}^{k_0+\lambda} c_{\ell_1}^{k_1+\lambda} \cdots c_{\ell_m}^{k_m+\lambda} h^{k_0+k_1+\cdots+k_m+(m+1)\lambda} \\ &= h^{(m+1)(\lambda+1)} \sum_{k_0=0}^{\infty} \sum_{k_1=0}^{\infty} \cdots \sum_{k_m=0}^{\infty} h^{k_0+k_1+\cdots+k_m} \delta_{\boldsymbol{k}} \mathscr{L}_{\boldsymbol{k}}, \end{aligned}$$

where

$$\delta_{\boldsymbol{k}} = \sum_{\boldsymbol{\ell} \in \Lambda_m^\nu} b_{\boldsymbol{\ell}} c_{\ell_0}^{k_0+\lambda} c_{\ell_1}^{k_1+\lambda} \cdots c_{\ell_m}^{k_m+\lambda}, \qquad \boldsymbol{k} \in (\mathbb{Z}^+)^{m+1}. \tag{3.6}$$

Comparing (3.5) and (3.6), we deduce an order condition for the quadrature formula:

Proposition 9 *The quadrature method* (3.2) *is of order* $p \in \mathbb{N}$, *i.e.* $Q(h) = I(h) + \mathcal{O}(h^{p+1})$ *for all sufficiently smooth functions* a, *if and only if*

$$\delta_{\boldsymbol{k}} = \gamma_{\boldsymbol{k}}, \qquad \boldsymbol{k} \in (\mathbb{Z}^+)^{m+1}, \quad k_0 + k_1 + \cdots + k_m \le p - (m+1)(\lambda+1). \tag{3.7}$$

Letting

$$p_j(t) := \sum_{i=1}^{\nu} u_i(t) c_i^j, \qquad j \in \mathbb{Z}^+,$$

we can simplify (3.6) by substituting the definition (3.3) of $b_{\boldsymbol{\ell}}$. The outcome is

$$\delta_{\boldsymbol{k}} = \int_{\mathscr{S}} p_{k_0+\lambda}(\kappa_0) p_{k_1+\lambda}(\kappa_1) \cdots p_{k_m+\lambda}(\kappa_m) \mathrm{d}\boldsymbol{\kappa}, \qquad \boldsymbol{k} \in (\mathbb{Z}^+)^{m+1}. \tag{3.8}$$

It follows at once from the properties of Lagrange cardinal polynomials u_i that

$$p_j(t) = t^j + \omega(t) e_j(t), \qquad j \in \mathbb{Z}^+, \tag{3.9}$$

where

$$\omega(t) := \prod_{k=1}^{\nu} (t - c_k)$$

and $e_j \in \mathbb{P}_{j-\nu}$, the set of polynomials of degree $j - \nu$. (We let $\mathbb{P}_{j-\nu} = \{0\}$ for $j < \nu$.) Substituting (3.9) into (3.8), we obtain

$$\delta_{\boldsymbol{k}} = \int_{\mathscr{S}} \prod_{j=0}^{m} \left[\kappa_j^{k_j+\lambda} + \omega(\kappa_j) e_{k_j+\lambda}(\kappa_j) \right] \mathrm{d}\boldsymbol{\kappa}. \tag{3.10}$$

Altogether, we have 2^{m+1} terms in the integrand. One of these, namely

$$\kappa_0^{k_0+\lambda} \kappa_1^{k_1+\lambda} \cdots \kappa_m^{k_m+\lambda},$$

is precisely the integrand in (3.5). We wish to explore the conditions that ensure that all the remaining $2^{m+1}-1$ terms vanish.

Given such a term, $F(\kappa_0,\kappa_1,\ldots,\kappa_m)$, say, there exists an index $r\in\{0,1,\ldots,m\}$ such that

$$F(\kappa_0,\kappa_1,\ldots,\kappa_m)=\kappa_0^{k_0+\lambda}\kappa_1^{k_1+\lambda}\cdots\kappa_{r-1}^{k_{r-1}+\lambda}\omega(\kappa_r)e_{k_r+\lambda}(\kappa_r)\cdots.$$

Suppose that $r\geq 1$. In that case we execute $(r-1)$ exchanges of the order of integration so that κ_r is the last to be integrated. We commence by exchanging the order of κ_r and κ_{r-1}. The outcome is

$$\int_0^1\int_0^{\kappa_{i_0}}\cdots\int_0^{\kappa_{i_{r-3}}}\int_0^{\kappa_{i_{r-2}}}\int_{\psi_r}^{\chi_r}\int_0^{\kappa_{i_r}}\cdots\int_0^{\kappa_{i_{m-1}}}F(\kappa_0,\kappa_1,\ldots,\kappa_m)$$
$$\mathrm{d}\kappa_m\cdots\mathrm{d}\kappa_{r+1}\,\mathrm{d}\kappa_{r-1}\,\mathrm{d}\kappa_r\,\mathrm{d}\kappa_{r-2}\cdots\mathrm{d}\kappa_0,$$

where

$$(\psi_r,\chi_r)=\begin{cases}(\kappa_r,\kappa_{i_{r-2}}), & i_{r-1}=r-1,\\ (0,\kappa_{i_{r-1}}), & i_{r-1}\in\{0,1,\ldots,r-2\}.\end{cases}$$

Continuing in this manner, we arrive at

$$\int_0^1\int_{\psi_1}^{\chi_1}\int_{\psi_2}^{\chi_2}\cdots\int_{\psi_m}^{\chi_m}F(\kappa_0,\kappa_1,\ldots,\kappa_m)\,\mathrm{d}\kappa_m\cdots\mathrm{d}\kappa_{r+1}\,\mathrm{d}\kappa_{r-1}\cdots\mathrm{d}\kappa_0\,\mathrm{d}\kappa_r,$$

where

$$\psi_j,\chi_j\in\begin{cases}\{0,\kappa_r,\kappa_0,\kappa_1,\ldots,\kappa_{j-2}\}, & j=1,2,\ldots,r\\ \{0,\kappa_0,\kappa_1,\ldots,\kappa_{j-1},1\}, & j=r+1,\ldots,m.\end{cases}$$

Relabelling the variables, we deduce that

$$\int_{\mathscr{S}}F(\kappa_0,\kappa_1,\ldots,\kappa_m)\mathrm{d}\boldsymbol{\kappa}=\int_0^1\omega(\kappa_0)e_{k_r+\lambda}(\kappa_0)\int_{\mathscr{A}}K(\kappa_1,\kappa_2,\ldots,\kappa_m)\mathrm{d}\boldsymbol{\kappa},\qquad(3.11)$$

where

$$\begin{aligned}&\mathscr{A}=\{(\kappa_1,\kappa_2,\ldots,\kappa_m)\in\mathbb{R}^m\,:\,\psi_j\leq\kappa_j\leq\chi_j,\ j=1,2,\ldots,m\}\\ &\left.\begin{aligned}&\psi_j\in\{0,\kappa_0,\kappa_1,\ldots,\kappa_{j-1}\},\\ &\chi_j\in\{\kappa_0,\kappa_1,\ldots,\kappa_{j-1},1\},\end{aligned}\right\}\quad j=1,2,\ldots,m,\end{aligned}$$

and

$$K(\kappa_1,\kappa_2,\ldots,\kappa_m)=\prod_{j=1}^m\tilde{p}_j(\kappa_j).$$

Each $\tilde{p}_j(t)$ in the above definition is either $\omega(t)e_{\ell_j+\lambda}(t)$ or $t^{\ell_j+\lambda}$, where

$$\ell_j=\begin{cases}k_{j-1}, & j=1,2,\ldots,r,\\ k_j, & j=r+1,\ldots,m.\end{cases}$$

For example,

$$\begin{aligned}&\int_0^1\int_0^{\kappa_0}\int_0^{\kappa_1}\int_0^{\kappa_1}\kappa_0^{k_0+\lambda}\kappa_1^{k_1+\lambda}\kappa_2^{k_2+\lambda}\omega(\kappa_3)e_{k_3+\lambda}(\kappa_3)\mathrm{d}\kappa_3\,\mathrm{d}\kappa_2\,\mathrm{d}\kappa_1\,\mathrm{d}\kappa_0\\ =&\int_0^1\omega(\kappa_0)e_{k_3+\lambda}(\kappa_0)\int_{\kappa_0}^1\int_{\kappa_0}^{\kappa_1}\int_0^{\kappa_2}\kappa_1^{k_0+\lambda}\kappa_2^{k_1+\lambda}\kappa_3^{k_2+\lambda}\mathrm{d}\kappa_3\,\mathrm{d}\kappa_2\,\mathrm{d}\kappa_1\,\mathrm{d}\kappa_0,\end{aligned}$$

hence

$$(\psi_1,\chi_1)=(\kappa_0,1),\quad(\psi_2,\chi_2)=(\kappa_0,\kappa_1),\quad(\psi_3,\chi_3)=(0,\kappa_2)$$

and

$$\tilde{p}_j(t)=t^{k_j+\lambda},\qquad j=1,2,3.$$

Each $\tilde{p}_j$ is a polynomial of degree $\ell_j+\lambda$. Therefore, and bearing in mind the definition of (ψ_i,χ_i), $i=1,2,\ldots,m$, it follows at once by induction that

$$\begin{aligned}&\tilde{p}_m(\kappa_m)\in\mathbb{P}_{\ell_m+\lambda}[\kappa_m]\\ \Rightarrow\quad&\int_{\psi_m}^{\chi_m}\tilde{p}_m(\kappa_m)\mathrm{d}\kappa_m\in\mathbb{P}_{\ell_m+\lambda_1}[\kappa_0,\ldots,\kappa_{m-1}]\\ \Rightarrow\quad&\int_{\psi_{m-1}}^{\chi_{m-1}}\int_{\psi_m}^{\chi_m}\tilde{p}_{m-1}(\kappa_{m-1})\tilde{p}_m(\kappa_m)\mathrm{d}\kappa_m\,\mathrm{d}\kappa_{m-1}\in\mathbb{P}_{\ell_{m-1}+\ell_m+2(\lambda+1)}[\kappa_0,\ldots,\kappa_{m-2}]\\ \Rightarrow\quad&\cdots\\ \Rightarrow\quad&\int_{\psi_1}^{\chi_1}\cdots\int_{\psi_m}^{\chi_m}\tilde{p}_1(\kappa_1)\cdots\tilde{p}_m(\kappa_m)\mathrm{d}\kappa_m\cdots\mathrm{d}\kappa_1\in\mathbb{P}_{\ell_1+\cdots+\ell_m+m(\lambda+1)}[\kappa_0]\\ \Rightarrow\quad&\int_{\mathscr{A}}K(\kappa_1,\ldots,\kappa_m)\mathrm{d}\kappa_m\cdots\mathrm{d}\kappa_1\in\mathbb{P}_{\ell_1+\cdots+\ell_m+m(\lambda+1)}[\kappa_0].\end{aligned}$$

Since $\ell_1+\cdots+\ell_m=k_0+\cdots+k_{r-1}+k_{r+1}+\cdots+k_m$ and $e_{k_r+\lambda}\in\mathbb{P}_{k_r+\lambda-\nu}$, it follows from (3.11) that

$$\int_{\mathscr{S}}F(\kappa_0,\kappa_1,\ldots,\kappa_m)\mathrm{d}\boldsymbol{\kappa}=\int_0^1\omega(\kappa)q(\kappa)\mathrm{d}\kappa,\tag{3.12}$$

where

$$q\in\mathbb{P}_{k_0+k_1+\cdots+k_m+(m+1)(\lambda+1)-\nu-1}.$$

Theorem 10 *Let us suppose that the polynomial ω obeys the orthogonality conditions*

$$\int_0^1\omega(\kappa)\kappa^{j-1}\mathrm{d}\kappa=0,\qquad j=1,2,\ldots,r.\tag{3.13}$$

Then $Q(h)$ is an order-$(\nu+r)$ approximation to the multivariate integral $I(h)$.

Proof Subject to (3.13), it follows from (3.12) that

$$k_0+k_1+\cdots+k_m\le r+\nu-(m+1)(\lambda+1)$$

implies

$$\int_{\mathscr{S}}F(\kappa_0,\kappa_1,\ldots,\kappa_m)\mathrm{d}\boldsymbol{\kappa}=0.$$

This is true with regard to all the $2^{m+1}-1$ terms in the integrand. In other words, just one term contributes to the integral (3.10) and we deduce that $\gamma_{\boldsymbol{k}} = \delta_{\boldsymbol{k}}$. The theorem now follows from the order condition (3.7) $\square$

Corollary *Let* $(c_1, c_2, \ldots, c_\nu)$ *be the nodes of Gaussian quadrature in* $[0,1]$. *Then* $Q(h)$ *is a quadrature of order* 2ν.

To rephrase the theorem and its corollary, the underlying order conditions are nothing else but the usual orthogonality conditions that guarantee the order of a univariate quadrature. All the necessary integrals can thus be evaluated to order p by evaluating the function a at just $\lfloor (p+1)/2 \rfloor$ Gauss–Legendre points in $[0,1]$ or, for that matter, at $\lfloor p/2 \rfloor + 1$ Gauss–Radau points there.

As a trivial example, we choose $\lambda = 0$, $\nu = 2$ and the Gauss–Legendre points

$$c_1 = \tfrac{1}{2} - \tfrac{1}{6}\sqrt{3}, \qquad c_2 = \tfrac{1}{2} + \tfrac{1}{6}\sqrt{3}.$$

Therefore

$$u_1(t) = \tfrac{1}{2} - (t - \tfrac{1}{2})\sqrt{3}, \qquad u_2(t) = \tfrac{1}{2} + (t - \tfrac{1}{2})\sqrt{3}.$$

Brief calculation affirms that the fourth-order quadrature is

$$\int_0^h \int_0^\kappa \mathscr{L}(a(\kappa), a(\xi))\,\mathrm{d}\xi\,\mathrm{d}\kappa \approx h^2[\tfrac{1}{8}\mathscr{L}_{1,1} + (\tfrac{1}{8} - \tfrac{1}{12}\sqrt{3})\mathscr{L}_{1,2} + (\tfrac{1}{8} + \tfrac{1}{12}\sqrt{3})\mathscr{L}_{2,1} + \tfrac{1}{8}\mathscr{L}_{2,2}].$$

In the special case when

$$\mathscr{L}(x,y) = [x,y],$$

which is of the concern in this paper, obvious cancellations yield

$$\int_0^h \int_0^\kappa [a(\kappa), a(\xi)]\mathrm{d}\xi\,\mathrm{d}\kappa \approx -\frac{\sqrt{3}}{6} h^2 [a(c_1 h), a(c_2 h)].$$

Likewise,

$$\begin{aligned}
\int_0^h H_{\omega_2}(\kappa)\mathrm{d}\kappa &= \int_0^h \left[\left[a(\kappa), \int_0^\kappa a(\xi)\mathrm{d}\xi\right], \int_0^\kappa a(\rho)\mathrm{d}\rho\right]\mathrm{d}\kappa \\
&\approx h^3\{-(\tfrac{3}{80} + \tfrac{1}{16}\sqrt{3})[[a(c_1h), a(c_2h)], a(c_1h)] \\
&\quad + (\tfrac{3}{80} - \tfrac{1}{16}\sqrt{3})[[a(c_1h), a(c_2h)], a(c_2h)]\} \\
&= -h^3[[a(c_1h), a(c_2h)], (\tfrac{3}{80} + \tfrac{1}{16}\sqrt{3})a(c_1h) - (\tfrac{3}{80} - \tfrac{1}{16}\sqrt{3})a(c_2h)]
\end{aligned}$$

and

$$\begin{aligned}
\int_0^h H_{\omega_3}(\kappa)\mathrm{d}\kappa &= \int_0^h \left[a(\kappa), \int_0^\kappa \left[a(\xi), \int_0^\xi a(\rho)\mathrm{d}\rho\right]\mathrm{d}\xi\right]\mathrm{d}\kappa \\
&\approx h^3\{(\tfrac{3}{80} - \tfrac{1}{48}\sqrt{3})[a(c_1h), [a(c_1h), a(c_2h)]] \\
&\quad - (\tfrac{3}{80} + \tfrac{1}{48}\sqrt{3})[a(c_2h), [a(c_1h), a(c_2h)]]\} \\
&= h^3[(\tfrac{3}{80} - \tfrac{1}{48}\sqrt{3})a(c_1h) - ((\tfrac{3}{80} + \tfrac{1}{48}\sqrt{3})a(c_2h), [a(c_1h), a(c_2h)]].
\end{aligned}$$

Recall, however, from (2.15) that $\int H_{\omega_2}$ and $\int H_{\omega_3}$ need be evaluated as part of a linear combination. Taking this into account, we obtain

$$f_0^2 f_2 \int_0^h H_{\omega_2}(\kappa)\mathrm{d}\kappa - f_0 f_1^2 \int_0^h H_{\omega_3}(\kappa)\mathrm{d}\kappa \approx h^3[[a(c_1h), a(c_2h)], b_1 a(c_1 h) - b_2 a(c_2 h)],$$

where

$$\begin{aligned} b_1 &= (\tfrac{3}{80} + \tfrac{1}{16}\sqrt{3}) f_0^2 f_2 + (\tfrac{3}{80} - \tfrac{1}{48}\sqrt{3}) f_0 f_1^2, \\ b_2 &= (\tfrac{3}{80} - \tfrac{1}{16}\sqrt{3}) f_0^2 f_2 + (\tfrac{3}{80} + \tfrac{1}{48}\sqrt{3}) f_0 f_1^2. \end{aligned}$$

In particular, if $f_0 = 1$, $f_1 = \frac{1}{2}$ and $f_2 = \frac{1}{12}$, in line with (2.4), then $b_1 = b_2 = \frac{1}{80}$ and

$$f_0^2 f_2 \int_0^h H_{\omega_2}(\kappa)\mathrm{d}\kappa - f_0 f_1^2 \int_0^h H_{\omega_3}(\kappa)\mathrm{d}\kappa \approx \tfrac{1}{80} h^3[[a(c_1h), a(c_2h)], a(c_1 h) - a(c_2 h)],$$

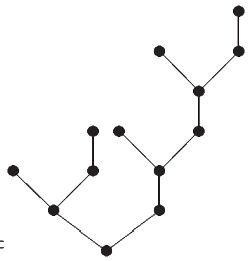
We thus deduce from our analysis and Theorem 6 that a fourth-order truncation of the Magnus series requires just two evaluations of a and the computation of only two commutators.

4 Reducing the number of commutators

A careful reader should have observed in the last section that there is a very large scope in reducing the number of commutators that need be evaluated to attain order 4. The number of function evaluations being determined solely by the order of the underlying method, the computation of commutators is a major expense of our algorithms, hence it makes sense to discuss in a more orderly fashion how to exploit the Lie-algebraic setting to reduce the number of commutators in a general case.

Another pertinent observation from the last section is that, although a definition of the weights by the formula (3.8) makes it amenable to successful order analysis, it is not of a form suitable to a (possibly symbolic) manipulation. Recall that the terms in a Magnus expansion are indexed by binary trees and are derived naturally in terms of the composition rules from Section 2. We wish to redefine the weights $b_{\boldsymbol{\ell}}$ in a similar fashion. It is a tribute to the power of graph theory to illuminate the matter at hand that both goals – reduction in the number of commutators and a recursive formula for quadrature weights – can be accomplished by the same mechanism. This is the theme of the present section. Our conclusion is (we believe) striking. Recall that we need to implement the multivariate quadrature (3.2) for all trees of requisite order and that the number of such trees grows exponentially with m. Yet, as it turns out, just $p-2$ binary trees determine the number of commutators that need be computed to attain order p. This renders our computational algorithm significantly cheaper and more competitive with alternative numerical approaches.

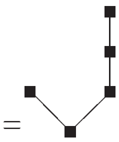
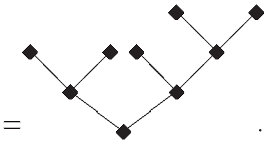
Let τ be an arbitrary binary tree that has been constructed by the composition rules of Section 2. We factorize τ into two trees, the *I-tree* (integration tree) and *C-tree* (commutation tree) in the following manner. The I-tree is formed from τ by pruning all the vertices with two children. (By 'pruning' we mean a progression in a monotone ordering, from the 'foliage', the top of the tree, down to the root.) Similarly, the C-tree is formed by pruning all the vertices with a single child. These concepts are made considerably clearer upon an examination of an example. For instance, let us consider the tree

$\tau =$  $\in \mathscr{T}_{13},$

which corresponds to the Magnus expansion term

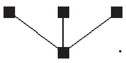
$$\int_0^t \left[\left[a(\kappa_0), \int_0^{\kappa_0} a(\kappa_1)\mathrm{d}\kappa_1\right], \int_0^{\kappa_0} \left[a(\kappa_2), \int_0^{\kappa_2} \left[a(\kappa_3), \int_0^{\kappa_3} a(\kappa_4)\mathrm{d}\kappa_4\right] \mathrm{d}\kappa_3\right] \mathrm{d}\kappa_2\right] \mathrm{d}\kappa_0.$$

Our factorization yields

I-tree $\tau^{\mathrm{I}} =$  and C-tree $\tau^{\mathrm{C}} =$  .

For clarity, we denote the I-tree and the C-tree of τ by τ^{I} and τ^{C} respectively and use "■" and "◆" to distinguish between their vertices.

Every C-tree is a *strict* binary tree: each vertex has either two children or none. An I-tree, however, need not be binary at all. For example,

$\omega_8^{\mathrm{I}} =$  .

It is easy to verify that the number of vertices in an I-tree τ^{I} is exactly the same as the number of integrals in $\int H_\tau$. Moreover, suppose that H_τ has been derived from H_{τ_1} and H_{τ_2} by the second composition rule from Section 2, i.e. that (2.16) holds. Let us define by $\mathscr{S}$ and $\mathscr{S}_j$ the simplices of integration in τ and in τ_j, $j = 1, 2$, respectively. Counting the number of integrals in each term, we deduce at once that

$$\mathrm{ord}\,\tau^{\mathrm{I}} = \mathrm{ord}\,\tau_1^{\mathrm{I}} + \mathrm{ord}\,\tau_2^{\mathrm{I}}.$$

Letting $m = \mathrm{ord}\,\tau$, we set

$$B_{\tau,\boldsymbol{\ell}}(t) := u_{\ell_0}(t) \int_0^t\int_0^{\kappa_{i_1}} \cdots \int_0^{\kappa_{i_{m-1}}} \prod_{i=1}^m u_{\ell_i}(\kappa_i)\mathrm{d}\kappa_m\,\mathrm{d}\kappa_{m-1}\cdots\mathrm{d}\kappa_1, \qquad \boldsymbol{\ell} \in \Lambda_m^\nu,$$

therefore, by (3.3)

$$b_{\boldsymbol{\ell}} = \int_0^1 B_{\tau,\boldsymbol{\ell}}(t)\mathrm{d}t. \tag{4.1}$$

Similar definitions pertain to τ_1 and τ_2. It is an immediate consequence of (2.16) that

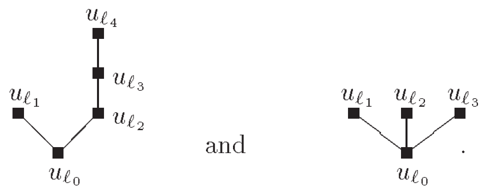
$$B_{\tau,\boldsymbol{\ell}}(t) = \int_0^t B_{\tau_1,\boldsymbol{\ell}_1}(\kappa) \int_0^\kappa B_{\tau_2,\boldsymbol{\ell}_2}(\xi)\mathrm{d}\xi\mathrm{d}\kappa, \tag{4.2}$$

where

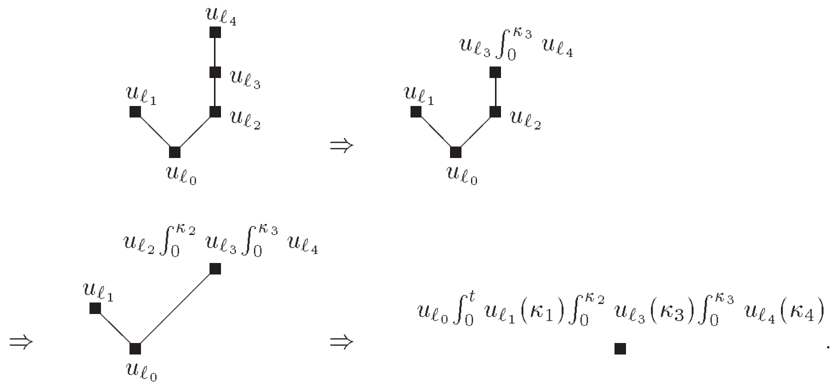
$$\boldsymbol{\ell} = (\boldsymbol{\ell_1}, \boldsymbol{\ell_2}), \qquad \boldsymbol{\ell}_i \in \{1, 2, \ldots \nu\}^{\mathrm{ord}\,\tau_i}, \quad i = 1, 2.$$

The weight $b_{\boldsymbol{\ell}}$ can be computed recursively by means of the formula (4.2), followed by the integral (4.1).

An alternative approach is, given $\boldsymbol{\ell} \in \Lambda_m^\nu$, to label all the vertices of an I-tree by the cardinal Lagrange polynomials u_{ℓ_i} in a *reverse natural ordering:* we label the root with u_{ℓ_0} and then progress to label all the remaining vertices so that each child is always labelled after its parent and a child to the left is always labelled first. Thus, for example,



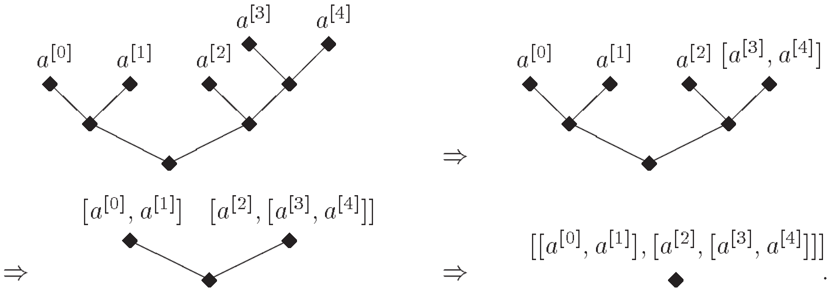
Next, the I-tree is *pruned.* Whenever a childless vertex is removed, the label of its parent is multiplied by the integral of the label of the vertex in question. Thus, for example



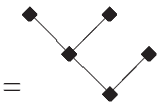
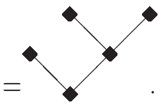
The outcome, as is trivial to prove, is the polynomial $B_{\tau,\boldsymbol{\ell}}$. Finally, we use (4.1) to convert it to the weight $b_{\boldsymbol{\ell}}$.

We next turn our attention to C-trees. Provided that $\tau \in \mathscr{T}_{3m+1}$, we deduce at once that its C-tree has order $2m+1$, since τ contains exactly m vertices with a single child. Moreover, it is trivial to observe that the C-tree has exactly $m+1$ top (i.e., childless) vertices.

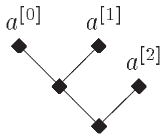
The C-tree determines the integrand similarly to the I-tree yielding the domain of integration. Similar connection extends to quadrature formulae (3.2): while the I-tree has just been exploited in the derivation of $b_{\boldsymbol{\ell}}$, we can use the C-tree to determine the structure of $\mathscr{L}(a(c_{\ell_0}h), a(c_{\ell_1}h), \ldots, a(c_{\ell_m}h))$. It follows from our original definition of the connection between trees and expansion terms in the Magnus series that the latter term can be obtained as follows. We label the top vertices of the C-tree, progressing from the left rightwards, by $a(c_{\ell_0}h), a(c_{\ell_1}h), \ldots, a(c_{\ell_m}h)$. Next we prune the tree. Each time a pair of children is pruned, their parent receives the label which is the commutator of their labels. For example, letting $a^{[i]} := a(c_{\ell_i}h)$, $i = 0, 1, \ldots, m$,

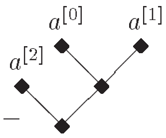


The C-tree is instrumental not just in regard to the recovery of the exact form of commutators but also in exploiting symmetries to eliminate many of the commutators, thereby decreasing a great deal the computational expense. Recall from Section 3 that H_{ω_2} and H_{ω_3} require the calculation of exactly the same commutators, albeit with a different labelling of the indices. This kind of symmetry is easily revealed from the structure of the C-tree. Thus,

$\tau^{\mathrm{C}}_{\omega_2} =$  and $\tau^{\mathrm{C}}_{\omega_3} =$  .

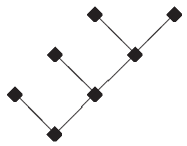
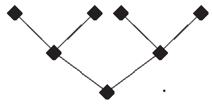
Bearing in mind the relationship between C-trees and commutators, we observe that rotating a C-tree about a vertical axis is equivalent to exchanging the terms in the underlying commutator. In other words,



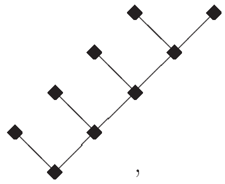
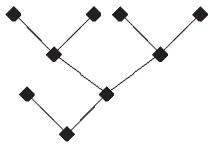
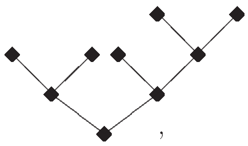
$\sim [[a^{[0]}, a^{[1]}], a^{[2]}] = -[a^{[2]}, [a^{[0]}, a^{[1]}]] \sim \; -$


and there is no need to evaluate the second commutator. Of course, we need to keep track of the exchange of indices, but this can be done easily.

In general, we say that two strictly binary trees, τ_1 and τ_2, say, are *equivalent* if τ_2 can be converted to τ_1 by a finite number of rotations with respect to vertical axes. Only a single representer from a class of equivalent trees need be evaluated for every index $\boldsymbol{\ell}$. Hence, it is of interest to compare the number of equivalent trees to the overall number of strictly binary trees of any given order $2m+1$. We recall from Section 2 that there are exactly $\theta_m = (2m)!/[m!(m+1)!]$ members in $\mathscr{T}_{3m+1}$, hence this is also the number of strictly binary trees of order $2m+1$. Let $\tilde{\theta}_m$ denote the number of equivalent strictly binary trees of order $2m+1$. Trivially, $\tilde{\theta}_0 = \tilde{\theta}_1 = 1$ and we have already seen that also $\tilde{\theta}_2 = 1$. It follows easily from Table 1 that $\tilde{\theta}_3 = 2$, with the representers

$\omega_4, \omega_5, \omega_6, \omega_8 \to$  $\omega_7 \to$  . (4.3)

Likewise, for $m = 4$ we may choose the representers

 ,  and  ,

therefore $\tilde{\theta}_4 = 3$.

In general, $\tilde{\theta}_m$ is known in combinatorics as the mth *Wedderburn–Etherington number* [6]. It is easy to affirm the recursive formula

$$\left.\begin{aligned} \tilde{\theta}_0 &= 1, \\ \tilde{\theta}_{2m-1} &= \tfrac{1}{2} \sum_{j=0}^{2m-2} \tilde{\theta}_j \tilde{\theta}_{2m-j-2} + \tfrac{1}{2} \tilde{\theta}_{m-1}, \\ \tilde{\theta}_{2m} &= \tfrac{1}{2} \sum_{j=0}^{2m-1} \tilde{\theta}_j \tilde{\theta}_{2m-j-1}, \end{aligned}\right\} \quad m \in \mathbb{N}$$

and it follows after an elementary manipulation that the generating function

$$\tilde{\Theta}(z) = \sum_{m=0}^{\infty} \tilde{\theta}_m z^m$$

obeys the functional equation

$$\tilde{\Theta}(z) = 1 + \tfrac{1}{2} z [\tilde{\Theta}(z)]^2 + \tfrac{1}{2} z \tilde{\Theta}(z^2).$$

Neither an exact formula for $\{\tilde{\theta}_m\}_{m \in \mathbb{Z}^+}$ nor an asymptotic expansion are known [6]. Yet, as can be seen from Table 2, the procedure of lumping all equivalent trees together saves a substantial proportion of computational cost.

Redundancy of strictly binary trees is just one mechanism that allows us to reduce the number of commutators that need be computed. Other devices are the antisymmetry of the commutator and the Jacobi identity. We demonstrate in the sequel that an exploitation of these two devices reduces the extent of computation in the implementation of our quadrature formulae to just *a single tree* for every $m \geq 0$.

m	all C-trees	equivalence classes of C-trees
0	1	1
1	1	1
2	2	1
3	5	2
4	14	3
5	42	6
6	132	11

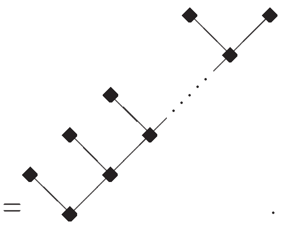
Table 2: The number of C-trees and of equivalence classes of C-trees for $m = 0, 1, \ldots, 6$.

We denote by $\mathscr{V}_m$ the set of all the strictly binary trees of order $2m+1$ (that is, all the C-trees that correspond to trees in $\mathscr{T}_{3m+1}$). Given $\tau \in \mathscr{V}_m$ and $a_0, a_1, \ldots, a_m \in \mathfrak{g}$, we say that $h_\tau(a_0, a_1, \ldots, a_m) \in \mathfrak{g}$ is a *realisation* of τ if it is obtained by the nested action of m commutators, consistently with our connection between commutation and C-trees. Thus, for example,

$$h_{\omega_2^{\mathrm{C}}}(a_0, a_1, a_2) = [a_0, [a_1, a_2]] \qquad \text{and} \qquad h_{\omega_7^{\mathrm{C}}}(a_0, a_1, a_2, a_3) = [[a_0, a_1], [a_2, a_3]].$$

We let $\mathscr{F}_m^\nu$ stand for the linear subset of $\mathfrak{g}$ which is generated by all realisations $h_\tau(a^{[\ell_0]}, a^{[\ell_1]}, \ldots, a^{[\ell_m]})$, where τ ranges across $\mathscr{V}_m$ and $\boldsymbol{\ell} \in \Lambda_m^\nu$. The dimension of $\mathscr{F}_m^\nu$ is denoted by $W_{m,\nu}$. Clearly, it represents the number of commutators that must be calculated in the implementation of the quadrature formulae (3.2) for all $\int H_\tau$ with $\tau \in \mathscr{T}_{3m+1}$. We prove in Appendix A that in general $W_{2,\nu} = \frac{1}{3}(\nu^2 - 1)\nu$ and $W_{3,\nu} = \frac{1}{4}(\nu^2 - 1)\nu^2$.[3]

We select a particular tree in $\mathscr{V}_m$, namely

$\varphi^{[m]} =$  .

Therefore, $\varphi^{[2]} = \omega_2^{\mathrm{C}}$ and $\varphi^{[3]} = \omega_4^{\mathrm{C}}$. Each realisation $\varphi^{[m]}$ is easily identified with a 'repeated' commutator,

$$h_{\varphi^{[m]}}(a_0, a_1, \ldots, a_m) = [a_0, [a_1, \ldots, [a_{m-1}, a_m] \cdots]].$$

We adopt the notation

$$[\ell_0, \ell_1, \ldots, \ell_m] = h_{\varphi^{[m]}}(a^{[\ell_0]}, a^{[\ell_1]}, \ldots, a^{[\ell_m]}).$$

[3] The dimension might be reduced if there are linear dependencies between the $a^{[j]}$ and their commutators. In an extreme case, if all the elements $a^{[j]}$ commute then $\mathscr{F}_m^\nu = \emptyset$. Moreover, needless to say that it cannot exceed the dimension of $\mathfrak{g}$ when the Lie algebra is finite-dimensional. We henceforth disregard these phenomena.

Let $\mathscr{K}_m^\nu$ be the linear space spanned by all the realisations of $\varphi^{[m]}$. Then, according to [20, Theorem 3.1, p. 71], the Lie algebra $\mathscr{K}^\nu$, generated by the free system of generators $\{a^{[1]}, a^{[2]}, \ldots, a^{[\nu]}\}$ can be written in the form

$$\mathscr{K}^\nu = \bigoplus_{r=1}^{\infty} \mathscr{K}_r^\nu.$$

In particular, every term that can be generated from these elements by m commutators belongs to

$$\bigoplus_{r=1}^{m} \mathscr{K}_r^\nu.$$

We deduce that $\mathscr{F}_m^\nu$ is contained in the above set and conclude that

$$\bigoplus_{r=1}^{m} \mathscr{F}_r^\nu = \bigoplus_{r=1}^{m} \mathscr{K}_r^\nu. \tag{4.4}$$

Given that $\mathscr{K}_r^\nu$ for $r = 1, 2, \ldots, m-1$, would have been already evaluated, we conclude that, provided that we have calculated all the commutators corresponding to the realisations of $\varphi^{[m]}$ in $\{a^{[0]}, a^{[1]}, \ldots, a^{[m]}\}$, we can compute all of $\mathscr{F}_m^\nu$, hence all the quadrature formulae allowing to advance from order m to order $m+1$.

This analysis affirms our observation that the realisations of $\varphi^{[2]}$ and $\varphi^{[3]}$ can be used to construct all other commutators of their orders, and it extends it to all $\varphi^{[m]}$. Moreover, the dimension of $\mathscr{K}_m^\nu$ is known [20, p. 71], hence

$$W_{m,\nu} = \dim \mathscr{K}_m^\nu = \frac{1}{m+1} \sum_{d|(m+1)} \mu(d) \nu^{(m+1)/d}, \tag{4.5}$$

where the sum is carried out over all the divisors of $m+1$ and the *Möbius function* $\mu(d)$ equals $(-1)^k$ if d is a product of k distinct primes, otherwise (i.e., when d is not square-free) it is zero [15]. Thus,

$$\begin{aligned}
W_{2,\nu} &= \tfrac{1}{3}(\nu^2 - 1)\nu, \\
W_{3,\nu} &= \tfrac{1}{4}(\nu^2 - 1)\nu^2, \\
W_{4,\nu} &= \tfrac{1}{5}(\nu^4 - 1)\nu, \\
W_{5,\nu} &= \tfrac{1}{6}(\nu^3 + \nu - 1)(\nu^2 - 1)\nu.
\end{aligned}$$

Unfortunately, neither (4.4) nor (4.5) are accompanied by a *constructive* proof, which can illuminate a numerical procedure whereby the least possible number of commutators is computed. Appendix A is concerned with a constructive evaluation of $W_{m,\nu}$ for $m = 2, 3$, whereas Appendix B demonstrates that the calculation of $W_{m,\nu}$ linear combinations of $h_{\varphi^{[m]}}$ suffices for the implementation of quadrature formulae for $m = 4, 5$. The development of a constructive numerical approach for all m and ν is a subject of ongoing research.

5 Magnus series and iterated commutators

The method of *Magnus series* and the method of *iterated commutators* [12] represent alternative means to represent and discretize the solution of the system (1.1). Although they share the important attribute of respecting Lie-algebraic structure, the two methods are, in a sense, based on 'orthogonal' reasoning. While Magnus series is based on a single exponential of an infinite (or, subject to truncation, 'long') expansion, the method of iterated commutators represents the solution as an infinite product of exponentials, each with a simple argument, and it approximates the solution by a finite product of this type. It is natural to consider an approach that borrows elements from both Magnus series and iterated commutators.

Lemma 11 *Let y be the solution of* (1.1) *and set*

$$x(t) = \mathrm{e}^{-\varrho(t)} y(t), \qquad t \geq 0,$$

where ϱ is an arbitrary, sufficiently smooth function. Then x obeys the differential equation

$$\begin{aligned} & x' = bx, \quad t \geq 0, \qquad x(0) = \mathrm{Id}, \\ \textit{where} \qquad & b(t) = \sum_{k=0}^{\infty} \frac{1}{k!} \mathrm{ad}^k(a, \varrho) - \sum_{k=0}^{\infty} \frac{1}{(k+1)!} \mathrm{ad}^k(\varrho', \varrho) \end{aligned} \tag{5.1}$$

and Id *is the identity. Moreover, if $a, \varrho : \mathbb{R}^+ \to \mathfrak{g}$ then also $b : \mathbb{R}^+ \to \mathfrak{g}$, consequently $x(t) \in G$ for every $t \geq 0$.*

Proof Formally differentiating x we deduce at once that

$$b(t) = \left(\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{e}^{-\varrho(t)} \right) \mathrm{e}^{\varrho(t)} + \mathrm{e}^{-\varrho(t)} a(t) \mathrm{e}^{\varrho(t)}, \qquad t \geq 0.$$

We next replace σ with $-\varrho$ in the proof of Theorem 1, concluding that

$$\sum_{m=0}^{k} (-1)^m \binom{k}{m} \varrho^m \varsigma \varrho^{k-m} = \mathrm{ad}^k(\varsigma, \varrho), \qquad k \in \mathbb{Z}^+ \tag{5.2}$$

and

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{e}^{-\varrho(t)} \right) \mathrm{e}^{\varrho(t)} = -\sum_{k=0}^{\infty} \frac{1}{(k+1)!} \mathrm{ad}^k(\varrho', \varrho). \tag{5.3}$$

Employing (5.2), we also conclude that

$$\begin{aligned} \mathrm{e}^{-\varrho(t)} a \mathrm{e}^{\varrho(t)} &= \sum_{\ell=0}^{\infty} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\ell!} \varrho^\ell a \varrho^k \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\ell=0}^{k} (-1)^\ell \binom{k}{\ell} \varrho^\ell a \varrho^{k-\ell} = \sum_{k=0}^{\infty} \frac{1}{k!} \mathrm{ad}^k(a, \varrho). \end{aligned} \tag{5.4}$$

Putting (5.3) and (5.4) together, we obtain the explicit form of the function b in (5.1). The proof of the lemma is concluded by observing that both (5.3) and (5.4) are producing terms in $\mathfrak{g}$ as long as $a(t), \varrho(t) \in \mathfrak{g}$ for $t \geq 0$. $\square$

Note that letting $\varrho(t) = \int_0^t a(\kappa)\mathrm{d}\kappa$ results in the formula (1.5) with $a_m \equiv a$.

We let $a_0 \equiv a$ and replace the Magnus expansion of σ, where $y(t) = \exp \sigma(t)$, with $\sigma_{0,p_0} \equiv \sigma_{p_0}$, where $p_0 \in \mathbb{Z}^+$. In accordance with Theorem 6, we note that

$$y_{[0]}(t) := \mathrm{e}^{\sigma_{0,p_0}(t)} y_0 = y(t) + \mathcal{O}\big(t^{p_0+2}\big) . \tag{5.5}$$

Letting $\varrho \equiv \sigma_{0,p_0}$, we form $a_1 \equiv b$ and note that (5.5) implies that $x(t) = \mathrm{Id} + \mathcal{O}\big(t^{p_0+2}\big)$ and $a_1(t) = \mathcal{O}\big(t^{p_0+1}\big)$. Next we truncate the Magnus expansion of (5.1) as in (2.19), where $p = p_1$. The outcome is $\sigma_{1,p_1} \equiv \sigma_{p_1}$ which, after exponentiation, yields the approximant

$$y_{[1]}(t) = \mathrm{e}^{\sigma_{0,p_0}(t)} \mathrm{e}^{\sigma_{1,p_1}(t)} y_0, \qquad t \geq 0.$$

To examine the order of $y_{[1]}$ we note that Theorem 6 need be now applied with $\lambda = p_0 + 1$. Therefore

$$y_{[1]}(t) = y(t) + \mathcal{O}\Big(t^{(p_0+1)(p_1+1)} + 1\Big) . \tag{5.6}$$

The general pattern emerges. Given $a_m(t) = \mathcal{O}(t^{\gamma_m})$, $m \in \mathbb{N}$, where

$$\begin{aligned} \gamma_0 &= 0 \\ \gamma_m &= (p_{m-1} + 1)(\gamma_{m-1} + 1), \quad m \in \mathbb{N}, \end{aligned} \tag{5.7}$$

we approximate the solution of

$$x' = a_m x, \quad t \geq 0, \qquad x(0) = \mathrm{Id},$$

by $\exp \sigma_{x,p_m}$. The outcome is the approximant

$$y_{[m]}(t) = \mathrm{e}^{\sigma_{0,p_0}(t)} \mathrm{e}^{\sigma_{1,p_1}(t)} \cdots \mathrm{e}^{\sigma_{m,p_m}(t)} y_0 = y(t) + \mathcal{O}\big(t^{\gamma_m+1}\big) , \qquad t \geq 0.$$

Unless we decide to terminate, we next generate a_{m+1} by letting $a = a_m$, $\varrho = \sigma_{m,p_m}$ in (5.1).

Note that (5.7) is consistent with (5.5) and (5.6). Letting $p_m \equiv 1$ we recover the standard iterated commutators from [12, 23]. With greater generality, choosing $p_m \equiv r \in \mathbb{N}$, we can verify at once that

$$\gamma_m = \frac{r+1}{r}[(r+1)^m - 1], \qquad m \in \mathbb{Z}^+.$$

Therefore the order increases exponentially.

Blending Magnus series with iterated commutators yields an abundant choice of discretization methods for every order $p \geq 3$. Each method corresponds to specific choice of $m \in \mathbb{N}$ and $p_0, p_1, \ldots, p_{m-1} \in \mathbb{N}$ such that $\gamma_m \geq p$. It is natural to search for a method which is, in some well-defined sense, 'optimal', the criterion being either the computational cost or 'nice' qualitative features. In a future paper we address ourselves to complexity issues associated with different methods of this kind and demonstrate that distinct criteria of computational cost (e.g., the relative cost of commutators and of function evaluations) often lead to different optimal methods.

6 Numerical examples and concluding remarks

The method of Magnus series is considerably more than just a numerical algorithm. By carrying out the full expansion or, alternatively, truncating (2.6) and subjecting the outcome to perturbation analysis, it should be possible to derive a wealth of qualitative results about linear systems (1.1). This, however, should not obscure the potential of Magnus series as a computational procedure.

The main purpose of this section is to present a number of preliminary numerical results. Our goal is neither to investigate in depth the implementation of Magnus series as a numerical algorithm nor to present a compendium of comparative numerical results that might act as a guide to pros and cons of different Lie-group solvers. More modestly, we intend merely to demonstrate that the method of Magnus series, which at first glance might appear to be exotic and bizarre, can be at a relatively modest expense harnessed to produce results which display advantageous behaviour when compared with classical numerical schemes. To this end we compare three methods, all of order 4. Specialising to the linear system (1.1) and letting $t_n = nh$, $y_n \approx y(t_n)$, where $n \in \mathbb{Z}^+$ and $h > 0$ is the step-length, these methods are

1. *RK4:* Explicit Runge–Kutta

$$\begin{aligned} k_1 &= a(t_n)y_n, \\ k_2 &= a(t_n + \tfrac{1}{2}h)(y_n + \tfrac{1}{2}hk_1), \\ k_3 &= a(t_n + \tfrac{1}{2}h)(y_n + \tfrac{1}{2}hk_2), \\ k_4 &= a(t_{n+1})(y_n + hk_3), \\ y_{n+1} &= y_n + \tfrac{1}{6}h(k_1 + 2k_2 + 2k_3 + k_4); \end{aligned}$$

2. *GL4:* Gauss–Legendre Runge–Kutta

$$\begin{aligned} k_1 &= a((\tfrac{1}{2} - \tfrac{\sqrt{3}}{6})h)[y_n + \tfrac{1}{4}hk_1 + (\tfrac{1}{4} - \tfrac{\sqrt{3}}{6})hk_2], \\ k_2 &= a((\tfrac{1}{2} + \tfrac{\sqrt{3}}{6})h)[y_n + (\tfrac{1}{4} + \tfrac{\sqrt{3}}{6})hk_1 + \tfrac{1}{4}hk_2], \\ y_{n+1} &= y_n + \tfrac{1}{2}h(k_1 + k_2); \end{aligned}$$

3. *MG4:* Truncated Magnus expansion with Gaussian points,

$$\begin{aligned} a_{[1]} &= a(t_n + (\tfrac{1}{2} - \tfrac{\sqrt{3}}{6})h), \qquad a_{[2]} = a(t_n + (\tfrac{1}{2} + \tfrac{\sqrt{3}}{6})h), \\ \tilde{\sigma} &= \tfrac{1}{2}h(a_{[1]} + a_{[2]}) + \tfrac{\sqrt{3}}{12}h^2[a_{[2]}, a_{[1]}] + \tfrac{1}{80}h^3[a_{[2]} - a_{[1]}, [a_{[2]}, a_{[1]}]], \\ y_{n+1} &= \mathrm{e}^{\tilde{\sigma}} y_n, \end{aligned}$$

   with the exponential function calculated to machine accuracy by the MATLAB function `expm`.

Note that each method requires exactly two function evaluations per step, provided that $a(t_{n+1})$ is re-used in the next step for *RK4*.

We have applied these methods to the following three ordinary differential systems:

A. $y'' + ty = 0$, $y(0) = 1$, $y'(0) = 0$.

The equation was converted to a two-dimensional vector system with

$$a(t) = \begin{bmatrix} 0 & 1 \\ -t & 0 \end{bmatrix}, \qquad t \geq 0,$$

and integrated in the range $0 \leq t \leq 100$. Note that the exact solution, a linear combination of *Airy functions* $\mathrm{Ai}(-t)$ and $\mathrm{Bi}(-t)$ [1, p. 446], is asymptotically unstable [2] and that it displays oscillations of progressively increasing frequency. Formally, conversion of the equation to a vector system yields a fundamental solution that evolves on the special linear group $\mathrm{SL}(\mathbb{R}, 2)$, but this is of little significance: it is the highly-oscillatory behaviour of the solution that presents the most formidable computational challenge.

B. The 10×10 system with

$$[a(t)]_{k,\ell} = \begin{cases} t \sin \frac{2k\pi}{11}, & k = \ell, \\ \cos \frac{2\pi k t}{11}, & k = \ell - 1, \\ -\cos \frac{2\pi \ell t}{11}, & k = \ell + 1, \\ 0, & |k - \ell| \geq 2, \end{cases} \qquad k, \ell = 1, 2, \ldots, 10,$$

with $y(0) = \mathrm{Id}$ and $0 \leq t \leq 5$. Note that $\mathrm{tr}\, a(t) = 0$, hence $a(t) \in \mathfrak{sl}(\mathbb{R}, 10)$. Therefore y lies in the special linear group, i.e. $\det y(t) \equiv 1$.

C. Another 10×10 system, namely

$$[a(t)]_{k,\ell} = \begin{cases} \mathrm{i}\, t \sin \frac{2\pi k}{11}, & k = \ell, \\ \cos \frac{\pi k t}{5}, & k = \ell - 1, \\ -\cos \frac{\pi \ell t}{5}, & k = \ell + 1, \\ 0, & |k - \ell| \geq 2, \end{cases} \qquad k, \ell = 1, 2, \ldots, 10,$$

again with $y(0) = \mathrm{Id}$ and $0 \leq t \leq 10$. This time $a^*(t) + a(t) \equiv 0$ and $\mathrm{tr}\, a(t) = 0$, therefore $a(t) \in \mathfrak{su}(\mathbb{R}, 10)$: $y(t)$ is unitary and $\det y(t) \equiv 1$ for all $t \geq 0$.

Figure 1 displays the error of *RK4* for problem **A**. Although the error decays consistently with order 4 when the step size h is being refined, it starts from a very substantial base. This can be attributed to the unstable and highly-oscillatory nature of the exact solution of problem **A** and means that an exceedingly small step size is required for the attainment of reasonable accuracy.

The implicit, A-stable method *GL4* is only marginally better, as is evident from Figure 2. Again, the error is attenuated in line with h but, as was the case with *RK4*, a very small step size is required to counteract the deterioration in numerical precision. The performance of *GL4* is disappointing because, according to conventional numerical wisdom, we might have expected it to perform much better than *RK4* by virtue of its A-stability.

The situation is drastically different when problem **A** is discretized with *MG4*, as can be ascertained from Figure 3. The error for the coarsest step size, $h = \frac{1}{10}$, is more than five significant digits more accurate than for the other methods! In general, it

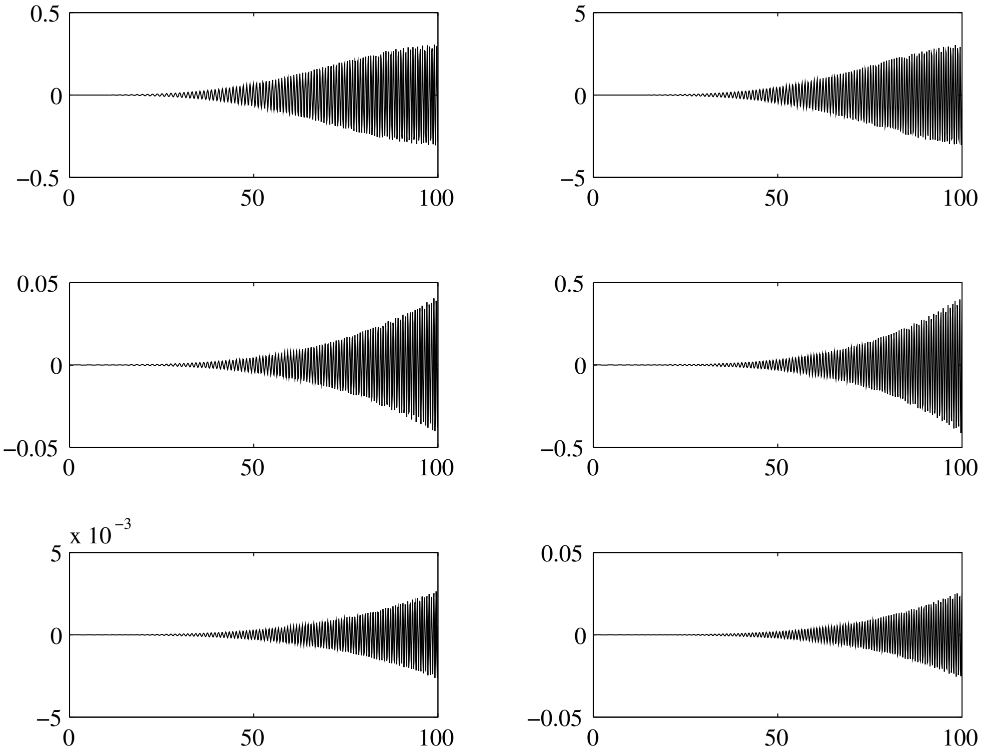


Figure 1 The error in the solution of the problem **A** by *RK4* for $0 \le t \le 100$. The first column displays the error in y and the second in y' for step sizes $h = \frac{1}{10}$ (top row), $h = \frac{1}{20}$ (second row) and $h = \frac{1}{40}$ (bottom row).

appears that the Magnus series approach is superior, in comparison with classical methods, not just with regard to the invariance of a Lie-group structure but also in the general issue of the recovery of qualitative features and robustness with regard to 'difficult' phenomena like high oscillation or complicated asymptotics. Similar pleasing behaviour is probably associated with other Lie-group methods, in particular with iterated commutators [23]. This, we believe, is a significant observation, which should act as a spur for further research.

This is perhaps the place to comment that our comparison was solely in terms of accuracy (and, in the sequel, departure from invariants) for identical step-length sequences. An alternative, equally legitimate criterion is a comparison with regard to computational expense. We have not done this in general and our programs have been neither optimized for speed nor written with a variable step-size and an error controller. It might be worthwhile to mention, however, that *MG4*, after a minor optimization to account for the special feature of the problem **A** (in particular, with an explicit evaluation of the 2×2 exponential) performed significantly better (counting flops) than the MATLAB `ode45` subroutine (a variable-step implementation of a fourth-order Runge–Kutta scheme).

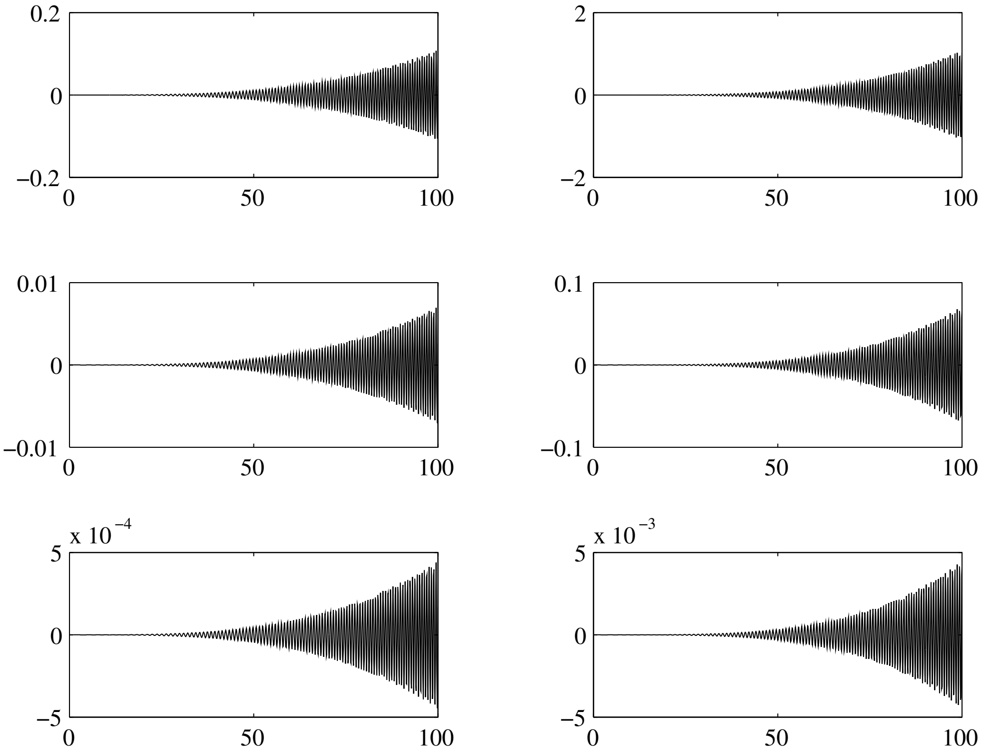


Figure 2 The error in the solution of the problem **A** by *GL4*. The interpretation of different sub-figures is the same as for Figure 1.

Figure 4 displays the Euclidean norm of the error in the solution of problem **B** by the three methods for four step-sizes, $h = \frac{1}{10}, \frac{1}{20}, \frac{1}{50}, \frac{1}{100}$. Note that *GL4* is marginally better than *RK4*, while *MG4*, which starts similarly, accumulates error much slower than the other two methods: at $t = 5$ it is better roughly by a factor of one hundred.

The exact solution of problem **B** is unstable and the extent of instability grows with increasing t. This is reflected by progressive deterioration in the absolute error for all three methods in Figure 4.

The main motivation for the use of a Magnus expansion is not to enhance accuracy but to force the solution to respect a Lie-group structure. Insofar as problem **B** is concerned, the Lie group is $\mathrm{SL}(\mathbb{R}, 10)$, hence $\det y(t) \equiv 1$, $t \geq 0$. This is true by design (to machine accuracy) for *MG4*, while both *RK4* and *GL4* depart from the manifold. This departure is illustrated (for the same sequence of step-sizes as before) in Figure 5.

This is perhaps the place to comment on the retention of invariants by classical numerical methods. *Multistep* methods score the worst and it is proved in [13] that they retain only linear invariants. Therefore, except for the trivial case of *general linear groups* $\mathrm{GL}(\mathbb{R}, d)$ and $\mathrm{GL}(\mathbb{C}, d)$, they should not be used when the retention of a Lie-group structure is at issue. Certain Runge–Kutta methods – *GL4*, but not *RK4* –

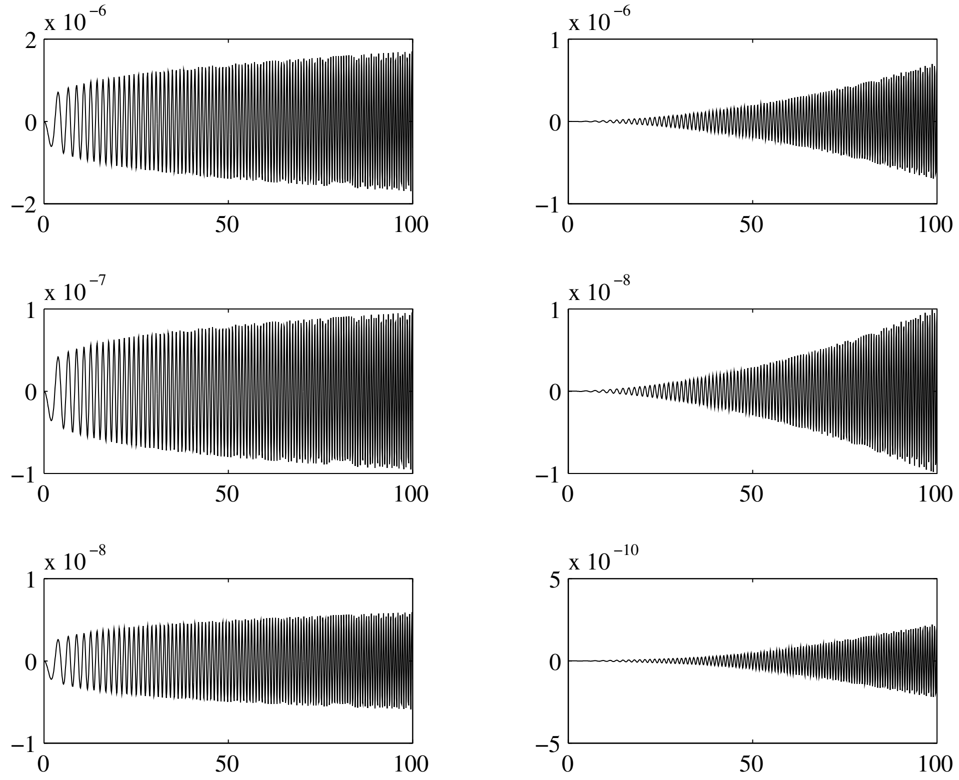


Figure 3 The error in the solution of the problem **A** by *MG4.* The interpretation of different sub-figures is the same as for Figures 1 and 2.

are somewhat better, since they can recover quadratic invariants [3]. Hence they can be safely used with the *orthogonal group* $\mathrm{O}(\mathbb{R}, d)$, the *unitary group* $\mathrm{U}(\mathbb{C}, d)$ and the *symplectic group* $\mathrm{Sp}(\mathbb{R}, 2d)$. Virtually no non-quadratic manifolds can be retained by Runge–Kutta methods [4] and, in particular, no Runge–Kutta may respect manifolds which are level sets of multivariate polynomials of (total) degree ≥ 3 [4]. Hence, no classical method is assured of retaining $\mathrm{SL}(\mathbb{R}, d)$ for $d \geq 3$, since the condition $\det y \equiv 1$ for a $d \times d$ matrix y is expressible as a level set of a d-degree polynomial. Seen in this light, Figure 5 is hardly surprising.

Our final numerical example is problem **C** and the relevant results are displayed in Figure 6. The absolute numerical error follows the same pattern as for problem **B**, namely it accumulates slower with *GL4* than with *RK4,* and yet slower with *MG4.*

Recall that, for the present example, $y(t) \in \mathrm{SU}(\mathbb{C}, 10) = \mathrm{U}(\mathbb{C}, 10) \cap \mathrm{SL}(\mathbb{C}, 10)$. In other words, $\bar{y}(t)^{\mathrm{T}} y(t) \equiv \mathrm{Id}$ and $\det y(t) \equiv 1$. The Magnus expansion retains, by design, both invariants, and we know that the Gauss–Legendre Runge–Kutta method *GL4* retains the first and violates the second. The classical Runge–Kutta method *RK4* respects neither invariant. All this is demonstrated in Figure 6.

We hasten to reiterate that our numerical results are not intended to present a comprehensive study, merely to provide an evidence of computational potential.

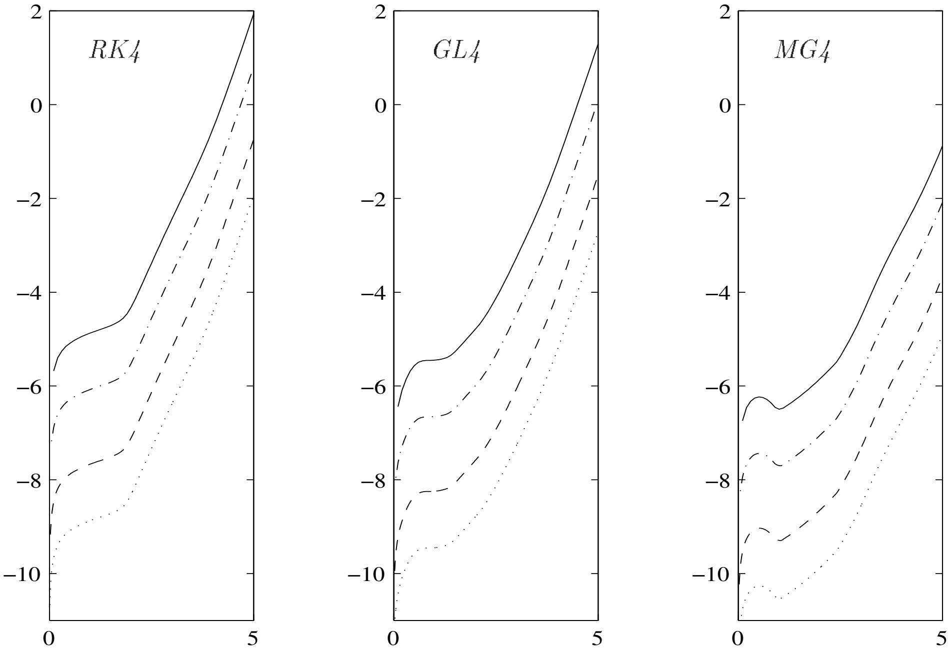


Figure 4 The error $\log_{10} \|y_n - y(t_n)\|_2$ for the three numerical methods for problem **B** and $0 \leq t \leq 5$. The solid, dot-dash, dash-dash and dotted lines correspond to $h = \frac{1}{10}, \frac{1}{20}, \frac{1}{50}$ and $\frac{1}{100}$ respectively.

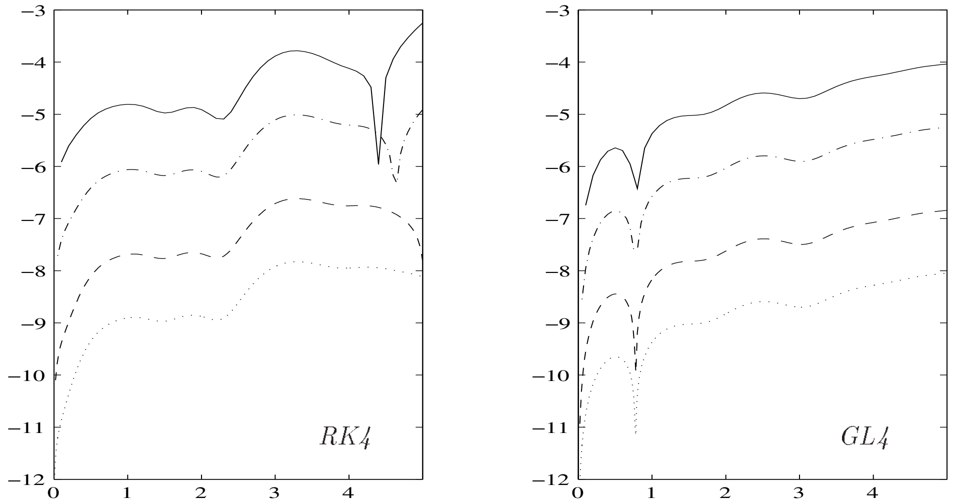


Figure 5 The error $\log_{10} |\det y_n - 1|$ for *RK4* and *GL4*, applied to problem **B**. The interpretation of different lines is the same as in Figure 4.

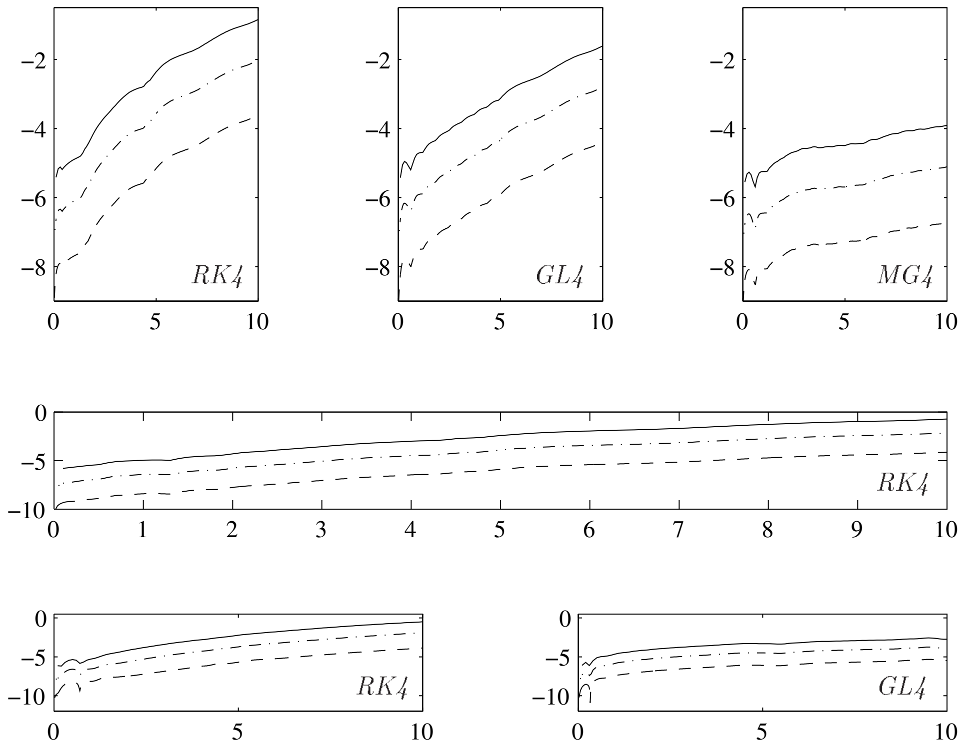


Figure 6 Computational results for problem **C**, $0 \le t \le 10$. The top row displays the absolute error $\log_{10} \|y_n - y(t_n)\|_2$: The solid, dot-dash and dash-dash lines correspond to $h = \frac{1}{10}, \frac{1}{20}$ and $h = \frac{1}{50}$ respectively. The middle row displays the orthogonality error $\log_{10} \|\bar{y}_n^{\mathrm{T}} y_n - \mathrm{Id}\|_2$ for *RK4*. Finally, the bottom row shows $\log_{10} |\det y_n - 1|$ for *RK4* and *GL4*.

A future paper will address itself to detailed complexity analysis of Magnus series and of their different combinations, *á la* Section 5, with iterated commutators.

This is the place to mention that the technique of Magnus series is not the only numerical method which is assured to stay on a Lie group. A number of alternative approaches have emerged in the last few years: the methods of *rigid frames* [8, 21], *discrete gradients* [22] and, perhaps most promisingly, Runge–Kutta methods corrected for a Lie group [17]. It is not the purpose of this paper to weigh the pros and cons of alternative techniques, except for declaring that, in the present, nascent state-of-the-art in numerical methods on differentiable manifolds it is perhaps premature to draw definite conclusions.

To conclude this paper, we recapitulate upon its three main results. Firstly, we have formally introduced Magnus series for Lie-group linear equations (1.1) and established a relationship between its terms and a subset of binary trees. This connection is the key to the understanding and use of Magnus series, since it allows for its recursive evaluation and leads to a convergence proof. Secondly, we have demonstrated that all the integrals which are used in a discretized version of Magnus series can be approximated by using a single set of univariate quadrature points. Hence, an order-p numerical method requires just $\lfloor(p+1)/2\rfloor$ function evaluations. Thirdly, using combinatorial arguments and comparing the dimension of subspaces in the Lie algebra $\mathfrak{g}$, we have proved that it is possible to reduce the number of commutators which are necessary to obtain an order-p discretization. Specifically, just $p-2$ C-trees determine the commutators that need be evaluated, while the number of all C-trees increases exponentially with p.

We believe that the approach of Magnus series is of interest both as an analytic construct and as a numerical tool. Needless to say, much remains to be done. In particular, we mention the implementation of Magnus series when $a(t)$ is a differential operator, constructive derivation of the least-dimensional (i.e., of dimension W_m^ν) basis of $\mathscr{F}_m^\nu$, and an effective approximation of the exponential which, respecting Lie groups, does not negate the most important feature of Magnus series, their retention of Lie-group structure. We hope to return to these themes in future papers.

A Calculation of $W_{2,\nu}$ and $W_{3,\nu}$

The derivation of $W_{m,\nu}$, $m=2,3$, in this section is much more than an example, illustrating the explicit formula (4.5): it also presents a constructive means for the formation of a basis of commutators, which is necessary in the implementation of the quadrature formulae of Section 3.

We recall from Section 4 the abbreviated notation

$$[\ell_0,\ell_1,\ldots,\ell_m]=h_{\varphi^{[m]}}(a^{[\ell_0]},a^{[\ell_1]},\ldots,a^{[\ell_m]}).$$

Insofar as $m=2$ is concerned, we have just one C-tree, $\varphi^{[2]}$. Although there are ν^3 terms in Λ_2^ν, we can reduce the count to $\frac{1}{2}(\nu-1)\nu^2$ by observing that

$$[\ell_0,\ell_1,\ell_2]+[\ell_0,\ell_2,\ell_1]=0 \tag{A.1}$$

and, by the Jacobi identity (1.2),

$$[\ell_0,\ell_1,\ell_2]+[\ell_1,\ell_2,\ell_0]+[\ell_2,\ell_0,\ell_1]=0. \tag{A.2}$$

Because of $(A.1)$, we can assume, without loss of generality, that $\ell_1<\ell_2$, otherwise the term either vanishes (when $\ell_1=\ell_2$) or equals $-[\ell_0,\ell_2,\ell_1]$. Moreover, if, in addition, $\ell_0<\ell_1$ then we can exploit $(A.2)$ to express the underlying term as a linear combination of other terms,

$$[\ell_0,\ell_1,\ell_2]=[\ell_1,\ell_0,\ell_2]-[\ell_2,\ell_0,\ell_1].$$

Therefore, we need to retain just the terms in Λ_2^ν such that $\ell_0\ge\ell_1$ and $\ell_1\le\ell_2-1$. There are precisely $W_{2,\nu}=\frac{1}{3}(\nu^2-1)\nu$ such terms.

According to (4.3), there are two C-trees of order $2m+1$ for $m=3$, namely $\varphi^{[3]}=\omega_4^{\mathrm{C}}$ and ω_7^{C}. We denote

$$h_{\omega_7^{\mathrm{C}}}(a^{[\ell_0]},a^{[\ell_1]},a^{[\ell_2]},a^{[\ell_3]})=[[\ell_0,\ell_1],[\ell_2,\ell_3]]$$

and observe that, by the Jacobi identity,

$$[[\ell_0,\ell_1],[\ell_2,\ell_3]]+[[\ell_1,\ell_0],[\ell_2,\ell_3]],[[\ell_0,\ell_1],[\ell_2,\ell_3]]+[[\ell_2,\ell_3],[\ell_0,\ell_1]]=0.$$

Consequently, we may assume without loss of generality that $(\ell_0,\ell_1)\prec(\ell_2,\ell_3)$, namely that (ℓ_0,ℓ_1) precedes (ℓ_2,ℓ_3) in the increasing *lexicographic* order. It is an easy calculation to affirm that the outcome is just

$$3\binom{\nu+1}{4} \tag{A.3}$$

terms.

The contribution of $\varphi^{[3]}$ is more difficult to evaluate. Clearly,

$$[\ell_0,\ell_1,\ell_2,\ell_3]+[\ell_0,\ell_1,\ell_3,\ell_2]=0,$$

therefore we can discard all the terms with $\ell_2\geq\ell_3$. This leaves us with $\frac{1}{2}(\nu-1)\nu^3$ commutators. Next we observe that, by the Jacobi identity and trivial manipulation,

$$[\ell_0,\ell_1,\ell_2,\ell_3]=[\ell_1,\ell_0,\ell_2,\ell_3]+[[\ell_0,\ell_1],[\ell_2,\ell_3]].$$

Since we have already accounted for ω_7^{C}, we deduce that we can, without loss of generality, discard all terms with $\ell_0>\ell_1$. There are $\frac{1}{4}(\nu-1)^2\nu^2$ such terms, hence we are left with $\frac{1}{4}(\nu^2-1)\nu^2$ commutators.

Our next step is to discard terms that can be obtained by applying the Jacobi identity to the subtree $\tau^{[2]}$. The latter results in

$$[\ell_0,\ell_1,\ell_2,\ell_3]+[\ell_0,\ell_2,\ell_3,\ell_1]+[\ell_0,\ell_3,\ell_1,\ell_2]=0$$

and it is nontrivial only if the integers ℓ_1,ℓ_2 and ℓ_3 are distinct. There are $\binom{\nu}{3}$ such triplets, but not all can be realised for $\ell_0\leq\ell_1$ and $\ell_2<\ell_3$: the exception is when $\ell_1,\ell_2,\ell_3<\ell_0$. In other words, for every $\ell_0=4,5,\ldots,\nu$ we cannot discard (or have already discarded) $\binom{\ell-1}{3}$ triplets. Easy calculation affirms that we are allowed to discard precisely $3\binom{\nu+1}{4}$ terms. This matches $(A.3)$, the contribution of $h_{\omega_7^{\mathrm{C}}}$, and we deduce that, indeed, $W_{3,\nu}=\frac{1}{4}(\nu^2-1)\nu^2$.

B Reducing $\mathscr{F}_m^\nu$ to linear combinations of $h_{\varphi^{[m]}}$ for $m=4,5$

It is trivial that just linear combinations of $h_{\varphi^{[m]}}$ need be computed for $m=0,1,2$ and we have seen in Section A that this is also the case for $m=3$. In this section we show how to represent all the elements in $\mathscr{F}_m^\nu$ as linear combinations of $h_{\varphi^{[m]}}$ for $m=4,5$. All the results have been obtained by using the Jacobi identity, either on the whole tree or on sub-trees and translated to the terminology of commutators:

In the case $m=4$ there are just three C-trees and

$$[a^{[\ell_0]},[[a^{[\ell_1]},a^{[\ell_2]}],[a^{[\ell_3]},a^{[\ell_4]}]]]=[\ell_0,\ell_1,\ell_2,\ell_3,\ell_4]-[\ell_0,\ell_2,\ell_1,\ell_3,\ell_4],$$
$$[[a^{[\ell_0]},a^{[\ell_1]}],[a^{[\ell_2]},[a^{[\ell_3]},a^{[\ell_4]}]]]=[\ell_0,\ell_1,\ell_2,\ell_3,\ell_4]-[\ell_1,\ell_0,\ell_2,\ell_3,\ell_4].$$

Insofar as $m=5$ is concerned, we have six C-trees and their representation in terms of $\varphi^{[5]}$ is

$$[[a^{[\ell_0]},a^{[\ell_1]}],[a^{[\ell_2]},[a^{[\ell_3]},[a^{[\ell_4]},a^{[\ell_5]}]]]] = [\ell_0,\ell_1,\ell_2,\ell_3,\ell_4,\ell_5]-[\ell_1,\ell_0,\ell_2,\ell_3,\ell_4,\ell_5],$$

$$[a^{[\ell_0]},[[a^{[\ell_1]},a^{[\ell_2]}],[a^{[\ell_3]},[a^{[\ell_4]},a^{[\ell_5]}]]]] = [\ell_0,\ell_1,\ell_2,\ell_3,\ell_4,\ell_5]-[\ell_0,\ell_2,\ell_1,\ell_3,\ell_4,\ell_5]$$

$$[a^{[\ell_0]},[a^{[\ell_1]},[[a^{[\ell_2]},a^{[\ell_3]}],[a^{[\ell_4]},a^{[\ell_5]}]]]] = [\ell_0,\ell_1,\ell_2,\ell_3,\ell_4,\ell_5]-[\ell_0,\ell_1,\ell_3,\ell_2,\ell_4,\ell_5],$$

$$\begin{aligned}[[a^{[\ell_0]},a^{[\ell_1]}],[[a^{[\ell_2]},a^{[\ell_3]}],[a^{[\ell_4]},a^{[\ell_5]}]]] &= [\ell_0,\ell_1,\ell_2,\ell_3,\ell_4,\ell_5]-[\ell_1,\ell_0,\ell_2,\ell_3,\ell_4,\ell_5]\\ &\quad -[\ell_0,\ell_1,\ell_3,\ell_2,\ell_4,\ell_5]+[\ell_1,\ell_0,\ell_3,\ell_2,\ell_4,\ell_5],\end{aligned}$$

$$[[a^{[\ell_0]},[a^{[\ell_1]},a^{[\ell_2]}]],[a^{[\ell_3]},[a^{[\ell_4]},a^{[\ell_5]}]]] = [\ell_2,\ell_1,\ell_0,\ell_3,\ell_4,\ell_5]-[\ell_0,\ell_2,\ell_1,\ell_3,\ell_4,\ell_5].$$

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