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Time-symmetry and high-order Magnus methods

A. Iserles, S. P. Nørsett and A. F. Rasmussen

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Department of Applied Mathematics and Theoretical Physics
Silver Street
Cambridge
England CB3 9EW

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by

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Abstract

The subject of this paper is the investigation of the *Magnus expansion* of a solution of the linear differential equation $y' = a(t)y$, $y(0) \in G$, where G is a Lie group and $a : \mathbb{R}^+ \to \mathfrak{g}$, $\mathfrak{g}$ being the Lie algebra of G. We commence with a brief survey of recent work in this area. Next, building on earlier work of Iserles and Nørsett, we prove that an appropriate truncation of the expansion is time-symmetric. Moreover, we develop a 6th-order Lie-group solver based on the Magnus expansion which requires just three function evaluations and the calculation of seven commutators. The paper is accompanied by a number of numerical experiments.

1 Introduction

The conventional means to calculate a numerical solution of an ordinary differential equations is by using one of the classical methods, e.g. Runge–Kutta or linear multistep schemes, typically with variable step-size and error control. It is a matter of long-term experience, underpinned by a great deal of powerful analysis, that this approach is satisfactory for many problems and probably the method of choice for general equations. The situation is different, however, if we are in possession of qualitative information with regard to the underlying equation and wish to recover it under discretization. In particular, if we wish to respect invariants, Iserles (1997) proved that all linear multistep methods fail to respect nonlinear invariants. The situation is somewhat better for Runge–Kutta methods, some of which respect quadratic invariants (Cooper 1987), but a recent, yet-unpublished result of Iserles and Zanna restricts the range of invariants that can be conserved by any Runge–Kutta methods to little more than quadratic. These observations underpin much of the recent effort to develop novel families of numerical integrators, which are designed to replicate exactly invariants, strong integrals and symmetries of the underlying differential system, an activity sometimes known as *geometric integration.*

Perhaps the most powerful general technique in geometric integration is the deployment of *Lie-group solvers.* The main reason is that many invariants (orthogonality, unitarity, volume conservation, ...) can be formulated in terms of Lie groups. Moreover, let $\mathcal{M}$ be a homogeneous space $\mathcal{M}$: a smooth manifold which is subjected to a transitive action of a Lie group G (Olver 1995). Munthe-Kaas & Zanna (1997) proved that, provided we can integrate numerically on G, we can amend our algorithm so as to stay on $\mathcal{M}$. This extends the approach of Lie-group solvers to, among many others, spheres, tori and isospectral manifolds.

A number of Lie-group algorithms have been proposed and studied in the last few years: the rigid-frame technique of Crouch and Grossman (Crouch & Grossman 1993, Owren & Marthinsen 1997), Runge–Kutta–Munthe-Kaas schemes (Munthe-Kaas 1997, Munthe-Kaas 1998) and Fer expansions (Iserles 1984, Zanna 1996). Recently, Iserles & Nørsett (1997) have introduced the very powerful technique of *Mag-*

nus expansions. The approach itself dates to the seminal paper of Magnus (1954) and Magnus expansions have received wide exposure in mathematical physics' literature as perturbative expansions of linear differential systems. Their systematic use as numerical integrators introduces a number of important issues which have been considered in (Iserles & Nørsett 1997) and, more recently, in (Iserles, Marthinsen & Nørsett 1998) and (Zanna 1997).

This paper follows in the footsteps of (Iserles & Nørsett 1997). We address ourselves to the linear matrix system

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

where $y_0 \in G$ and $a : \mathbb{R}^+ \to \mathfrak{g}$. Here G is a matrix Lie group, while $\mathfrak{g}$ is its *Lie algebra.* While referring the reader to (Olver 1995, Varadarajan 1984) for Lie-group terminology, we comment that most of this paper can be perfectly well understood by restricting the attention to the case when G coincides with the *orthogonal group* $\mathrm{O}_n(\mathbb{R})$ (the set of all $n \times n$ real orthogonal matrices), whereby $\mathfrak{g} = \mathfrak{so}_n(\mathbb{R})$ is the Lie algebra of $n \times n$ real skew-symmetric matrices. The main idea behind the Magnus technique is to represent the solution in the form $y(t) = \mathrm{e}^{\sigma(t)} y_0$, where the matrix function σ evolves on $\mathfrak{g}$, and seek an expansion to σ in a form that involves the matrix function a in repeated commutation and integration. We defer a more comprehensive review of the method to Section 2. In Section 3 we investigate the order of magnitude of terms in the Magnus expansion. This leads to a proof of an important feature of such expansions: appropriately truncated, they are *time-symmetric.* This immediately results in a number of benefits and reduced implementation costs. In Section 4 we describe in detail a Magnus method of order 6 which has been designed to reduce complexity and economise in the number of calculations. Finally, Section 5 displays a number of computational results which illustrate the power of the Magnus algorithm.

We mention in passing that, although our exposition is restricted to the linear ordinary differential system (1.1), much of our analysis can be extended to the nonlinear case along the lines of (Zanna 1997).

2 Magnus series

A Lie group G is a smooth manifold endowed with a multiplicative group structure, consistent with the underlying topology of the manifold. The set $\mathrm{GL}_n(\mathbb{R})$ of all $n \times n$ real matrices is a Lie group (the *general linear group*), while a Lie group $G \subseteq \mathrm{GL}_n(\mathbb{R})$ is called a *matricial Lie group.* Standard examples include $\mathrm{T}_n(\mathbb{R})$ (the set of upper-tridiagonal matrices), $\mathrm{O}_n(\mathbb{R})$ (the orthogonal group), $\mathrm{SL}_n(\mathbb{R})$ (the special linear group of matrices with a unit determinant), $\mathrm{SO}_n(\mathbb{R})$ (the special orthogonal group, $\mathrm{O}_n(\mathbb{R}) \cap \mathrm{SL}_n(\mathbb{R})$), the symplectic group $\mathrm{Sp}_n(\mathbb{R})$ and much more. It is possible to define Lie groups over other fields but this greater generality does not help to elucidate the argument of this paper and we forthwith, without loss of generality, restrict ourselves to Lie groups over reals.

The tangent space of a Lie group at identity is a *Lie algebra:* a linear space equipped with a binary, linear, skew-symmetric operation often called *commutation* or a *Lie bracket.* For further reference we note that the commutator obeys the *Jacobi* *identity*

$$[x,[y,z]]+[y,[z,x]]+[z,[x,y]]=O, \qquad x,y,z\in\mathfrak{g}. \tag{2.1}$$

In the case of matricial Lie groups, this binary operation is just the standard additive commutator, $[x,y]=xy-yx$.

The Lie algebra corresponding to $\mathrm{T}_n(\mathbb{R})$ is the set of $n\times n$ real strictly upper-triangular matrices. Likewise, the Lie algebra $\mathfrak{so}_n(\mathbb{R})$ of both $\mathrm{O}_n(\mathbb{R})$ and $\mathrm{SO}_n(\mathbb{R})$ consists of $n\times n$ real skew-symmetric matrices. Further examples can be found in (Olver 1995, Varadarajan 1984).

Given an element $x\in\mathfrak{g}$, we can return to the group by exponentiation, $\mathrm{e}^{tx}\in G$, $t\in\mathbb{R}$, which in the case of matricial Lie groups corresponds to the standard matrix exponential. This is a motivation behind the idea of representing the solution of (1.1) in the form $y(t)=\mathrm{e}^{\sigma(t)}y_0$, $t\ge 0$: as long as we approximate σ by another element of $\mathfrak{g}$, we can be assured that the outcome evolves on G. Unlike the group G, its Lie algebra $\mathfrak{g}$ is a *linear space.* It is considerably easier to restrict a numerical solution to the latter set and this explains why so many Lie-group solvers commence by mapping the problem to the underlying algebra (Iserles & Nørsett 1997, Munthe-Kaas 1997, Zanna 1996).

The linear differential equation (1.1) can be translated to the underlying algebra (and to the terminology of the the function σ), and this has been already described by Hausdorff (1906):

$$\sigma'=\sum_{k=0}^{\infty}\frac{\mathrm{B}_k}{k!}\mathrm{ad}_{\sigma}^{k}a, \quad t\ge 0, \qquad \sigma(0)=0, \tag{2.2}$$

where $\{\mathrm{B}_k\}_{k=0}^{\infty}$ are *Bernoulli numbers* (Abramowitz & Stegun 1965), while the *adjoint operator* $\mathrm{ad}_x^k y$ is defined by iterated commutation:

$$\begin{aligned}&\mathrm{ad}_x^0 y=y,\\ &\mathrm{ad}_x^k y=[x,\mathrm{ad}_x^{k-1}y], \qquad k\in\mathbb{N}.\end{aligned}$$

On the face of it, (2.2) is hardly an improvement over (1.1), being a nonlinear equation and involving an infinite sum. Fortunately, an observation of Wilhelm Magnus (1954) demonstrates that (2.2) possesses a great deal of structure which can be harnessed to produce accurate and relatively affordable approximants. He showed that

$$\begin{aligned}\sigma(t)=&\int_0^t a(\xi_1)\mathrm{d}\xi_1-\tfrac12\int_0^t\int_0^{\xi_1}[a(\xi_2),a(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1\\ &+\tfrac14\int_0^t\int_0^{\xi_1}\int_0^{\xi_2}[[a(\xi_3),a(\xi_2)],a(\xi_1)]\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1\\ &+\tfrac1{12}\int_0^t\int_0^{\xi_1}\int_0^{\xi_1}[a(\xi_3),[a(\xi_2),a(\xi_1)]]\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1+\cdots\end{aligned} \tag{2.3}$$

and this expression has been widely used, mainly in mathematical physics, as a means to derive a perturbation solution of (1.1).

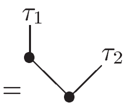
The derivation of a Magnus expansion beyond the terms prescribed in (2.3), as well as its effective numerical implementation, were taken up by Iserles & Nørsett (1997). The general Magnus expansion of σ has the form

$$\sigma(t) = \sum_{m=0}^{\infty} \sum_{\tau \in \mathbb{T}_m} \alpha(\tau) \int_0^t H_\tau(\xi)\mathrm{d}\xi, \qquad t \geq 0, \tag{2.4}$$

where the set $\mathbb{T}_m$ will be defined soon, $\alpha(\tau)$ are scalars and $H_\tau(t) \in \mathfrak{g}$ are functions of t that depend upon a and which, to be consistent with (2.3), are likely to involve integrals and nested commutators. The first main idea in (Iserles & Nørsett 1997) is to associate each term in (2.4) with a *rooted tree,* according to the following prescription:

$$\bullet \;\sim a(t) \tag{2.5}$$

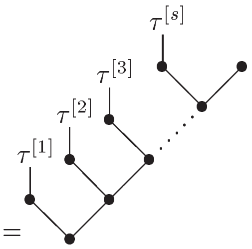
and, recursively,

$\tau =$ 

$$\Rightarrow \qquad H_\tau(t) = \left[\int_0^t H_{\tau_1}(\xi)\mathrm{d}\xi, H_{\tau_2}(t) \right]. \tag{2.6}$$

Thus, appending a root to a tree corresponds to the integration of the underlying Magnus term, while joining two trees with a common root signifies commutation. The set $\mathbb{T}_m$ contains all trees with $3m+1$ vertices that can be obtained with the operation (2.6) (that is, 'integrate the first term and commute the outcome with the second term').

The coefficient $\alpha(\tau)$ is set to one for the trivial tree (2.5). Otherwise, every $\tau \in \mathbb{T}_m$, $m \geq 1$, can be written in a unique fashion in the form

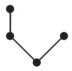
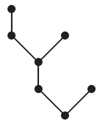
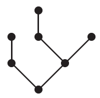
$\tau =$ 

(2.7)

where the number $s \leq m$ is called the *width* of τ. In that case

$$\alpha(\tau) = \frac{\mathrm{B}_s}{s!} \prod_{l=1}^{s} \alpha(\tau^{[l]}). \tag{2.8}$$

The Magnus terms corresponding to (2.2) are thus

τ	$H_\tau(t)$	$\alpha(\tau)$
	$a(t)$	1
	$\int_0^t [a(\xi), a(t)]\mathrm{d}\xi$	$\frac{1}{2}$
	$\int_0^t \int_0^{\xi_1} [[a(\xi_2), a(\xi_1)], a(t)]\mathrm{d}\xi_2 \mathrm{d}\xi_1$	$\frac{1}{4}$
	$\int_0^t \int_0^t [a(\xi_1), [a(\xi_2), a(t)]]\mathrm{d}\xi_2 \mathrm{d}\xi_1$	$\frac{1}{12}$

and it is easy to generate further terms, whether by hand or symbolic calculation, for as long as necessary (Engø, Marthinsen & Munthe-Kaas 1997).

Insofar as an efficient numerical procedure for the solution of (1.1) is concerned, the formal Magnus expansion is just the first step. As can be ascertained at once by inspection, numerical implementation of a Magnus expansion requires the computation of a large number of multivariate integrals over different convex polyhedra. A *sine qua non* of a viable numerical procedure is an effective and cheap evaluation of such integrals. Fortunately, this can be done by exploiting the fact that the integrand is always of the form $\mathcal{L}(a(\xi_1), a(\xi_2), \ldots, a(\xi_m))$, where $\mathcal{L}$ is a multilinear function. Let $c_1, c_2, \ldots, c_\nu$ be distinct quadrature points in $[0,1]$, set $\lambda_k \in \mathbb{P}_{\nu-1}[t]$ as the kth cardinal Lagrange polynomial and assume that the univariate quadrature formula

$$\int_0^1 f(\xi)\mathrm{d}\xi \approx \sum_{k=1}^{\nu} b_k f(c_k), \qquad b_k = \int_0^1 \lambda_k(\xi)\mathrm{d}\xi, \quad k = 1, 2, \ldots, \nu, \tag{2.9}$$

is of order $p \in \{\nu, \nu+1, \ldots, 2\nu\}$. Every integral in a Magnus expansion is over a convex polyhedron of the general form

$$\mathcal{S}_h = \{(\xi_1, \xi_2, \ldots, \xi_m) \,:\, 0 < \xi_1 < h,\ \ 0 < \xi_j < \xi_{i_j},\ j = 2, 3, \ldots, m\},$$

where

$$i_j \in \{1, 2, \ldots, j-1\}.$$

We approximate

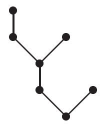
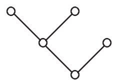
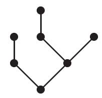
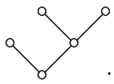
$$\int_{\mathcal{S}_h} \mathcal{L}(a(\xi_1), \ldots, a(\xi_m))\mathrm{d}\xi_m \cdots \mathrm{d}\xi_1 \approx h^m \sum_{\boldsymbol{l} \in \boldsymbol{C}_m^\nu} b_{\boldsymbol{l}} \mathcal{L}(a(c_{l_1}h), \ldots, a(c_{l_m}h)), \tag{2.10}$$

where $\boldsymbol{C}_m^\nu$ is the set of all combinations $\boldsymbol{l} = (l_1, l_2, \ldots, l_m)$ from the set $\{1, 2, \ldots, \nu\}$ and

$$b_{\boldsymbol{l}} := \int_{\mathcal{S}_1} \prod_{j=1}^{\nu} \lambda_{l_j}(\xi_j)\mathrm{d}\xi_m \cdots \mathrm{d}\xi_1, \qquad \boldsymbol{l} \in \boldsymbol{C}_m^\nu.$$

An important result of (Iserles & Nørsett 1997) is that the multivariate quadrature formula (2.10) shares the order p of the univariate approximation (2.9). In other words, in terms of function evaluations *the cost of all the multivariate quadratures needed to approximate the Magnus expansion to given order is exactly the same as the cost of a single univariate quadrature formula.*

The apparent downside of (2.10) is that it requires the evaluation of a very large number of commutators: recall that each $\mathcal{L}$ is made out of commutators and, needless to say, the number of combinations increases exponentially with m. Fortunately, two devices come to our rescue, both based on the rich range of symmetries of the commutator operation. Firstly, given a tree τ, let us designate by τ^{c} (thereafter called 'the C-tree of τ') the strictly binary tree which is obtained from τ by excising all the vertical edges and fusing their endpoint vertices. We say that two C-trees are *equivalent* if one can be converted to the other by rotation with respect to a vertical axis. For example, herewith the C-trees corresponding to the only two terms with two commutators:

 $\Rightarrow$  and  $\Rightarrow$  .

Clearly, they can be converted to each other by a single vertical rotation, and this means that, for each combination $\boldsymbol{l} \in \mathrm{C}_3^{\nu}$ there exists another 3-tuple $\boldsymbol{k} \in \mathrm{C}_3^{\nu}$ such that $\mathcal{L}_1(a(c_{l_1}h), a(c_{l_2}h), a(c_{l_3}h)) = -\mathcal{L}_2(a(c_{k_1}h), a(c_{k_2}h), a(c_{k_3}h))$, where $\mathcal{L}_1$ and $\mathcal{L}_2$ are the integrands of the two integrals, respectively. In general, it is not the number of trees that matters in numerical calculation but the number of equivalence classes of C-trees (Iserles & Nørsett 1997).

Even more important are the savings that follow by using the *Jacobi identity,* since many commutators can be expressed as a linear combination of other commutators. This has been already observed in (Iserles & Nørsett 1997), but the most significant result in this area is the important paper of Munthe-Kaas & Owren (1998), who employ the theory of graded free Lie algebras to reduce the volume of computation in Magnus expansions and other Lie-group methods.

We conclude this section by describing the order-4 discretized Magnus expansion from (Iserles & Nørsett 1997). Its detailed derivation draws upon the range of ideas and techniques that have been described above. Thus, to time-step from t_N to $t_{N+1} = t_N + h$ we evaluate the matrix a at the Gaussian points,

$$a_1 = a(t_N + (\tfrac{1}{2} - \tfrac{\sqrt{3}}{6})h), \qquad a_2 = a(t_N + (\tfrac{1}{2} + \tfrac{\sqrt{3}}{6})h),$$

whence

$$\sigma_{N+1} = \tfrac{1}{2}(a_1 + a_2) + \tfrac{\sqrt{3}}{12}h^2[a_2, a_1] + \tfrac{1}{80}h^3[a_2 - a_1, [a_2, a_1]] \tag{2.11}$$

and $y_{N+1} = \mathrm{e}^{\sigma_{N+1}} y_N$.

3 Trees, order and time-symmetry

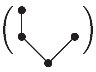
The first step in implementing the Magnus expansion (2.4) for either numerical or perturbative ends is a truncation of infinite series. It has been proved in (Iserles

& Nørsett 1997) that, except for $m = 0$, $\tau \in \mathbb{T}_m$ implies $H_\tau(t) = \mathcal{O}\big(t^{\beta+1}\big)$, where $\beta \geq m+1$. Therefore, for every $p \geq 2$, the function

$$\sigma_p(t) := \sum_{m=0}^{p-2} \sum_{\tau \in \mathbb{T}_m} \alpha(\tau) \int_0^t H_\tau(\xi) \mathrm{d}\xi \tag{3.1}$$

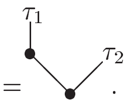
approximates σ to order p, i.e. $\sigma_p(t) - \sigma(t) = \mathcal{O}\big(t^{p+1}\big)$. Our claim is that similar goal can be attained, in general, with far fewer terms.

Given $\tau \in \mathbb{T}_m$ for some $m \in \mathbb{Z}^+$, we define the *power* of τ, denoted by $\operatorname{pwr} \tau$, as the least integer k such that $H_\tau(t) = \mathcal{O}\big(t^k\big)$ for *every* sufficiently smooth matrix function a. We designate by $\mathbb{F}_k$ the set of all the trees τ of power $k \geq 0$. Clearly $\operatorname{pwr}(\bullet) = 0$ and it is easy to verify by direct calculation that

pwr () $= 2$.

With little more effort, we can completely elucidate the power of every tree τ from the recursive rules that have been employed in its construction at the first place.

Lemma 1 *Suppose that*

$\tau =$  .

Then

$$\operatorname{pwr} \tau = \begin{cases} \operatorname{pwr} \tau_1 + \operatorname{pwr} \tau_2 + 1, & \tau_1 \neq \tau_2, \\ \operatorname{pwr} \tau_1 + \operatorname{pwr} \tau_2 + 2, & \tau_1 = \tau_2. \end{cases} \tag{3.2}$$

Proof Suppose that

$$H_{\tau_l}(t) = c_l t^{p_l} + d_l t^{p_l+1} + \mathcal{O}\big(t^{p_l+2}\big),$$

where $p_l = \operatorname{pwr} \tau_l$, $l = 1, 2$. Then

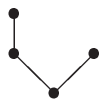
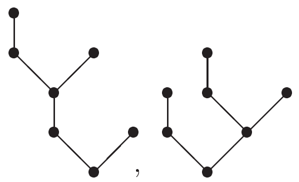
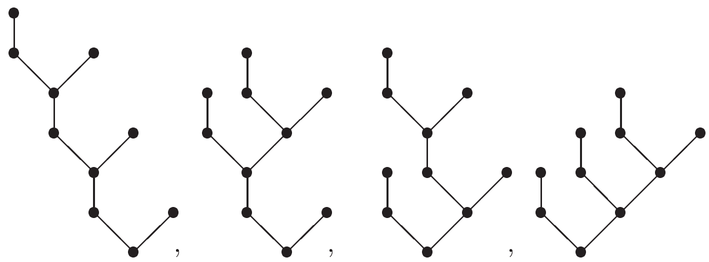
$$\begin{aligned} H_\tau(t) &= \left[\int_0^t H_{\tau_1}(\xi)\mathrm{d}\xi, H_{\tau_2}(t)\right] \\ & \left[\tfrac{1}{p_1+1} c_1 t^{p_1+1} + \tfrac{1}{p_1+2} d_1 t^{p_1+2} + \cdots,\; c_2 t^{p_2} + d_2 t^{p_2+1} + \cdots\right] \\ &= \tfrac{1}{p_1+1}[c_1, c_2] t^{p_1+p_2+1} + \left(\tfrac{1}{p_1+1}[c_1, d_2] - \tfrac{1}{p_1+2}[c_2, d_1]\right) t^{p_1+p_2} + \cdots. \end{aligned}$$

The required result follows, since $\tau_1 = \tau_2$ implies $c_1 = c_2$. □

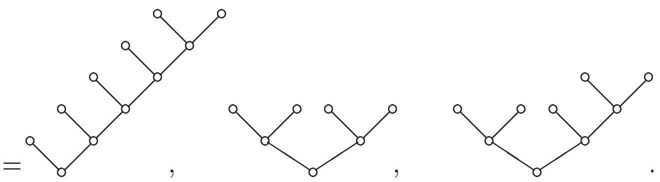
The first few sets $\mathbb{F}_m$ are displayed in Table 1. It is clear (and the point will be pursued further in the sequel) that truncating the Magnus expansion by power, rather than by the number of vertices, leads to significant savings.

Similarly to Section 2, in the context of quadrature it is convenient to consider equivalence classes of C-trees in $\mathbb{F}_k$. Thus, we denote by $\mathbb{F}_k^{\mathrm{c}}$ the set of all the equivalence

Table 1: The sets $\mathbb{F}_k$. Note that $\mathbb{F}_1 = \emptyset$

The set	The trees
$\mathbb{F}_0$	
$\mathbb{F}_2$	
$\mathbb{F}_3$	
$\mathbb{F}_4$	

classes of C-trees in $\mathbb{F}_k$. It follows that $\mathbb{F}^{\mathrm{c}}_k$, $k = 0, 2, 3, 4, 5$, are simpletons, while (choosing appropriate representatives)

$\mathbb{F}^{\mathrm{c}}_6 =$ 

Our next step it to investigate the size of the sets $\mathbb{F}_k$ and $\mathbb{F}^{\mathrm{c}}_k$, since this sheds light on the gain in efficiency that we can expect when using the *canonical expansion*

$$\tilde{\sigma}_p(t) = \sum_{k=0}^{p-1} \sum_{\tau \in \mathbb{F}_k} \alpha(\tau) \int_0^t H_\tau(\xi) \mathrm{d}\xi \tag{3.3}$$

in preference to (3.1).

Let $\varphi_k := \#\mathbb{F}_k$ and $\varphi^{\mathrm{c}}_k := \#\mathbb{F}^{\mathrm{c}}_k$, $k \in \mathbb{Z}^+$. Given $\tau \in \mathbb{F}_k$, $k \in \mathbb{N}$, it must have been obtained *either* from $\tau_1 \in \mathbb{F}_{k_1}$ and $\tau_2 \in \mathbb{F}_{k_2}$, $\tau_1 \neq \tau_2$, such that $k_1 + k_2 = k - 1$, *or* $\tau_1 = \tau_2 \in \mathbb{F}_{k_1}$ and $2k_1 = k - 2$ (in the latter case k must be even). This gives the following recurrences,

$$\begin{aligned}
\varphi_0 &= 1, \\
\varphi_{2k11} &= \sum_{l=0}^{2k-2} \varphi_l \varphi_{2k-2-l} - \varphi_{k-1}, \qquad k \in \mathbb{N}, \\
\varphi_{2k} &= \sum_{l=0}^{2k-1} \varphi_l \varphi_{2k-1-l} + \varphi_{k-1}, \qquad k \in \mathbb{N}.
\end{aligned}$$

Letting $\Phi(z) = \sum_{k=0}^{\infty} \varphi_k z^k$ be the generating function of the sequence $\{\varphi_k\}_{k=0}^{\infty}$, we can obtain from the above the functional equation

$$\Phi(z) = 1 + z[\Phi(z)]^2 + z(z-1)\Phi(z^2).$$

The latter equation has not proved helpful in elucidating the asymptotic behaviour of the sequence $\{\varphi_k\}_{k=0}^{\infty}$. Instead, we have resorted to numerical means, which seem to indicate that

$$\limsup_{k\to\infty} \varphi_k^{1/k} \approx 3.1167417747. \tag{3.4}$$

This should be compared with $\theta_m = \#\mathbb{T}_m$ which obeys $\limsup_{m\to\infty} \theta_m^{1/m} = 4$ (Iserles & Nørsett 1997).

Similarly to θ_m and φ_k, we let θ_m^{c} and φ_k^{c} denote the cardinality of the sets $\mathbb{T}_m^{\mathrm{c}}$ and $\mathbb{F}_k^{\mathrm{c}}$ respectively. The sequence $\{\theta_m^{\mathrm{c}}\}_{m=0}^{\infty}$ has been identified in (Iserles & Nørsett 1997) with *Wedderburn–Ethrington numbers* and it is known that $\limsup_{m\to\infty} {\theta_m^{\mathrm{c}}}^{1/m} \approx 2.483253536$. To investigate the asymptotic behaviour of the sequence $\{\varphi_k^{\mathrm{c}}\}_{k=0}^{\infty}$ we again form the recurrence relations and the generating function $\Phi^{\mathrm{c}}(z) := \sum_{k=0}^{\infty} \varphi_k^{\mathrm{c}} z^k$.

We can obtain an element in $\mathbb{F}_{2s}^{\mathrm{c}}$ in one of two ways. Firstly, we can combine $\tau_1 \in \mathbb{F}_l^{\mathrm{c}}$ with $\tau_2 \in \mathbb{F}_{2s-l-1}^{\mathrm{c}}$ for some $0 \le l \le s-1$. Secondly, we can obtain an element in $\mathbb{F}_{2s}^{\mathrm{c}}$ by combining each element in $\mathbb{F}_{s-1}^{\mathrm{c}}$ with itself. Altogether, we have

$$\varphi_{2s}^{\mathrm{c}} = \sum_{l=0}^{s-1} \varphi_l^{\mathrm{c}} \varphi_{2s-l-1}^{\mathrm{c}} + \varphi_{s-1}^{\mathrm{c}} = \tfrac{1}{2} \sum_{l=0}^{2s-1} \varphi_l^{\mathrm{c}} \varphi_{2s-l-1}^{\mathrm{c}} + \varphi_{s-1}^{\mathrm{c}}, \qquad s \in \mathbb{N}.$$

Likewise, for $\mathbb{F}_{2s+1}^{\mathrm{c}}$, we combine $\tau_1 \in \mathbb{F}_l^{\mathrm{c}}$ with $\tau_2 \in \mathbb{F}_{2s-l}^{\mathrm{c}}$, where $0 \le l \le s-1$. Moreover, when $l = s$ and both τ_1 and τ_2 lie in $\mathbb{F}_s^{\mathrm{c}}$, we have $\frac{1}{2}(\varphi_s^{\mathrm{c}} - 1)\varphi_s^{\mathrm{c}}$ combination of distinct terms (as well as φ_s^{c} combinations of identical terms, which are counted in $\mathbb{F}_{2s+2}^{\mathrm{c}}$). Therefore,

$$\varphi_{2s+1}^{\mathrm{c}} = \tfrac{1}{2} \sum_{l=0}^{2s} \varphi_l^{\mathrm{c}} \varphi_{2s-l}^{\mathrm{c}} - \tfrac{1}{2}\varphi_s^{\mathrm{c}}.$$

Brief manipulation affirms the identity

$$\Phi^{\mathrm{c}}(z) = 1 + \tfrac{1}{2} z[\Phi^{\mathrm{c}}(z)]^2 + (z^2 - \tfrac{1}{2}z)\Phi^{\mathrm{c}}(z^2). \tag{3.5}$$

Lemma 2 *It is true that*

$$\limsup_{k\to\infty} \varphi_k^{\mathrm{c}\,1/k} = 2. \tag{3.6}$$

Proof We commence by noting that Φ^{c} has a finite radius $r \geq 0$ of convergence about the origin, since it diverges for $z = 1$. Moreover, $r \geq \frac{1}{4}$, because $\sum_{i=0}^{k} \varphi_k^{\mathrm{c}} \leq \sum_{i=0}^{k} \theta_i$ and $\sum_{m=0}^{\infty} \theta_m z^m$ has the radius of convergence $\frac{1}{4}$ (Iserles & Nørsett 1997).

Since $\varphi_k^{\mathrm{c}} \geq 0$, it follows that for every $|z| < r$

$$|\Phi^{\mathrm{c}}(z)| \leq \sum_{k=0}^{\infty} \varphi_k^{\mathrm{c}} |z|^k = \Phi^{\mathrm{c}}(|z|).$$

Therefore $|\Phi^{\mathrm{c}}(z)| \leq \Phi^{\mathrm{c}}(\frac{1}{2})$, $|z| < \frac{1}{2}$, provided that Φ^{c} is summable at $\frac{1}{2}$. Letting $z = \frac{1}{2}$ in (3.5), we readily obtain $\Phi^{\mathrm{c}}(\frac{1}{2}) = 2$. Consequently, $r \geq \frac{1}{2}$.

Suppose next that r exceeds $\frac{1}{2}$. Therefore $z = \frac{1}{2}$ is within the domain of convergence and $\mathrm{d}\Phi^{\mathrm{c}}(\frac{1}{2})/\mathrm{d}z$ is well-defined. Differentiating the functional equation yields

$$\frac{\mathrm{d}\Phi^{\mathrm{c}}(z)}{\mathrm{d}z} = \tfrac{1}{2}[\Phi^{\mathrm{c}}(z)]^2 + z\Phi^{\mathrm{c}}(z)\frac{\mathrm{d}\Phi^{\mathrm{c}}(z)}{\mathrm{d}z} + (2z - \tfrac{1}{2})\Phi^{\mathrm{c}}(z^2) + 2z(z^2 - \tfrac{1}{2}z)\frac{\mathrm{d}\Phi^{\mathrm{c}}(z^2)}{\mathrm{d}z}$$

and, letting $z = \frac{1}{2}$, we obtain $\Phi^{\mathrm{c}}(\frac{1}{4}) = -4$. This is clearly impossible, since the power series of Φ^{c} has nonnegative coefficients. Therefore it is impossible for r to exceed $\frac{1}{2}$ and we deduce that this is the radius of convergence of the series.

The lemma follows from the root test for convergence, since

$$2 = \frac{1}{r} = \limsup_{k\to\infty} \varphi_k^{1/k}.$$

$\square$

Table 2 displays the numbers $\theta_m, \theta_m^{\mathrm{c}}, \varphi_m$ and φ_m^{c} and it it clear that the overall number of trees in the expansion is reduced a great deal by opting for the canonical expansion (3.3) in place of (2.4), whether with explicit integrals or with quadrature formulae.

The canonical expansion (3.3) has another important and most welcome characteristics: as we are about to prove, it is time-symmetric.

A dynamical system

$$x(t) = X_{t-t_0} x(t_0), \qquad t \geq 0,$$

is said to be *time-symmetric* if

$$X_t \circ X_{-t} = \mathrm{Id}, \qquad t \geq 0, \tag{3.7}$$

in other words when, for any $t_0 < t_1$, the integration from t_0 to t_1, followed by integration from t_1 back to t_0, recovers exactly the initial value (Sanz-Serna & Calvo 1994). Time-symmetry is important in the context of symplectic integration (Reich 1996) but, within the present context, its main importance is that it implies that $X_t = \mathrm{e}^{F_t}$, where F_t can be expanded in *odd* powers of t (Hairer & Wanner 1991). For

Table 2: The cardinality of different sets of binary trees.

m	θ_m	φ_m	θ_m^{c}	φ_m^{c}
0	1	1	1	1
1	1	0	1	0
2	2	1	1	1
3	5	2	2	1
4	14	4	3	1
5	42	8	6	1
6	132	21	11	3
7	429	52	23	4
8	1430	138	46	7
9	4862	362	98	11
10	16796	980	207	20

completeness, we sketch the proof of this classical result. Thus, assuming arbitrarily high smoothness, we can expand

$$X_t = \sum_{l=0}^{\infty} x_l (t\mathrm{D})^l,$$

where D is the differential operator – this is equivalent to the statement that

$$X_t g(t_0) = \sum_{l=0}^{\infty} x_l t^l g^{(l)}(t_0)$$

for every analytic function g and for every t in the domain of analyticity. We stipulate that the generating function

$$x(z) = \sum_{l=0}^{\infty} x_l z^l$$

is analytic for sufficiently small $|z|$ and that $x_0 = 1$, the latter being necessary for consistency. It is now trivial to verify that

$$\begin{aligned} X_t \circ X_{-t} &= \sum_{l=0}^{\infty} x_l (t\mathrm{D})^l \sum_{j=0}^{\infty} x_j (-t\mathrm{D})^j \\ &= \sum_{l=0}^{\infty} \left[\sum_{j=0}^{l} (-1)^j x_j x_{l-j} \right] (t\mathrm{D})^l. \end{aligned}$$

Therefore, (3.7) is equivalent to

$$\sum_{j=0}^{l} (-1)^j x_j x_{l-j} = 0, \qquad l \in \mathbb{N},$$

and this, in turn, is equivalent to $x(z)x(-z) \equiv 1$. Since $x(0) = 1$, the analytic function g is nonzero in a sufficiently small neighbourhood of the origin, where $f(z) := \log x(z)$ is well-defined. We deduce that f is analytic and odd, therefore

$$f(z) = \sum_{l=0}^{\infty} f_l z^{2l+1}.$$

By construction, f is the generating function of F_t, hence we conclude that

$$F_t = \sum_{l=0}^{\infty} f_l (t\mathrm{D})^{2l+1}.$$

Theorem 3 *Let $X_t y_0 = \mathrm{e}^{\tilde{\sigma}_p(t)} y_0$, where $\tilde{\sigma}_p$ is the truncated canonical Magnus expansion (3.3). The X_t is time-symmetric.*

Proof To persuade ourselves that the assertion of the theorem makes sense, we let

$$\sigma(t) = \int_0^t a(\xi)\mathrm{d}\xi - \tfrac{1}{2}\int_0^t \int_0^{\xi_1} [a(\xi_2), a(\xi_1)]\mathrm{d}\xi_1 \mathrm{d}\xi_2 + \cdots$$

be the Magnus expansion corresponding to the equation (1.1) and denote by ρ the Magnus expansion of the equation

$$z' = -a(t_1 - t)z, \quad t \geq 0, \qquad z(0) = y(t_1). \tag{3.8}$$

Brief calculation affirms that

$$\rho(t) = -\int_0^t a(t_1 - \xi)\mathrm{d}\xi - \tfrac{1}{2}\int_0^t \int_0^{\xi_1} [a(t_1 - \xi_2), a(t_1 - \xi_1)]\mathrm{d}\xi_2 \mathrm{d}\xi_1 + \cdots,$$

therefore

$$\rho(t_1) = -\int_0^{t_1} a(\xi)\mathrm{d}\xi - \tfrac{1}{2}\int_0^{t_1} \int_{\xi_1}^{t_1} [a(\xi_2), a(\xi_1)]\mathrm{d}\xi_2 \mathrm{d}\xi_1.$$

According to (3.7), time-symmetry is equivalent to the statement that, for every $t_1 \geq 0$, integrating (1.1) from $t = 0$ to $t = t_1$, followed by the integration of (3.8) in the same range, must bring us back to the initial condition. Since the exact differential equation is time-symmetric, it is true that

$$\sigma(t_1) + \rho(t_1) \equiv 0. \tag{3.9}$$

This can be verified at once for the first few terms, since

$$\int_0^{t_1} \int_0^{t_1} [a(\xi_2), a(\xi_1)]\mathrm{d}\xi_2 \mathrm{d}\xi_1 \equiv 0$$

and we may deduce that the truncated canonical expansion is time-symmetric for $p = 0, 1$.

More importantly, our analysis points out a strategy for the proof of the theorem. The identity (3.9) is always true for sufficiently small $t_1 > 0$. Let

$$\gamma_l(t) := \sum_{\tau\in\mathbb{F}_l} \alpha(\tau) \int_0^t H_\tau(\xi)\mathrm{d}\xi, \qquad l \in \mathbb{Z}^+,$$

and denote by $\delta_l(t)$ the corresponding terms for ρ. Hence

$$\tilde{\sigma}_p = \sum_{l=0}^{p} \gamma_l, \qquad \tilde{\rho}_p = \sum_{l=0}^{p} \delta_l$$

and $\gamma_l(t), \delta_l(t) = \mathcal{O}\big(t^l\big)$. We have already proved that $\gamma_l(t) + \delta_l(t) \equiv 0$, $l = 0, 1$. Suppose that

$$\gamma_l(t) + \delta_l(t) \equiv 0, \qquad l = 0, 1, \ldots, p-1,$$

and assume that, given a matrix function a, there exists $\tilde{p} \geq p$ such that

$$\gamma_p(t) + \delta_p(t) = ct^{\tilde{p}} + \mathcal{O}\big(t^{\tilde{p}+1}\big), \qquad c \neq 0.$$

Suppose first that $\tilde{p} = p$. Then we reach a contradiction, since

$$\sum_{l=0}^{\infty}[\gamma_l(t) + \delta_l(t)] \equiv 0, \qquad \sum_{l=0}^{p}[\gamma_l(t) + \delta_l(t)] = ct^p + \mathcal{O}\big(t^{p+1}\big)$$

implies that

$$\sum_{l=p+1}^{\infty} [\gamma_l(t) + \delta_l(t)] = \mathcal{O}(t^p),$$

which is impossible.

Assume thus that $\tilde{p} > p$. It is easy to verify that there exists $q > p$ such that

$$\sum_{l=p}^{q}[\gamma_l(t) + \delta_l(t)] = e_1 t^q + \mathcal{O}\big(t^{q+1}\big), \qquad e_1 \neq 0.$$

For example, if $\tilde{p} = p + 1$, we let $q = \tilde{p}$, if $\tilde{p} = p + 2$ and $\gamma_{p+1}(t) + \delta_{p+1}(t) = \mathcal{O}\big(t^{\hat{p}}\big)$ then $q = \min\{\tilde{p}, \hat{p}\}$ and so on. This is a contradiction, since, again,

$$\sum_{l=0}^{\infty}[\gamma_l(t) + \delta_l(t)] \equiv 0, \qquad \sum_{l=0}^{q}[\gamma_l(t) + \delta_l(t)] = e_1 t^q + \mathcal{O}\big(t^{q+1}\big),$$

imply

$$\sum_{l=q+1}^{\infty} [\gamma_l(t) + \delta_l(t)] = -e_1 t^q + \mathcal{O}\big(t^{q+1}\big),$$

in variance with the definition of γ_l and δ_l. We therefore deduce that no such $\tilde{p}$ exists, hence $\gamma_l + \delta_l \equiv 0$ for all $l \in \mathbb{Z}^+$ and the truncated canonical Magnus expansion is time-symmetric. □

Theorem 4 *The order of the truncated canonical Magnus expansion (3.3) is* $2\lfloor (p+1)2/\rfloor$.

Proof Because of time-symmetry, both $\sigma(t)$ and $\sigma_p(t)$ can be expanded in odd powers of t. Therefore

$$\sigma_p(t) = \sigma(t) + \mathcal{O}\big(t^{\hat{p}+1}\big)\,,$$

where $\hat{p}$ is even. The theorem follows since, by construction, $\hat{p} \ge p$. $\square$

It is important to bear in mind that we did not prove that every term $\int_0^t H_\tau(\xi)\mathrm{d}\xi$ such that $\tau \in \mathbb{F}_{2s-1}$, say, is necessarily $\mathcal{O}\big(t^{2s+1}\big)$: it is the linear combination of terms that increases the order! Foe example, let us consider the case $p = 3$. There are exactly two terms in $\mathbb{F}_3$ and it is possible to show that

$$\begin{aligned} I_1(t) &:= \int_0^t\int_0^{\xi_1}\int_0^{\xi_2} [[a(\xi_3), a(\xi_2)], a(\xi_1)]\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1 = -\tfrac{1}{24}[[\beta,\alpha],\alpha]t^4 + \mathcal{O}\big(t^5\big)\,,\\ I_2(t) &:= \int_0^t\int_0^{\xi_1}\int_0^{\xi_1} [a(\xi_3), [a(\xi_2), a(\xi_1)]]\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1 = \tfrac{1}{8}[[\beta,\alpha],\alpha]t^4 + \mathcal{O}\big(t^5\big)\,,\end{aligned}$$

where $a(t) = \alpha + \beta t + \mathcal{O}\big(t^2\big)$ (Iserles et al. 1998). Therefore

$$\tfrac{1}{4}I_1(t) + \tfrac{1}{24}I_2(t) = \mathcal{O}\big(t^5\big)\,.$$

Note that Theorems 3 and 4 leave the integrals intact, while numerical implementation of Magnus expansions requires the replacement of integrals by quadrature. However, it is trivial to ascertain that the multivariate quadrature methods from Section 2 are time-symmetric, provided that the quadrature points $c_1, c_2, \ldots, c_\nu$ are symmetric with respect to the point $\frac{1}{2}$. This corresponds to their two natural choices, as either Gauss–Legendre or Gauss–Lobatto points.

An immediate consequence of Theorem 4 and the last paragraph is that the last term in (2.11) can be removed without affecting the order. In other words, the scheme

$$\sigma_{n+1} = \tfrac{1}{2}(a_1 + a_2) + \tfrac{\sqrt{3}}{12}h^2[a_2, a_1]$$

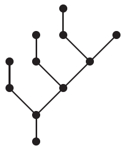
is of order 4.

Time-symmetry has proved itself important in the context of symplectic integration because it leads to superior long-term behaviour of the numerical solver (Reich 1996). It makes sense to suspect that it plays similar role in the context of Magnus series, but this question has not yet been investigated.

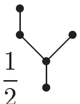
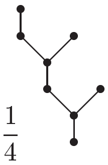
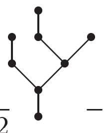
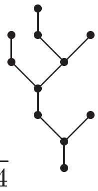
4 An order-6 Magnus expansion

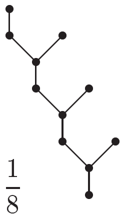
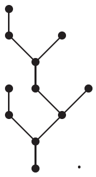
According to Theorem 4, we need to let $p = 5$ in the canonical expansion (3.3) to obtain order 6. According to Table 2, this results in eight trees, except that (adding an extra root to emphasize that we are dealing with $\int_0^t H_\tau(\xi)\mathrm{d}\xi$, rather than with

$H_\tau(t)$) the coefficient of



is zero. Mildly abusing notation, we write the truncated canonical Magnus expansion corresponding to the order-6 method in the form

$\tilde{\sigma}_5(t) =$ $-\frac{1}{2}$  $+\frac{1}{4}$  $+\frac{1}{12}$  $-\frac{1}{24}$ 

$-\frac{1}{8}$  $-\frac{1}{24}$  . (4.1)

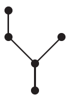
Requiring order 6, we employ Gauss–Legendre quadrature with $\nu = 3$, therefore

$$c_1 = \tfrac{1}{2} - \tfrac{\sqrt{15}}{10} \qquad c_2 = \tfrac{1}{2}, \qquad c_3 = \tfrac{1}{2} + \tfrac{\sqrt{15}}{10}.$$

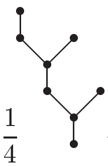
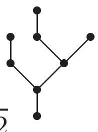
Letting $a_l = a(t_N + c_l h)$, $l = 1, 2, 3$, we commence by evaluating the first integral,

 $\Rightarrow \quad h(\tfrac{5}{18}a_1 + \tfrac{4}{9}a_2 + \tfrac{5}{18}a_3).$ (4.2)

Likewise, we use the approach of Section 2 to approximate the second integral,

 $\Rightarrow \quad \sqrt{15}h^2(\tfrac{1}{27}[a_1, a_2] + \tfrac{1}{54}[a_1, a_3] + \tfrac{1}{27}[a_2, a_3]).$ (4.3)

In principle, we could have continued with the multivariate quadrature formulae from (Iserles & Nørsett 1997) and Section 2 for subsequent integrals, accompanied if and when necessary by the Jacobi identity. Thus, for example,

$\frac{1}{4}$  $+\frac{1}{12}$  $\Rightarrow \quad h^3(\tfrac{47}{13608}[a_1, [a_1, a_2]] + \tfrac{5}{3024}[a_1, [a_1, a_3]]$

$$+ \tfrac{97}{13608}[a_1, [a_2, a_3]] - \tfrac{19}{3402}[a_2, [a_1, a_2]] + \tfrac{19}{3402}[a_2, [a_2, a_3]]$$

$$- \tfrac{97}{13608}[a_3, [a_1, a_2]] - \tfrac{5}{3024}[a_3, [a_1, a_3]] - \tfrac{47}{13608}[a_3, [a_2, a_3]]).$$ (4.4)

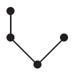
This, however, is suboptimal and we can do substantially better in terms of commutator evaluations by adopting a different approach. Suppose that

$$a(t) = \alpha + \beta t + \gamma t^2 + \delta t^3 + \cdots$$

and let

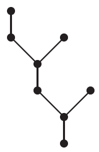
$$\mu = [\alpha, \delta], \quad \psi = [\beta, \gamma], \quad \zeta = [\alpha, \mu], \quad \tau = [\alpha, \psi], \quad \sigma = [\beta, \eta], \quad \xi = [\gamma, \theta].$$

We substitute the expansion of a into different terms. In the first instance we evaluate

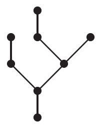


$$\Rightarrow \quad \tfrac{1}{2}\theta t^2 + \tfrac{2}{3}\eta t^3 + (\tfrac{3}{4}\mu + \tfrac{1}{6}\psi)t^4 + \cdots .$$

This is a starting point in expanding the two terms in $\mathbb{F}_3$, a task assisted by the techniques in (Iserles et al. 1998):

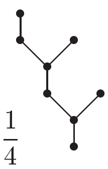
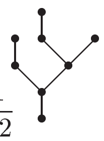


$$\Rightarrow \quad -\tfrac{1}{24}\rho h^4 - (\tfrac{1}{30}\omega + \tfrac{1}{30}\chi)h^5 - (\tfrac{1}{40}\zeta + \tfrac{1}{180}\tau + \tfrac{1}{36}\sigma + \tfrac{1}{36}\xi)h^6 - \cdots ,$$



$$\Rightarrow \quad \tfrac{1}{8}\rho h^4 + (\tfrac{2}{15}\omega + \tfrac{1}{20}\chi)h^5 + (\tfrac{1}{8}\zeta + \tfrac{1}{36}\tau + \tfrac{1}{18}\sigma + \tfrac{1}{36}\xi)h^6 + \cdots .$$

Adding up, we obtain

$\frac{1}{4}$  $+\ \frac{1}{12}$ 

$$\Rightarrow \quad (\tfrac{1}{360}\omega - \tfrac{1}{240}\chi)h^5 + (\tfrac{1}{240}\zeta + \tfrac{1}{1080}\tau - \tfrac{1}{432}\sigma - \tfrac{1}{216}\xi)h^6 + \cdots .$$

We aim to construct a quadrature formula of the form

$$h^3 \sum_{(k,l,j)\in\mathcal{B}} b_{k,l,j}[a_k, [a_l, a_j]], \tag{4.5}$$

where $\mathcal{B}$ is a set of indices. Thus, for example, in (4.4) we have

$$\mathcal{B} = \{(1,1,2), (1,1,3), (1,2,3), (2,1,2), (2,2,3), (3,1,2), (3,1,3), (3,2,3)\},$$

eight terms altogether. In the sequel we strive to find a *smaller* set $\mathcal{B}$. To this end we expand

$$\begin{aligned}[a_k,[a_l,a_j]] &= [\alpha + c_k h\beta + c_k^2 h^2\gamma, [\alpha + c_l h\beta + c_l^2 h^2\gamma + c_l^3 h^3\delta, \alpha + c_j h\beta \\ &\quad + c_j^2 h^2\gamma + c_j^3 h^3\delta]] \\ &= [\alpha + c_k h\beta + c_k^2 h^2\gamma, h(c_j - c_l)\theta + h^2(c_j^2 - c_l^2)\eta + h^3((c_j^3 - c_l^3)\mu \\ &\quad + c_j c_l (c_j - c_l)\psi)] \\ &= h(c_j - c_l)\rho + h^2\{(c_j^2 - c_l^2)\omega + c_k(c_j - c_l)\chi\} + h^3\{(c_j^3 - c_l^3)\zeta \\ &\quad + c_j c_l(c_j - c_l)\tau + c_k(c_j^2 - c_l^2)\sigma + c_k^2(c_j - c_l)\xi\} + \cdots .\end{aligned}$$

Therefore, comparing coefficients, order-6 conditions are

$$\begin{aligned}\sum_{\mathcal{B}} \tilde{b}_{k,l,j} &= 0, \\ \sum_{\mathcal{B}} (c_l + c_j)\tilde{b}_{k,l,j} &= \tfrac{1}{360}, \\ \sum_{\mathcal{B}} c_k \tilde{b}_{k,l,j} &= -\tfrac{1}{240}, \\ \sum_{\mathcal{B}} (c_l^2 + c_l c_j + c_j^2)\tilde{b}_{k,l,j} &= \tfrac{1}{240}, \\ \sum_{\mathcal{B}} c_j c_l \tilde{b}_{k,l,j} &= \tfrac{1}{1080}, \\ \sum_{\mathcal{B}} c_k(c_l + c_j)\tilde{b}_{k,l,j} &= -\tfrac{1}{432}, \\ \sum_{\mathcal{B}} c_k^2 \tilde{b}_{k,l,j} &= -\tfrac{1}{216},\end{aligned}$$

where $\tilde{b}_{k,l,j} = (c_j - c_l)b_{k,l,j}$.

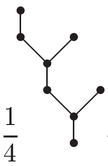
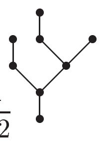
On the face of it, we have seven equations and need seven terms in $\mathcal{B}$ to satisfy them: this would represent a saving of just one term over (4.4). This estimate, however, is pessimistic, since it disregards symmetries in Gauss–Legendre nodes. `MATLAB` and `Maple` search has resulted in what appears to be the minimal set,

$$\mathcal{B} = \{(1,1,2),(1,2,3),(3,1,2),(3,2,3)\},$$

with

$$b_{1,1,2} = \tfrac{1}{432}, \quad b_{1,2,3} = \tfrac{5}{432}, \quad b_{3,1,2} = -\tfrac{5}{432}, \quad b_{3,2,3} = -\tfrac{1}{432}.$$

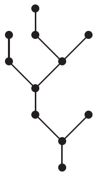
We have thus obtained the 6th-order quadrature

$\frac{1}{4}$  $+ \frac{1}{12}$ 

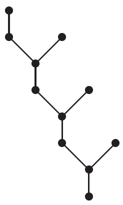
$$\Rightarrow \quad \tfrac{1}{432}h^3([a_1,[a_1,a_2]] + 5[a_1,[a_2,a_3]] - 5[a_3,[a_1,a_2]] - [a_3,[a_2,a_3]]) \tag{4.6}$$

which uses just four terms.

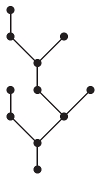
Finally, we need to approximate the integrals corresponding to the linear combination of the three terms in $\mathbb{F}_4$. We again expand each integral in power series,



$$\Rightarrow \quad -\tfrac{1}{40}[\alpha,\rho]h^5 - (\tfrac{1}{120}[\alpha,\chi] + \tfrac{1}{45}[\alpha,\omega] + \tfrac{1}{48}[\beta,\rho])h^6 + \cdots$$

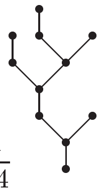
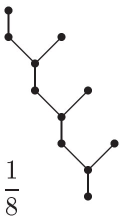
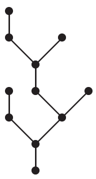


$$\Rightarrow \quad \tfrac{1}{120}[\alpha,\rho]h^5 + (\tfrac{1}{180}[\alpha,\chi] + \tfrac{1}{180}[\alpha,\omega] + \tfrac{1}{144}[\beta,\rho])h^6 + \cdots,$$



$$\Rightarrow \quad -\tfrac{1}{30}[\alpha,\rho]h^5 - (\tfrac{1}{36}[\alpha,\chi] + \tfrac{1}{36}[\alpha,\omega] + \tfrac{1}{72}[\beta,\rho])h^6 + \cdots.$$

Consequently,

$-\dfrac{1}{24}$  $-\dfrac{1}{8}$  $-\dfrac{1}{24}$ 

$$\Rightarrow \quad \tfrac{1}{720}[\alpha,\rho]h^5 + (\tfrac{7}{8640}[\alpha,\chi] + \tfrac{1}{720}[\alpha,\omega] + \tfrac{1}{1728}[\beta,\rho])h^6 + \cdots.$$

We seek a quadrature rule of the form

$$h^4 \sum_{(k,l,j,i)\in\mathcal{A}} b_{k,l,j,i}[a_k,[a_l,[a_j,a_i]]]. \tag{4.7}$$

Since

$$\begin{aligned}
[a_k,[a_l,[a_j,a_i]]] &= [\alpha + c_k h\beta, [\alpha + c_l h\beta, [\alpha + c_j h\beta + c_j^2 h^2\gamma, \alpha + c_i h\beta + c_i^2 h^2 \gamma]]] \\
&= [\alpha + c_k h\beta, [\alpha + c_l h\beta, h(c_i - c_j)\theta + h^2(c_i^2 - c_j^2)\eta]] \\
&= [\alpha + c_k h\beta, h(c_i - c_j)\rho + h^2((c_i^2 - c_j^2)\omega + c_l(c_i - c_j)\chi)] \\
&= h(c_i - c_j)[\alpha,\rho] + h^2\{c_l(c_i - c_j)[\alpha,\chi] + (c_i^2 - c_j^2)[\alpha,\omega] \\
&\quad + c_k(c_i - c_j)[\beta,\rho]\} + \cdots,
\end{aligned}$$

we obtain the order-6 conditions

$$\begin{aligned}
\sum_{\mathcal{A}} \tilde{b}_{k,l,j,i} &= \frac{1}{720}, \\
\sum_{\mathcal{A}} c_l \tilde{b}_{k,l,j,i} &= \frac{7}{8640}, \\
\sum_{\mathcal{A}} (c_i + c_j) \tilde{b}_{k,l,j,i} &= \frac{1}{720}, \\
\sum_{\mathcal{A}} c_k \tilde{b}_{k,l,j,i} &= \frac{1}{1728},
\end{aligned}$$

Remarkably, they can be satisfied by choosing just two terms,

$$\mathcal{A} = \{(3,1,1,3), (1,3,1,3)\},$$

with the weights

$$b_{3,1,1,3} = -\frac{1}{5184} + \frac{\sqrt{15}}{4320}, \qquad b_{1,3,1,3} = \frac{1}{5184} + \frac{\sqrt{15}}{4320}.$$

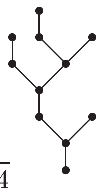
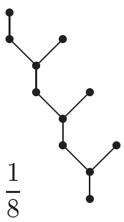
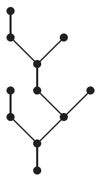
Perhaps even more remarkably, the Jacobi identity (2.1) gives

$$[a_3,[a_1,[a_1,a_3]]] + [a_1,[[a_1,a_3],a_3]] + [[a_1,a_3],[a_3,a_1]] = 0$$

therefore $[[a_1,a_3],[a_3,a_1]] = 0$ implies that

$$[a_3,[a_1,[a_1,a_3]]] = [a_1,[a_3,[a_1,a_3]]].$$

We conclude that the order-6 conditions can be satisfied by using just a single term in (4.7),

$$-\frac{1}{24}$$  $$-\frac{1}{8}$$  $$-\frac{1}{24}$$  $$\Rightarrow \quad \tfrac{\sqrt{15}}{2160} h^4 [a_1,[a_3,[a_1,a_3]]]. \qquad (4.8)$$

Totting up (4.2),(4.3),(4.6) and (4.8), we obtain the order-6 method

$$\begin{aligned}
\sigma_{n+1} = {} & \tfrac{1}{18} h (5a_1 + 8a_2 + 5a_3) - \tfrac{\sqrt{15}}{108} h^2 (2[a_1,a_2] + [a_1,a_3] + 2[a_2,a_3]) \\
& + \tfrac{1}{432} h^3 ([a_1,[a_1,a_2]] + 5[a_1,[a_2,a_3]] - 5[a_3,[a_1,a_2]] \\
& - [a_3,[a_2,a_3]]) + \tfrac{\sqrt{15}}{2160} h^4 [a_1,[a_3,[a_1,a_3]]].
\end{aligned} \qquad (4.9)$$

The implementation of (4.9) requires just three function evaluations, as well as the computation of seven commutators:

$$a_{1,2}=[a_1,a_2],\quad a_{1,3}=[a_1,a_3],\quad a_{2,3}=[a_2,a_3],$$
$$a_{1,3,1,2}=[a_1-5a_3,a_{1,2}],\quad a_{1,3,2,3}=[5a_1-a_3,a_{2,3}],\quad a_{1,3,1,3}=[a_1,[a_3,a_{1,3}]],$$

whereby the method reads

$$\begin{aligned}\sigma_{n+1}={}&\tfrac{1}{18}h(5a_1+8a_2+5a_3)-\tfrac{\sqrt{15}}{108}h^2(2a_{1,2}+a_{1,3}+2a_{2,3})\\&+\tfrac{1}{432}h^3(a_{1,3,1,2}+a_{1,3,2,3})+\tfrac{\sqrt{15}}{2160}h^4a_{1,3,1,3}.\end{aligned}$$

5 Numerical examples

The purpose of this section is neither to present a comprehensive numerical study of the Magnus algorithm nor to compare it with other numerical time-stepping methods. Our sole goal is to demonstrate that the practice complies with theory. To this end we present a small number of computational examples, all in a fixed step-size setting. We refer the reader to (Iserles et al. 1998) for the discussion of error-control and variable time-stepping strategies in the context of Magnus series.

Our first example is the equation

$$y'=\begin{bmatrix}0&1\\-\frac{1}{(1+t)^2}&0\end{bmatrix}y,\quad t\ge 0,\qquad y(0)=I, \tag{5.1}$$

which evolves on $\mathrm{SL}_2(\mathbb{R})$. The exact solution of (5.1) is

$$y(t)=\begin{bmatrix}(1+t)^{1/2}[\cos\theta(t)-\frac{\sqrt{3}}{3}\sin\theta(t)] & \frac{2\sqrt{3}}{3}(1+t)^{1/2}\sin\theta(t)\\ -\frac{2\sqrt{3}}{3}(1+t)^{-1/2}\sin\theta(t) & (1+t)^{-1/2}[\cos\theta(t)+\frac{\sqrt{3}}{3}\sin\theta(t)]\end{bmatrix},$$

where $\theta(t)=\frac{\sqrt{3}}{2}\log(1+t)$. Figure 1 displays $\log_{10}\|y_N-y(t_N)\|$ (i.e., the number of significant digits) for two methods, the 4th-order and the 6th-order Magnus algorithms from (Iserles & Nørsett 1997) and from the last section respectively, for three step-sizes: $h=\frac{1}{10},\frac{1}{20}$ and $\frac{1}{40}$. The main purpose of this example is to demonstrate that the behaviour is consistent with the stipulated order.

The second example is the equation

$$y'=\begin{bmatrix}0&1\\-t\sin^2 t&0\end{bmatrix}y,\quad t\ge 0,\qquad y(0)=I, \tag{5.2}$$

whose solution is highly oscillatory and of increasing amplitude. We have solved (5.2) with two 6th-order methods: the Magnus expansion (4.9) and the 7-stage explicit

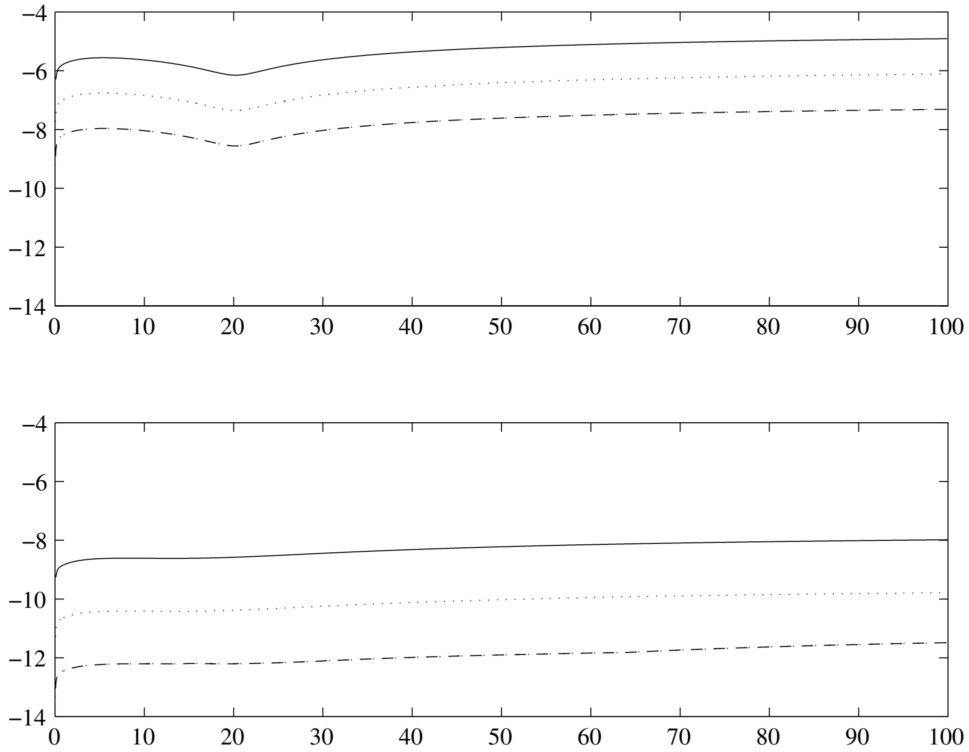


Figure 1: The number of significant digits in the solution of (5.1) by a 4th-order (upper figure) and 6th-order (lower figure) Magnus expanions. The solid line stands for $h = \frac{1}{10}$, the dot-dot line for $h = \frac{1}{20}$ and the dot-dash for $h = \frac{1}{40}$.

Runge–Kutta method with the Butcher tableau

$$\begin{array}{c|ccccccc}
0 & & & & & & & \\
\frac{1}{2} & \frac{1}{2} & & & & & & \\
\frac{2}{3} & \frac{2}{9} & \frac{4}{9} & & & & & \\
\frac{1}{3} & \frac{7}{36} & \frac{2}{9} & -\frac{1}{12} & & & & \\
\frac{5}{6} & -\frac{35}{144} & -\frac{55}{36} & \frac{35}{48} & \frac{15}{8} & & & \\
\frac{1}{6} & -\frac{1}{360} & -\frac{11}{36} & -\frac{1}{8} & \frac{1}{2} & \frac{1}{10} & & \\
1 & -\frac{41}{260} & \frac{22}{13} & \frac{43}{156} & -\frac{118}{39} & \frac{32}{195} & \frac{80}{39} & \\
\hline
 & \frac{13}{200} & 0 & \frac{11}{40} & \frac{11}{40} & \frac{4}{25} & \frac{4}{25} & \frac{13}{200}
\end{array} \tag{5.3}$$

(Hairer & Wanner 1991).

As can be observed in Figure 2, both methods have done very well in modelling a fairly complicated solution: the trajectories look virtually undistinguishable and, as a matter of fact, differ only in the fourth significant digit. Note that the solution of (5.2) lives on $\mathrm{SL}_2(\mathbb{R})$ and this feature is automatically captured by the Magnus

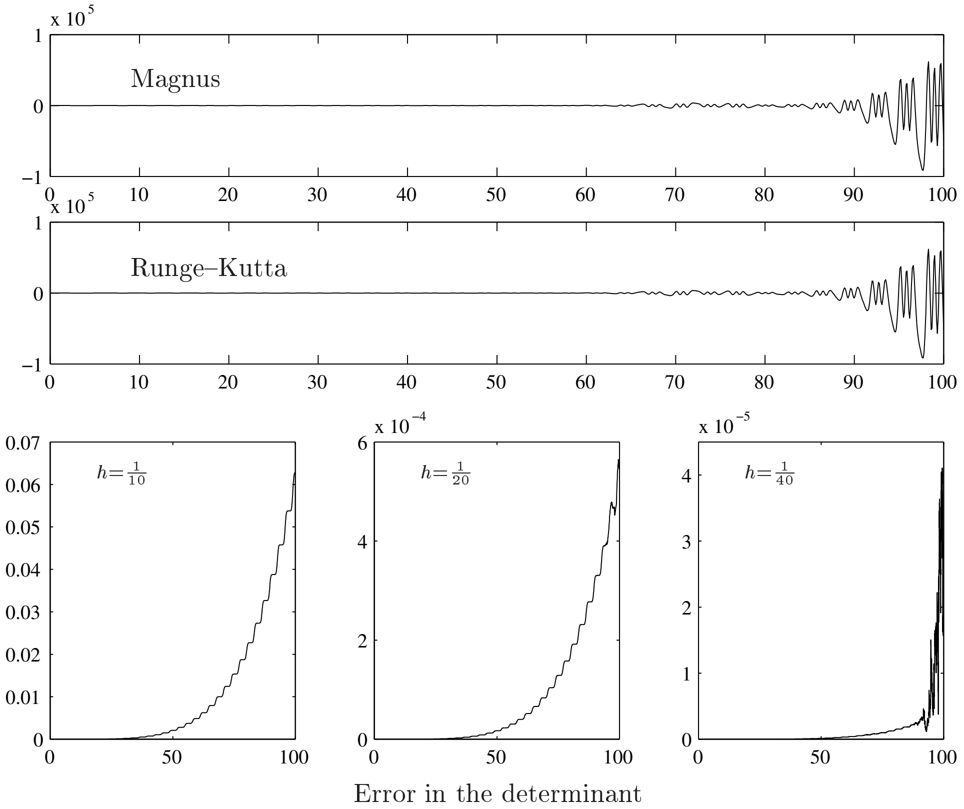


Figure 2: Numerical results for the equation (5.2). The top two figures display the $(1,1)$ component of y_n for the Magnus and Runge–Kutta methods respectively for $h = \frac{1}{10}$. The bottom three figures display $\log|\det y_n|$ for the Runge–Kutta scheme for different stepsizes.

expansion. Insofar as the Runge–Kutta is concerned, however, an exponential growth in $\log|\det y_n|$ can be observed in the figure.

Our final example is the $\mathrm{SO}_4(\mathbb{R})$ flow

$$y' = \begin{bmatrix} 0 & t\sin\frac{\pi t}{4} & 0 & 0 \\ -t\sin\frac{\pi t}{4} & 0 & t\sin\frac{\pi t}{2} & 0 \\ 0 & -t\sin\frac{\pi t}{2} & 0 & t\sin\frac{3\pi t}{4} \\ 0 & 0 & -t\sin\frac{3\pi t}{4} & 0 \end{bmatrix} y, \quad t \geq 0, \qquad y(0) = I. \quad (5.4)$$

The special orthogonal group being a compact manifold, the trajectory of $y(t)$ is bounded, and this is rendered correctly by the 6th-order Magnus expansion: the error is exactly as predicted by order considerations, while orthogonality error is nil by design. This, however, is not the case with the Runge–Kutta scheme (5.3) which, for the same step-size sequence, displays rapid onset of unstable behaviour and exponentially-growing amplitude. This phenomenon is expressed, as can be read at once from Figure 3, both in the solution trajectory y_n and in the orthogonality error $\|y_n^{\mathrm{T}} y_n - I\|$.

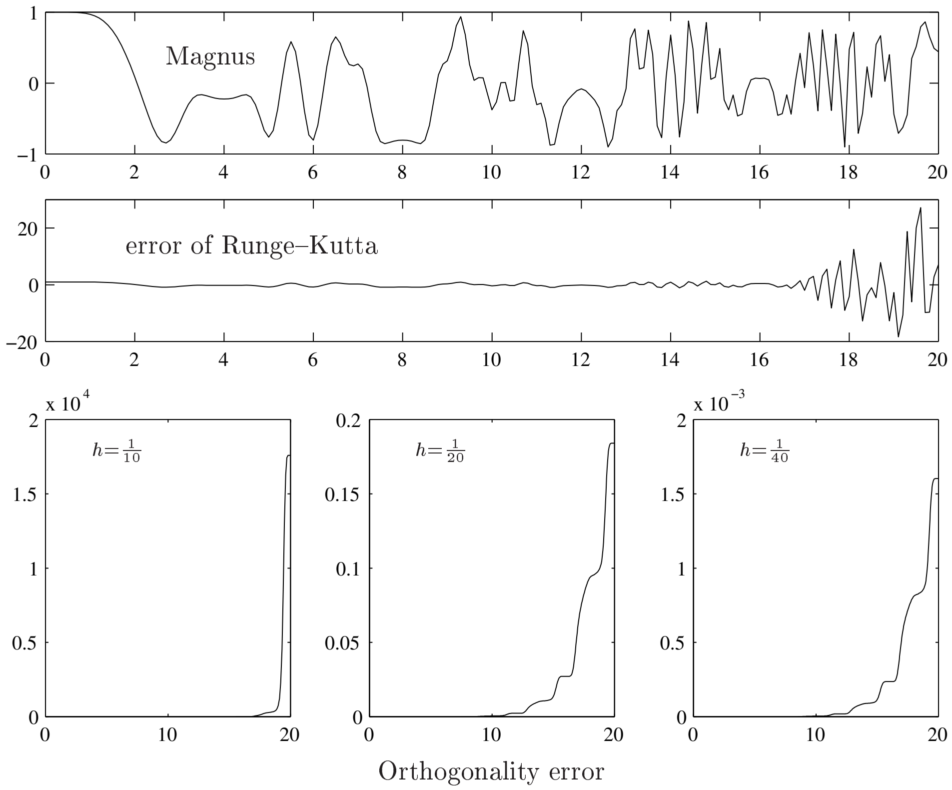


Figure 3: The $(1,1)$ component of the numerical solution of the orthogonal flow (5.4) by 6th-order Magnus and Runge–Kutta methods for $0 \leq t \leq 20$. The top figure displays the solution sequence for the Magnus method, with the *error* in the Runge–Kutta method (for $h = \frac{1}{10}$) underneath. Orthogonality error $\|y_n^{\mathrm{T}} y_n - I\|$ for the Runge–Kutta scheme with $h = \frac{1}{10}, \frac{1}{20}$ and $\frac{1}{40}$ is displayed at the bottom three figures.

This is an illustration of a phenomenon which is at the moment under active investigation, namely that in compact Lie groups Lie-group methods possess significantly better stability properties than more conventional time-stepping methods.

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