On Cayley-transform methods for the discretization of Lie-group equations

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Abstract

In this paper we develop in a systematic manner the theory of time-stepping methods based on the Cayley transform. Such methods can be applied to discretise differential equations that evolve in some Lie groups, in particular in the orthogonal group and the symplectic group. Unlike many other Lie-group solvers, they do not require the evaluation of matrix exponentials.

Similarly to the theory of Magnus expansions in (Iserles & Nørsett 1999), we identify terms in a *Cayley expansion* with rooted trees, which can be constructed recursively. Each such term is an integral over a polytope but all such integrals can be evaluated to high order by using special quadrature formulae similar to the construction in (Iserles & Nørsett 1999).

Truncated Cayley expansions (with exact integrals) need not be time-symmetric, hence the method does not display the usual advantages associated with time symmetry, e.g. even order of approximation. However, time symmetry (with its attendant benefits) is attained when exact integrals are replaced by certain quadrature formulae.

1 Quadratic Lie groups

The theme of this paper is geometric integration: numerical discretization of differential equations that respects their underlying geometry. It is increasingly recognised by numerical analysts and users of computational methods alike that geometric integration often represents a highly efficient and precise means toward obtaining a numerical solution, whilst retaining important qualitative attributes of the differential system (Budd & Iserles 1999).

Large number of differential equations with a wide range of practical applications evolve on Lie groups

$$G = \{A \in \mathrm{GL}_n(\mathbb{R}) \,:\, AJA^{\mathrm{T}} = J\}, \tag{1.1}$$

where $\mathrm{GL}_n(\mathbb{R})$ is the group of all $n \times n$ nonsingular real matrices and $J \in \mathrm{GL}_n(\mathbb{R})$ is given. (We refer the reader to (Carter, Segal & Macdonald 1995, Olver 1995, Varadarajan 1984) for an introduction to the theory of Lie groups.) Familiar examples are

- The *orthogonal group* $\mathrm{O}_n(\mathbb{R})$, whereby $J = I$, the identity matrix. This group plays an important role in a wide variety of applications, e.g. modelling of mechanical systems (Lewis & Simo 1994), processes in numerical linear algebra (Chu 1994), solution of isospectral flows (Calvo, Iserles & Zanna 1997) and evaluation of Lyapunov exponents (Dieci, Russell & van Vleck 1994). In some applications, as a matter of fact, one needs to consider the *Euclidean group* of affine

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translations of $\mathrm{O}_n(\mathbb{R})$ or the *special orthogonal group* $\mathrm{SO}_n(\mathbb{R}) = \mathrm{O}_n(\mathbb{R}) \cap \mathrm{SL}_n(\mathbb{R})$ of orthogonal matrices with unit determinant. In yet other applications it is not the group *per se* but its action on a *homogeneous space* which is of interest. Having said this, as long as we can discretise successfully equations evolving on a Lie group, we can do so in its connected components or in homogeneous spaces associated with it (Munthe-Kaas 1999).

  Important examples of homogeneous spaces which are acted upon by the orthogonal group are spheres and tori.

- The *symplectic group* Sp_n, whereby $J = \begin{bmatrix} O & I \\ -I & O \end{bmatrix}$ is the symplectic matrix. This group is germane to the investigation of Hamiltonian equations.
- The group $\mathrm{O}_{3,1}(\mathbb{R}) \subset \mathrm{GL}_4(\mathbb{R})$, whereby $J = \mathrm{diag}(1, 1, 1, -1)$, occurs in the study of special relativity. More specifically, the object of interest is the *Lorenz group* $\mathrm{SO}_{3,1}(\mathbb{R}) = \mathrm{O}_{3,1}(\mathbb{R}) \cap \mathrm{SL}_4(\mathbb{R})$, the connected component of $\mathrm{O}_{3,1}(\mathbb{R})$ consisting of matrices with determinant one (Carter et al. 1995).

It is perhaps natural to call G a *quadratic Lie group,* since its elements lie in a submanifold embedded in $\mathbb{R}^{n^2}$ which can be described by a set of quadratic equations. Yet, we use this name with a degree of caution, since the term *linear Lie groups* is sometimes used for all matrix Lie groups (Carter et al. 1995).

A natural complexification of (1.1) is

$$\{A \in \mathrm{GL}_n(\mathbb{C}) \,:\, AJA^{\mathrm{H}} = J\}, \tag{1.2}$$

where $J \in \mathrm{GL}_n(\mathbb{C})$ and $B^{\mathrm{H}} = \bar{B}^{\mathrm{T}}$. An important example of (1.2) is the *unitary group* $\mathrm{U}_n(\mathbb{C})$. We note in passing that the entire discussion of this paper can be reworded in an entirely transparent manner so that it caters for differential equations evolving on complex groups (1.2).

A differential equation evolving on a Lie group G (which need not be quadratic) can be always written in the form

$$Y' = A(t, Y)Y, \quad t \geq t_0, \qquad Y(t_0) = Y_0 \in G, \tag{1.3}$$

where $A : [t_0, \infty) \times G \to \mathfrak{g}$ and $\mathfrak{g}$ is the *Lie algebra* of G (Budd & Iserles 1999). The interpretation of (1.3) is almost self-evident since, $\mathfrak{g}$ being the tangent space of G at identity, it is true that $A(t, Y)Y \in \mathrm{T}G|_Y$, the tangent space at Y. Numerous discretization methods that retain the Lie-group structure of (1.3) follow a set pattern: Firstly, the equation is rendered in $\mathfrak{g}$: Letting $Y(t) = \mathrm{e}^{\Omega(t)} Y_0$, we obtain the *dexpinv equation*

$$\Omega' = \sum_{m=0}^{\infty} \frac{\mathrm{B}_m}{m!} \mathrm{ad}_{\Omega}^m A(t, \mathrm{e}^{\Omega} Y_0), \quad t \geq t_0, \qquad \Omega(t_0) = O, \tag{1.4}$$

where $\{\mathrm{B}_m\}_{m \geq 0}$ are Bernoulli numbers and ad_B is the *adjoint operator,*

$$\mathrm{ad}_B^m C = \begin{cases} C, & m = 0, \\ [B, \mathrm{ad}_B^{m-1} C], & m \geq 1 \end{cases}$$

(Hausdorff 1906, Iserles & Nørsett 1999, Munthe-Kaas 1998). Inasmuch as (1.4) is considerably more complicated than the Lie-group equation (1.3), it has a crucial and most welcome attribute: unlike a Lie group G, the Lie algebra $\mathfrak{g}$ is a linear space. Therefore, as long as the dexpinv equation (1.4) is discretized by using solely linear-space operations and commutators, the outcome will (to machine accuracy) reside in the correct configuration space $\mathfrak{g}$. Having advanced the solution in the Lie algebra, we complete the procedure by translating the new value back to the Lie group with the exponential map.

Several discretization methods are employing the above approach: Runge–Kutta–Munthe-Kaas schemes (Munthe-Kaas 1998), Fer and Magnus expansions (Fer 1958, Iserles & Nørsett 1999, Magnus 1954). Moreover, similar approach can be generalized to homogeneous spaces (Munthe-Kaas 1999).

Insofar as quadratic Lie groups (1.1) are concerned, the Lie algebra $\mathfrak{g}$ is of particularly simple form,

$$\mathfrak{g} = \{A \in \mathfrak{gl}_n(\mathbb{R}) \,:\, AJ + JA^{\mathrm{T}} = O\}, \tag{1.5}$$

where $\mathfrak{gl}_n(\mathbb{R})$ is the Lie algebra of all $n \times n$ real matrices. Arguably, the most computation-intensive stage in the implementation of Lie-group methods is the evaluation of the matrix exponential since for general Lie groups it is forbidden to replace e^z by an analytic (e.g., rational) approximant, as this might take us outside the Lie group (Kang & Zai-jiu 1995). This, however, is not the case when G is a quadratic Lie group, since $f(\mathfrak{g}) \subseteq G$ for every $f(z) = \mathrm{e}^{g(z)}$, where g is an odd analytic function (Celledoni & Iserles 1998). In particular, we may approximate the exponential by diagonal Padé approximants.

A particular example of such a function f is $\mathrm{cay}(z,\alpha) := (1+\alpha z)/(1-\alpha z)$, $\alpha \in \mathbb{R} \setminus \{0\}$: a *Cayley transform.* Indeed, a diagonal Padé approximant is nothing else but a product of Cayley transforms! Note that the evaluation of $\mathrm{cay}(B,\alpha)$ is considerably cheaper than that of e^B. Inasmuch as this provides a very attractive option in the context of aforementioned Lie-group methods, it has been realised few years ago that the Cayley transform can be used *directly,* in place of the exponential map (Lewis & Simo 1994). In other words, we do not use it to approximate the exponential but dispose of the latter altogether, solving instead for a function Ω such that

$$Y(t) = \mathrm{cay}(\Omega(t), \tfrac{1}{2})Y_0 = [I - \tfrac{1}{2}\Omega(t)]^{-1}[I + \tfrac{1}{2}\Omega(t)]Y_0. \tag{1.6}$$

(The choice of $\alpha = \frac{1}{2}$ is arbitrary but it ensures, as will be evident in the sequel, particularly simple form of various expansion coefficients, while retaining a sentimental link with the exponential: $\mathrm{cay}(z, \frac{1}{2}) = \mathrm{e}^z + \mathcal{O}(z^3)$.)

Differentiating (1.6) yields

$$Y' = \tfrac{1}{2}(I - \tfrac{1}{2}\Omega)^{-1}\Omega'(I - \tfrac{1}{2}\Omega)^{-1}(I + \tfrac{1}{2}\Omega)Y_0 + \tfrac{1}{2}(I - \tfrac{1}{2}\Omega)^{-1}\Omega' Y_0$$

and substitution in (1.3) results in

$$\tfrac{1}{2}(I - \tfrac{1}{2}\Omega)^{-1}\Omega'(I - \tfrac{1}{2}\Omega)^{-1}(I + \tfrac{1}{2}\Omega) + \tfrac{1}{2}(I - \tfrac{1}{2}\Omega)^{-1}\Omega' = A(t, \mathrm{cay}(\Omega),$$

where $\mathrm{cay}(z) \equiv \mathrm{cay}(z, \frac{1}{2})$. Multiplying by $(I - \frac{1}{2}\Omega)$ on the left and the right gives, after trivial manipulation, the *dcayinv equation*

$$\Omega' = \mathrm{dcay}_\Omega^{-1} A = A - \tfrac{1}{2}[\Omega, A] - \tfrac{1}{4}\Omega A \Omega, \quad t \geq t_0, \qquad \Omega(t_0) = O. \tag{1.7}$$

Two important observations pertain to equation (1.7).

1. We have already commented that implementing the dcayinv equation, in preference to the classical dexpinv equation (1.4), leads to considerably cheaper mapping of values from the algebra to the group. However, (1.7) has further important advantage: each function evaluation is itself much cheaper than in (1.4). Although the infinite series in the latter may be truncated (consistently with the order of the underlying approximation: cf. (Iserles, Nørsett & Rasmussen 1998) for details), the evaluation of each term therein requires the computation of one commutator.

2. Note the appearance of the *symmetric product* $\Omega A \Omega$ in (1.7). For general Lie algebras it need not be true that the symmetric product resides in $\mathfrak{g}$. Fortunately, (1.5) is not 'general' and it is easy to prove that $ABA \in \mathfrak{g}$ for every $A, B \in \mathfrak{g}$. This is an immediate consequence of the following result.

   Proposition 1 *Let $A, B, C \in \mathfrak{g}$, the Lie algebra $\mathfrak{g}$ having been defined in (1.5). Then $X := ABC + CBA \in \mathfrak{g}$.*

   Proof We wish to show that $XJ + JX^{\mathrm{T}} = O$. Observe though from (1.5) that $JZ^{\mathrm{T}} = -ZJ$ for every $Z \in \mathfrak{g}$. Therefore

$$\begin{aligned} JX^{\mathrm{T}} &= J(C^{\mathrm{T}}B^{\mathrm{T}}A^{\mathrm{T}} + A^{\mathrm{T}}B^{\mathrm{T}}C^{\mathrm{T}}) = (JC^{\mathrm{T}})B^{\mathrm{T}}A^{\mathrm{T}} + (JA^{\mathrm{T}})(B^{\mathrm{T}}C^{\mathrm{T}}) \\ &= (-CJ)(B^{\mathrm{T}}A^{\mathrm{T}}) + (-AJ)(B^{\mathrm{T}}C^{\mathrm{T}}) = -C(JB^{\mathrm{T}})A^{\mathrm{T}} - A(JB^{\mathrm{T}})C^{\mathrm{T}} \\ &= -C(-BJ)A^{\mathrm{T}} - A(-BJ)C^{\mathrm{T}} = CB(JA^{\mathrm{T}}) + AB(JC^{\mathrm{T}}) \\ &= CB(-AJ) + AB(-CJ) = -XJ \end{aligned}$$

   and it follows that $X \in \mathfrak{g}$, as required. □

The equation (1.7) can be easily solved with, say, an explicit Runge–Kutta method: a Cayley version of the Runge–Kutta methods in (Munthe-Kaas 1998). In the present paper we propose to pursue an alternative course of action, expanding the solution of (1.7) in a manner similar to *Magnus series.* We assume in the sequel for the sake of simplicity that the equation (1.3) is linear, hence that it reads $Y' = A(t)Y$, where $A : [t_0, \infty) \to \mathfrak{g}$. The reader is referred to (Diele, Lopez & Peluso 1998, Engø 1998, Lewis & Simo 1994, Marthinsen & Owren 1999) for examples of methods based on the Cayley transform and their applications and to (Zanna 1997) for a generalisation of Magnus expansions from linear to nonlinear equations.

Magnus series have been originally introduced by Wilhelm Magnus (1954) and have been used in a multitude of publications in theoretical physics, quantum chemistry, control theory, stochastic differential equations and, lately, geometric integration. In particular, Iserles & Nørsett (1999) have approached Magnus series in a systematic fashion as a *numerical* construct: deriving expansion coefficients in an organised, recursive manner and constructing efficient quadrature formulae for the numerous multivariate integrals that feature in this procedure. In essence, a Magnus expansion of (1.4) (assuming without loss of generality $t_0 = 0$) is

$$\begin{aligned}\Omega(t) = &\int_0^t A(\xi)\mathrm{d}\xi - \tfrac{1}{2}\int_0^t\int_0^{\xi_1}[A(\xi_2), A(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ &+ \tfrac{1}{4}\int_0^t\int_0^{\xi_1}\int_0^{\xi_2}[[A(\xi_3), A(\xi_2)], A(\xi_1)]\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ &+ \tfrac{1}{12}\int_0^t\int_0^{\xi_1}\int_0^{\xi_1}[A(\xi_3), [A(\xi_2), A(\xi_1)]]\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1 + \cdots.\end{aligned} \tag{1.8}$$

Using graph theory, it is possible to associate each term above with a specific *rooted binary tree,* whereby new terms can be generated by combining trees (Iserles & Nørsett 1999). In Section 2 we extend similar approach to the solution of (1.7). Thus, solving (1.7), the expansion (1.8) is replaced by

$$\begin{aligned}\Omega(t) = &\int_0^t A(\xi)\mathrm{d}\xi - \tfrac{1}{2}\int_0^t\int_0^{\xi_1}[A(\xi_2), A(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ &+ \tfrac{1}{4}\int_0^t\int_0^{\xi_1}\int_0^{\xi_2}[[A(\xi_3), A(\xi_2)], A(\xi_1)]\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ &- \tfrac{1}{4}\int_0^t\left[\int_0^{\xi_1} A(\xi_2)\mathrm{d}\xi_2\right]A(\xi_1)\left[\int_0^{\xi_1} A(\xi_3)\mathrm{d}\xi_3\right]\mathrm{d}\xi_1 + \cdots.\end{aligned} \tag{1.9}$$

The *Cayley series* (1.9) can be also analysed using graph theory, except that we need to use more complicated *bicolour trees.*

Numerical implementation of Cayley series necessitates the approximation of a large number of multivariate integrals. On the face of it, this is a formidable and computationally intensive task. Yet, using special quadrature formulae from (Iserles & Nørsett 1999), it is possible to derive high-order methods that require a surprisingly small number of function evaluations. More specifically, we need just ν function evaluations for a method of order 2ν, similarly to the familiar univariate Gaussian quadrature. This issue is addressed in Section 3.

Truncating a Magnus expansion in an appropriate manner results in a *time-symmetric* scheme (Iserles et al. 1998). This is important since time-symmetric schemes are always of an even order. Thus, truncating the expansion so that to ensure order $2\nu - 1$, say, automatically brings the order up to 2ν. In Section 4 we consider time symmetry for Cayley series. It turns out the, although a truncation of the series (with all integrals evaluated exactly) is not time-symmetric, the latter feature is restored, with all its attendant benefits, when the integrals are replaced by quadrature! Thus, perhaps surprisingly, a numerical method produces a better approximation of the solution of (1.7) than an 'exact' truncation of the Cayley series.

We reiterate that the remainder of this paper assumes that we are solving a linear equation. Inasmuch as the solution of linear equations in Lie groups is of considerable independent interest, our approach can be extended to nonlinear equations. This has been already done by Zanna (1997) for Magnus expansions and we are confident that her approach, based on collocation, can be extended to the present setting.

2 The Cayley expansion

2.1 Bicolour trees and the Cayley expansion

In this section we subject the Cayley expansion (1.9) to systematic analysis. We commence by denoting by $\mathcal{I}_m$ the portion of the Cayley expansion containing terms with precisely $m \geq 1$ integrals, hence

$$\begin{aligned}
\mathcal{I}_1(t) &= \int_0^t A(\xi)\mathrm{d}\xi, \\
\mathcal{I}_2(t) &= -\tfrac{1}{2}\int_0^t\int_0^{\xi_1}[A(\xi_2), A(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 \\
\mathcal{I}_3(t) &= \tfrac{1}{4}\int_0^t\int_0^{\xi_1}\int_0^{\xi_2}[[A(\xi_3), A(\xi_2)], A(\xi_1)]\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1 \\
&\quad -\tfrac{1}{4}\int_0^t\left[\int_0^{\xi_1}A(\xi_2)\mathrm{d}\xi_2\right]A(\xi_1)\left[\int_0^{\xi_1}A(\xi_2)\mathrm{d}\xi_2\right]\mathrm{d}\xi_1
\end{aligned}$$

and so on. Substituting

$$\Omega(t) = \sum_{m=1}^{\infty}\mathcal{I}_m \tag{2.1}$$

in (1.7) results in

$$\begin{aligned}
\sum_{m=1}^{\infty}\mathcal{I}_m(t) &= \int_0^t A(\xi)\mathrm{d}\xi - \tfrac{1}{2}\int_0^t\left[\sum_{m=1}^{\infty}\mathcal{I}_m(\xi), A(\xi)\right]\mathrm{d}\xi \\
&\quad -\tfrac{1}{4}\int_0^t\left[\sum_{m=1}^{\infty}\mathcal{I}_m(\xi)\right]A(\xi)\left[\sum_{m=1}^{\infty}\mathcal{I}_m(\xi)\right]\mathrm{d}\xi \\
&= \int_0^t A(\xi)\mathrm{d}\xi - \tfrac{1}{2}\sum_{m=2}^{\infty}\int_0^t[\mathcal{I}_{m-1}(\xi), A(\xi)]\mathrm{d}\xi \\
&\quad -\tfrac{1}{4}\sum_{m=3}^{\infty}\sum_{k=1}^{m-2}\int_0^t\mathcal{I}_{m-k-1}(\xi)A(\xi)\mathcal{I}_k(\xi)\mathrm{d}\xi.
\end{aligned}$$

Counting the number of integrals in each expression, we obtain the recursive formula

$$\mathcal{I}_m(t) = -\tfrac{1}{2}\int_0^t[\mathcal{I}_{m-1}(\xi), A(\xi)]\mathrm{d}\xi - \tfrac{1}{4}\sum_{k=1}^{m-2}\int_0^t\mathcal{I}_{m-k-1}(\xi)A(\xi)\mathcal{I}_k(\xi)\mathrm{d}\xi, \tag{2.2}$$

valid for every $m \geq 3$. Note that the term

$$\int_0^t\mathcal{I}_{m-k-1}(\xi)A(\xi)\mathcal{I}_k(\xi)\mathrm{d}\xi$$

for $2k \neq m-1$ does not, in general, belong to $\mathfrak{g}$. However, it is always matched in $\mathcal{I}_m$ with

$$\int_0^t\mathcal{I}_k(\xi)A(\xi)\mathcal{I}_{m-k-1}(\xi)\mathrm{d}\xi$$

and, according to Proposition 1, their sum yields an element in the Lie algebra.

A useful way of understanding the Cayley expansion (2.1) follows by associating its elements with a subset of *planar rooted binary trees,* similarly to the analysis of Magnus series in (Iserles & Nørsett 1999). We commence by noting that, by (2.2), each term V, say, in the linear combination $\mathcal{I}_m$, $m \geq 3$, is necessarily obtained in one of two ways: either

$$V(t) = \int_0^t [V_1(\xi), A(\xi)]\mathrm{d}\xi, \tag{2.3}$$

where V_1 is in $\mathcal{I}_{m-1}$ or there exist $V_1 \in \mathcal{I}_{m-k-1}$ and $V_2 \in \mathcal{I}_k$ for some $k \in \{1, 2, \ldots, m-2\}$ such that

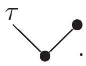
$$V(t) = \int_0^t V_1(\xi)A(\xi)V_2(\xi)\mathrm{d}\xi. \tag{2.4}$$

Thus, three devices are used in the recursion: integration, commutation with A and a product of three elements, the middle one being the matrix A. We establish an isomorphism between $V \in \mathcal{I}_m$, $m \geq 1$, and a subset of planar, binary rooted bicolour trees according to the following rules:

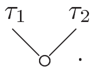
1. The matrix $A(t)$ corresponds to the trivial rooted tree $\bullet$.
2. Let the term $V_\tau(t)$ correspond to the tree τ. Then

   $\int_0^t V_\tau(\xi)\mathrm{d}\xi$ corresponds to 
.

3. Let the term $V_\tau(t)$ correspond to the tree τ. Then

   $[V_\tau(t), A(t)]$ corresponds to 
.

4. Let the terms $V_{\tau_1}(t)$ and $V_{\tau_2}(t)$ correspond to the trees τ_1 and τ_2 respectively. Then

   $V_{\tau_1}(t)A(t)V_{\tau_2}(t)$ corresponds to 
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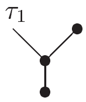
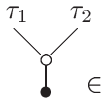
We denote by $\mathbb{T}_m$ the set of bicolour trees that correspond to terms in $\mathcal{I}_m$, $m \geq 1$. It follows at once that the elements of $\mathbb{T}_m$ can be composed recursively, consistently with the above rules,

1. $\mathbb{T}_1$ consists of a single element, ;
2. If $\tau_1 \in \mathbb{T}_{m-1}$, $m \geq 2$, then



$\in \mathbb{T}_m$; (2.5)

3. If $\tau_1 \in \mathbb{T}_{m-k-1}$, $\tau_2 \in \mathbb{T}_k$ for $m \geq 3$ and $1 \leq k \leq m-2$ then

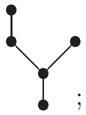


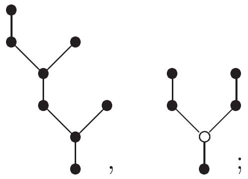
$$\in \mathbb{T}_m \; ; \tag{2.6}$$

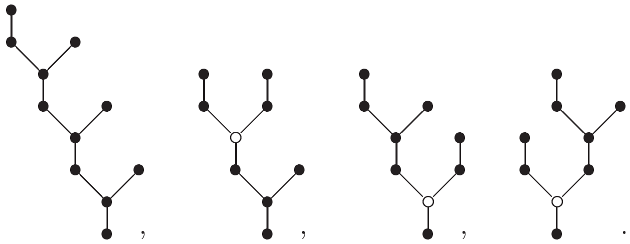
4. Every term in $\mathbb{T}_m$. $m \geq 2$, is necessarily derived by either (2.5) or (2.6).

We thus obtain

$\mathbb{T}_1$:


$\mathbb{T}_2$:


$\mathbb{T}_3$:


$\mathbb{T}_4$:


Let $\gamma(\tau)$ denote the number of white nodes in the tree $\tau \in \mathbb{T} = \cup_{m \geq 1} \mathbb{T}_m$. We are now equipped to represent explicitly the Cayley expansion (2.1).

Theorem 2 *The solution of the dcayinv equation (1.7) can be expanded in the form*

$$\Omega(t) = \sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{2^{m-1}} \sum_{\tau \in \mathbb{T}_m} (-1)^{\gamma(\tau)} V_\tau(t). \tag{2.7}$$

Proof By induction on $m \geq 1$. We have already observed that $\mathcal{I}_1 = \int_0^t A(\xi)\mathrm{d}\xi$. Otherwise, given any term V_τ with $\tau \in \mathbb{T}_m$, $m \geq 2$, there are exactly two possibilities, either (2.5) or (2.6). In the first case $\gamma(\tau) = \gamma(\tau_1)$, hence (2.2), (2.5) and the induction hypothesis imply that the coefficient in front of V_τ is

$$-\frac{1}{2} \times \frac{(-1)^{m-2+\gamma(\tau_1)}}{2^{m-2}} = \frac{(-1)^{m-1+\gamma(\tau)}}{2^{m-1}}.$$

In the second case $\gamma(\tau) = \gamma(\tau_1) + \gamma(\tau_2) + 1$. Thus, we deduce from (2.2), (2.6) and the induction assumption that the coefficient is

$$-\frac{1}{4} \times \frac{(-1)^{m-k-2+\gamma(\tau_1)}}{2^{m-k-2}} \times \frac{(-1)^{k-1+\gamma(\tau_2)}}{2^{k-1}} = \frac{(-1)^{m-1+\gamma(\tau)}}{2^{m-1}}.$$

Therefore (2.7) is true. $\square$

As we have already remarked, not every single term V_τ can be assured to lie in the Lie algebra. The simplest example is provided by the two leftmost terms in $\mathbb{T}_4$. We say that the trees $\tau_1, \tau_2 \in \mathbb{T}_m$ for some $m \geq 3$, such that $\gamma(\tau_1) = \gamma(\tau_2) \geq 1$, are *adjoint* if one can be obtained from the other by a vertical rotation with respect to a white node.

It follows at once from our construction and Proposition 1 that $V_{\tau_1}(t) + V_{\tau_2}(t) \in \mathfrak{g}$ whenever τ_1 and τ_2 are adjoint. Moreover, since $\gamma(\tau_1) = \gamma(\tau_2)$, the coefficients in front of $V_{\tau_1}(t)$ and $V_{\tau_2}(t)$ are the same. Therefore (2.7) implies that indeed $\Omega(t) \in \mathfrak{g}$, $t \geq 0$.

2.2 Counting trees

Our programme to prove convergence of the Cayley expansion (2.7) and to assess the computational expense of its implementation as a computational algorithm hinges upon estimates of the number of expansion terms. The simplest such estimate addresses itself to θ_m, the number of terms in $\mathbb{T}_m$. We commence by noting that $\theta_1 = \theta_2 = 1$, $\theta_3 = 2$, $\theta_4 = 4$.

Since each element of $\mathbb{T}_m$, $m \geq 3$, originates in either (2.5) or (2.6), we have the recurrence

$$\theta_m = \theta_{m-1} + \sum_{k=1}^{m-2} \theta_k \theta_{m-k-1}, \qquad m \geq 3. \tag{2.8}$$

Let

$$\theta(z) = \sum_{m=1}^{\infty} \theta_m z^{m-1}$$

be the generating function of the sequence $\{\theta_m\}_{m\geq 1}$. Multiplying (2.8) by z^{m-1}, summing up for $m \geq 3$ and adding $\theta_1 + \theta_2 z = 1 + z$ yields

$$\begin{aligned}
\theta(z) &= 1 + z + \sum_{m=3}^{\infty} \left(\theta_{m-1} + \sum_{k=1}^{m-2} \theta_k \theta_{m-k-1} \right) z^{m-1} \\
&= 1 + z + z \sum_{m=2}^{\infty} \theta_m z^{m-1} + \sum_{k=1}^{\infty} \theta_k \sum_{m=k+2}^{\infty} \theta_{m-k-1} z^{m-1} \\
&= 1 + z + z[\theta(z) - 1] + z^2 \sum_{k=1}^{\infty} \theta_k z^{k-1} \sum_{m=1}^{\infty} \theta_m z^{m-1}
\end{aligned}$$

and we deduce the functional equation

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

Since $\theta(0) = 1$, we conclude that

$$\theta(z) = \frac{1 - z - \sqrt{(1-3z)(1+z)}}{2z^2}.$$

Thus, θ is analytic at the origin with radius of convergence $\frac{1}{3}$ (the singularity at the origin is removable).

Lemma 3 *It is true that*

$$\limsup_{m\to\infty} \theta_m^{1/m} = 3. \tag{2.9}$$

Proof By the Cauchy principle of convergence, the reciprocal of the radius of convergence of θ at the origin is

$$\limsup_{m\to\infty} \theta_m^{1/m}.$$

□

We observe that in the case of a Magnus expansion the number of terms with m integrals grows like 4^m, hence (2.9) implies that the number of terms in a Cayley expansion grows (at least in an asymptotic sense) considerably slower.

Truncating the Cayley expansion (2.7) according to $\mathbb{T}_m$,

$$\Omega(t) \approx \Omega_{(p)}(t) = \sum_{m=1}^{p} \sum_{\tau\in\mathbb{T}_m} \alpha(\tau) V_\tau(t), \tag{2.10}$$

where $\alpha(\tau) = (-1)^{m+\gamma(\tau)-1}/2^{m-1}$, leads to an order-$p$ approximation. However, the same outcome can be obtained with a far smaller number of terms by taking heed of redundancies in expansion terms. Similarly to (Iserles et al. 1998), we say that the tree τ is of *power* s (denoted by $s = \operatorname{pwr}\tau$) if for every sufficiently smooth $A(t) \in \mathfrak{g}$ it is true that $V_\tau(t) = \mathcal{O}(t^s)$. An obvious alternative to (2.10) is the truncation

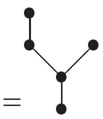
$$\Omega_{[p]}(t) = \sum_{m=1}^{p} \sum_{\tau\in\mathbb{F}_m} \alpha(\tau) V_\tau(t), \tag{2.11}$$

where $\mathbb{F}_m$ is the set of all trees of power $m \geq 1$.

Let ϕ_m be the number of terms in $\mathbb{F}_m$. Although clearly $\sum_{m=1}^{p} \phi_m \leq \sum_{m=1}^{p} \theta_m$, a more precise estimation of the ϕ_ms and of the savings inherent in (2.11) requires more effort.

Clearly, each tree $\tau \in \mathbb{F}_m$, $m \geq 2$, can be obtained via either (2.5) or (2.6). In the latter case it follows at once, counting integrals, that $\operatorname{pwr}\tau = \operatorname{pwr}\tau_1 + \operatorname{pwr}\tau_2 + 1$ and this cannot be improved for general matrices A.

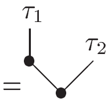
For trees obtained via (2.5), however, there are redundancies that can increase the estimate from the trivial inequality $\operatorname{pwr}\tau \geq \operatorname{pwr}\tau_1 + 1$. We commence by noting that, while the power of  is 1, the power of

$\tau =$ 

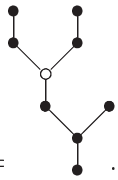
is 3. This can be easily affirmed by substituting the expansion $A(t) = A_0 + A_1 t + \cdots$ into

$$V_\tau(t) = \int_0^t \int_0^{\xi_1} [A(\xi_2), A(\xi_1)] \mathrm{d}\xi_2 \mathrm{d}\xi_1.$$

It has been observed in (Iserles et al. 1998), in the context of the Magnus expansion, that the power of

$\tau =$ 

is $\operatorname{pwr}\tau_1 + \operatorname{pwr}\tau_2 + 1$, except that when $\tau_1 = \tau_2$ then $\operatorname{pwr}\tau = \operatorname{pwr}\tau_1 + \operatorname{pwr}\tau_2 + 2$. In our case such increase in power takes place only when $\tau_1 = \tau_2 = \bullet$. Another power-increasing mechanism, however, follows from the interaction of white nodes with (2.5). For example, consider the tree

$\tau =$  .

Since $\operatorname{pwr}\tau_1 = 3$ and $\operatorname{pwr}\tau_2 = 0$, we may presume that $\operatorname{pwr}\tau = 4$, but this is an underestimate. Substituting $A(t) = A_0 + A_1 t + A_2 t^2 + \cdots$ into

$$V_\tau(t) = \int_0^t \left[\int_0^{\xi_1} \int_0^{\xi_2} A(\xi_3)\mathrm{d}\xi_3 A(\xi_2) \int_0^{\xi_2} A(\xi_3)\mathrm{d}\xi_3 \mathrm{d}\xi_2,\ A(\xi_1) \right] \mathrm{d}\xi_1$$

gives

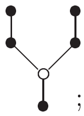
$$\left(\tfrac{1}{24}[A_0^3, A_1] - \tfrac{1}{40}A_0[A_0, A_1]A_0\right)t^5 + \mathcal{O}\left(t^6\right),$$

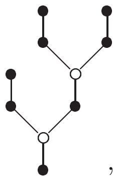
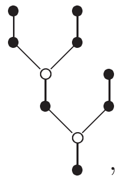
hence $\operatorname{pwr}\tau = 5$, the reason being that commutation kills the leading term in

$$\int_0^t [\tfrac{1}{3}A_0^3\xi^3 + \tfrac{1}{8}(A_0^2A_1 + 2A_0A_1A_0 + A_1A_0^2)\xi^4 + \cdots,\ A_0 + A_1\xi + \cdots]\mathrm{d}\xi.$$

To single out other trees that display similar increase in power, we let $\mathbb{T}^\circ$ be the set of all trees in $\mathbb{T}$ that contain no black nodes with two children (in other words, such that V_τ contains no commutators). Letting $\mathbb{T}^\circ_m = \mathbb{T}^\circ \cap \mathbb{T}_m$, $m \geq 1$, we have

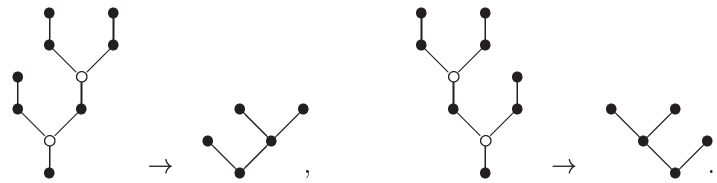
$\mathbb{T}^\circ_1$:  ;

$\mathbb{T}^\circ_3$:  ;

$\mathbb{T}^\circ_5$:  ,  ,

with $\mathbb{T}^\circ_2 = \mathbb{T}^\circ_4 = \emptyset$. In general, it is trivial to observe that $\mathbb{T}^\circ_{2m} = \emptyset$, $m \geq 1$, while each $\mathbb{T}^\circ_{2m+1}$ is isomorphic to the set of all *strictly binary rooted trees with* $2m+1$ *nodes.*

The isomorphism is provided by removing all vertical lines and colouring all nodes black, e.g.



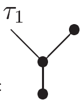
The number of strictly binary trees with $2m+1$ vertices is well known (Iserles & Nørsett 1999) and we deduce that

$$\phi_m^\circ = \#\mathbb{T}_m^\circ = \begin{cases} 0, & m = 2s, \\ (2s)!/[s!(s+1)!], & m = 2s+1. \end{cases}$$

The importance of $\mathbb{T}^\circ$ is underscored by the observation, trivially provable by induction, that, for $A(t) = A_0 + \mathcal{O}(t)$,

$$\tau_1 \in \mathbb{T}_{2m-1}^\circ \qquad \Rightarrow \qquad V_{\tau_1}(t) = cA_0^{2m-1}t^{2m-1} + \mathcal{O}\big(t^{2m}\big),$$

where $c \neq 0$ is a constant. (In particular, observe that $\mathbb{T}_{2m-1}^\circ \subseteq \mathbb{F}_{2m-1}$.) Therefore $[V_{\tau_1}(t), A(t)] = \mathcal{O}\big(t^{2m}\big)$ and we conclude that

$$\operatorname{pwr}\tau = 2m+1 \qquad \text{where} \qquad \tau =$$  $$\in \mathbb{T}_{2m-1}^\circ,$$

a gain of one unit.

We deduce that the numbers $\{\phi_m\}$ obey the recurrences

$$\begin{aligned} \phi_1 &= 1, \\ \phi_{2m} &= \phi_{2m-1} + \sum_{k=1}^{2m-2} \phi_{2m-k-1}\phi_k - \phi_{2m-1}^\circ, \qquad m \geq 1 \\ \phi_{2m+1} &= \phi_{2m} + \sum_{k=1}^{2m-1} \phi_{2m-k}\phi_k + \phi_{2m-1}^\circ, \qquad m \geq 1. \end{aligned} \tag{2.12}$$

The reason is that trees in $\mathbb{F}_m$ are composed exactly like trees in $\mathbb{T}_m$, via either (2.5) or (2.6), except that ϕ_{2m-1}° trees are 'upgraded' from $\mathbb{F}_{2m}$ to $\mathbb{F}_{2m+1}$ for all $m \geq 1$. Letting

$$\phi(z) = \sum_{m=1}^{\infty} \phi_m z^m$$

be the generating function of the sequence $\{\phi_m\}_{m\geq 1}$, long but straightforward algebra deduces from (2.12) that

$$\phi(z) = 1 - z + z^2 + z\phi(z) + z^2[\phi(z)]^2 - \sum_{m=1}^{\infty} \phi_{2m+1}^\circ z^{2m+1} + \sum_{m=1}^{\infty} \phi_{2m+1}^\circ z^{2m+2}.$$

However,

$$\sum_{m=1}^{\infty}\phi^{\circ}_{2m+1}z^{2m+1}=z\left[\sum_{m=0}^{\infty}\frac{(2m)!}{m!(m+1)!}z^{2m}-1\right]=\frac{1-2z^2-\sqrt{1-4z^2}}{2z}.$$

Summing up the last expression, we have used special functions,

$$\begin{aligned}\sum_{m=0}^{\infty}\frac{(2m)!}{m!(m+1)!}z^{2m} &= \sum_{m=0}^{\infty}\frac{(\frac12)_m}{(m+1)!}(2z)^{2m}=-\frac{1}{2z^2}\sum_{m=1}^{\infty}\frac{(-\frac12)_m}{m!}(2z)^{2m}\\ &= \frac{1}{2z^2}\left(1-{}_1F_0\left[\begin{matrix}-\frac12;\\ —;\end{matrix}4z^2\right]\right)=\frac{1}{2z^2}(1-\sqrt{1-4z^2}).\end{aligned}$$

Cf. (Rainville 1960) for relevant notation.

We conclude that the generating function ϕ satisfies the quadratic equation

$$z^2[\phi(z)]^2-(1-z)\phi(z)-\frac{1-3z-(1-z)\sqrt{1-4z^2}}{2z}=0$$

with the solution

$$\phi(z)=\frac{1-z-\sqrt{1-5z^2-2z(1-z)\sqrt{1-4z^2}}}{2z^2}. \tag{2.13}$$

Similarly to the proof of Lemma 3, we determine the rate of growth of $\{\phi_n\}$ by identifying the singularity of ϕ nearest to the origin. It is straightforward to ascertain that it is a branch point at $0.37063854143014207603\ldots$. Taking its reciprocal, we obtain

$$\limsup_{m\to\infty}\phi_m^{1/m}=2.6980464474671475136\ldots.$$

This represents substantial improvement over (2.9). The reduction in the number of terms when $\Omega_{(p)}$ is replaced by $\Omega_{[p]}$ is illustrated in Table 1. We note in passing that the number of trees of power p in a Magnus expansion grows like $(3.11674\ldots)^p$ (Iserles et al. 1998).

m	1	2	3	4	5	6	7	8	9	10	11	12	13	14
θ_m	1	1	2	4	9	21	51	127	323	835	2188	5798	15511	41835
ϕ_m	1	0	2	1	6	6	24	35	113	205	589	1217	3283	7339

Table 1: The number of terms in $\mathbb{T}_m$ and $\mathbb{F}_m$.

2.3 Convergence

In the present section we discuss conditions that assure the convergence of the Cayley expansion $\Omega_{(p)}$ as $p\to\infty$. We assume that $A\in \mathrm{C}^1[\mathfrak{g}]$ and let $K(t):=\int_0^t\|A(\xi)\|\mathrm{d}\xi$, where $\|\cdot\|$ is a norm. Given $X\in\mathfrak{g}$, we denote by κ a constant such that

$$\|[X,A]\|\le\kappa\|X\|\cdot\|A\|,\qquad A\in\mathfrak{g}.$$

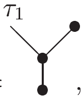
Trivially, we can always choose $\kappa = 2$. However, it is sometimes possible to find smaller bounds: it will be demonstrated in a forthcoming publication that we can always choose $\kappa = \sqrt{2}$ for $\mathfrak{g} = \mathfrak{so}_n(\mathbb{R})$ when $\|\cdot\|$ is the Frobenius norm. Even smaller bounds can be obtained in some algebras and it is an easy exercise to prove that we may take $\kappa = 1$ in $\mathfrak{so}_3(\mathbb{R})$, again with the Frobenius norm.

Lemma 4 *Given $\tau \in \mathbb{T}_m$, $m \geq 1$, it is true that*

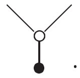
$$\|V_\tau(t)\| \leq \beta(\tau)\kappa^{m-2\gamma(\tau)-1}[K(t)]^m, \tag{2.14}$$

where

$\beta(\tau) = 1,\qquad \tau =$ ,

$\beta(\tau) = \dfrac{\beta(\tau_1)}{m},\qquad \tau =$ 

, (2.15)

$\beta(\tau) = \dfrac{\beta(\tau_1)\beta(\tau_2)}{m},\qquad \tau =$ 

.

Proof By induction on $m \geq 1$. The lemma is certainly true for the unique tree $\tau_0 \in \mathbb{T}_1$, since $\gamma(\tau_0) = 1$ and

$$\|V_{\tau_0}(t)\| = \left\|\int_0^t A(\xi)\mathrm{d}\xi\right\| \leq \int_0^t \|A(\xi)\|\mathrm{d}\xi = K(t),$$

consistently with (2.14).

Suppose that $m \geq 2$ and that $\tau \in \mathbb{T}_m$ has been derived using (2.5). Then $\tau_1 \in \mathbb{T}_{m-1}$, $\gamma(\tau) = \gamma(\tau_1)$ and

$$\begin{aligned}\|V_\tau(t)\| &= \left\|\int_0^t [V_{\tau_1}(\xi), A(\xi)]\mathrm{d}\xi\right\| \leq \kappa\int_0^t \|V_{\tau_1}(\xi)\|\cdot\|A(\xi)\|\mathrm{d}\xi \\ &\leq \kappa \times \beta(\tau_1)\kappa^{(m-1)-2\gamma(\tau_1)-1} \times \int_0^t [K(\xi)]^{m-1}K'(\xi)\mathrm{d}\xi \\ &= \frac{\beta(\tau_1)}{m}\kappa^{m-2\gamma(t)-1}[K(t)]^m.\end{aligned}$$

The remaining possibility is that $m \geq 3$ and $\tau \in \mathbb{T}_m$ has been obtained from (2.6). Therefore $\tau_1 \in \mathbb{T}_{m-k-1}$, $\tau_2 \in \mathbb{T}_k$ for some $k \in \{1, 2, \ldots, m-2\}$ and $\gamma(\tau) = \gamma(\tau_1) + \gamma(\tau_2) + 1$. We have

$$\begin{aligned}\|V_\tau(t)\| &= \left\|\int_0^t V_{\tau_1}(\xi)A(\xi)V_{\tau_2}(\xi)\mathrm{d}\xi\right\| \leq \int_0^t \|V_{\tau_1}(\xi)\|\cdot\|A(\xi)\|\cdot\|V_{\tau_2}(\xi)\|\mathrm{d}\xi \\ &\leq \beta(\tau_1)\kappa^{(m-k-1)-2\gamma(\tau_1)-1} \times \beta(\tau_2)\kappa^{k-2\gamma(\tau_2)-1} \times \int_0^t [K(\xi)]^{(m-k-1)+k}K'(\xi)\mathrm{d}\xi \\ &= \frac{\beta(\tau_1)\beta(\tau_2)}{m}\kappa^{m-2\gamma(\tau)-1}[K(t)]^m.\end{aligned}$$

This concludes the proof. $\square$

We let

$$T(z) := \sum_{m=1}^{\infty} \sum_{\tau\in\mathbb{T}_m} \beta(\tau)\kappa^{m-2\gamma(\tau)-1} z^m, \qquad z\in\mathbb{C}.$$

Because of (2.14) we can immediately deduce from (2.7) that

$$\|\Omega(t)\| \le \sum_{m=1}^{\infty} \frac{1}{2^{m-1}} \sum_{\tau\in\mathbb{T}_m} \|V_\tau(t)\| \le 2T(\tfrac{1}{2}K(t))$$

and, in particular, the Cayley expansion converges for $t\ge t_0$ if $\frac{1}{2}K(t)$ is within the radius of convergence of the Taylor expansion of T about the origin. Thus, the determination of this radius of convergence is of critical importance to convergence analysis.

Employing the recurrence (2.15), we observe that

$$\begin{aligned} T(z) = z + \tfrac{1}{2}\kappa z^2 + \sum_{m=3}^{\infty} \frac{1}{m} \Bigg[& \sum_{\tau_1\in\mathbb{T}_{m-1}} \beta(\tau_1)\kappa^{m-2\gamma(\tau_1)-1} \\ & + \sum_{k=1}^{m-2} \sum_{\tau_1\in\mathbb{T}_{m-k-1}} \sum_{\tau_2\in\mathbb{T}_k} \beta(\tau_1)\beta(\tau_2)\kappa^{m-2[\gamma(\tau_1)+\gamma(\tau_2)]-3} \Bigg] z^m. \end{aligned}$$

Differentiation with respect to z yields

$$\begin{aligned} T'(z) &= 1 + \kappa z + \kappa \sum_{m=2}^{\infty} \sum_{\tau\in\mathbb{T}_m} \beta(\tau)\kappa^{m-2\gamma(\tau)-1} z^m \\ &\quad + \sum_{m=2}^{\infty} \sum_{k=1}^{m-1} \sum_{\tau_1\in\mathbb{T}_{m-k}} \sum_{\tau_2\in\mathbb{T}_k} \beta(\tau_1)\beta(\tau_2)\kappa^{m-2[\gamma(\tau_1)+\gamma(\tau_2)]-2} z^m \\ &= 1 + \kappa z + \kappa[T(z) - z] \\ &\quad + \sum_{k=1}^{\infty} \sum_{m=1}^{\infty} \sum_{\tau_1\in\mathbb{T}_m} \sum_{\tau_2\in\mathbb{T}_k} \beta(\tau_1)\beta(\tau_2)\kappa^{m+k-2[\gamma(\tau_1)+\gamma(\tau_2)]-2} z^{m+k} \\ &= 1 + \kappa T(z) + [T(z)]^2. \end{aligned}$$

We thus deduce that the generating function T obeys the Riccati differential equation

$$T'(z) = 1 + \kappa T(z) + [T(z)]^2, \quad z\ge 0, \qquad T(0) = 0,$$

whose explicit solution for $\kappa\in[0,2)$ is

$$T(z) = \frac{\tan\lambda z}{\lambda - \frac{1}{2}\kappa\tan\lambda z},$$

where $\lambda = \sqrt{1-\kappa^2/4}$, while $\kappa = 2$ results in

$$T(z) = \frac{z}{1-z}.$$

Following our discussion, we observe that $T(K(t))$ is bounded (and the Cayley expansion converges) provided that $K(t)$ is smaller than $2z_\kappa$, where z_κ is the radius of convergence of T about the origin. We determine z_κ by identifying the singularity of T nearest the origin,

$$z_\kappa = \frac{\tan^{-1}(2\lambda/\kappa)}{\lambda}.$$

Since

$$z'_\kappa = -\frac{2\kappa}{(4-\kappa^2)^{3/2}}\left(\frac{(4-\kappa^2)^{1/2}}{\kappa} - \tan^{-1}\frac{(4-\kappa^2)^{1/2}}{\kappa}\right) < 0, \qquad \kappa \in (0,2),$$

it follows that z_κ decreases monotonically from $\lim_{\kappa\to 0} z_\kappa = \pi/2$ to $z_2 = 1$. As expected, the smaller κ, the more generous are the convergence conditions. We sum up the main result of our convergence analysis in the following theorem.

Theorem 5 *The Cayley expansion (2.7) converges for $t \geq t_0$ with respect to the norm $\|\cdot\|$, provided that*

$$\int_0^t \|A(\xi)\|\mathrm{d}\xi \leq 4\frac{\tan^{-1}(\sqrt{4-\kappa^2}/\kappa)}{\sqrt{4-\kappa^2}}. \tag{2.16}$$

Following upon our claim that we may take $\kappa = \sqrt{2}$ in the important case $\mathfrak{g} = \mathfrak{so}_n(\mathbb{R})$, $n \geq 4$, we deduce from (2.16) that in that case the Cayley expansion converges in the Frobenius norm whenever

$$\int_0^t \|A(\xi)\|_{\mathrm{F}}\mathrm{d}\xi \leq \frac{\sqrt{2}\pi}{2} \approx 2.221441460792.$$

3 Quadrature

3.1 Quadrature of multilinear forms

Simple choices of the matrix function $A(t)$, e.g. polynomial or trigonometric entries, lend themselves to exact evaluation, perhaps assisted by symbolic algebra. However, practical implementation of a Cayley expansion for general matrix functions $A(t)$ requires the discretization of integrals by quadrature. The number of terms increases exponentially, each term is a multivariate integral over a different polytope and multivariate quadrature is a notoriously difficult numerical task. Thus, it might be fair to advance the point of view that, even for moderate values of $p \geq 1$, the Cayley expansion (2.11) is too effort-consuming for practical use. Fortunately, nothing can be further from the truth! The redeeming feature of expansion terms in (2.11) is that they possess structure that can be exploited to a very good effect and this leads to affordable and precise quadrature schemes.

The situation is very similar to that of Magnus expansions: each term is of the form

$$I(h) = \int_{h\mathcal{S}} \mathcal{L}(A(\xi_1), A(\xi_2), \ldots, A(\xi_r))\,\mathrm{d}\xi_r\mathrm{d}\xi_{r-1}\cdots\mathrm{d}\xi_1, \tag{3.1}$$

where $\mathcal{L}$ is a *multilinear function* while $\mathcal{S} \subset \mathbb{R}^r$ is a polytope of the form

$$\mathcal{S} = \{\boldsymbol{x} \in \mathbb{R}^r \,:\, 0 \leq \xi_i \leq \xi_{l_i},\ i = 1, 2, \ldots, r\},$$

where $\xi_0 = 1$ and $\min\{1, i-1\} \le l_i \le i-1$, $i = 1, 2, \ldots, r$. Table 2 displays a number of examples that help to illustrate this observation.

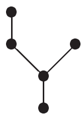
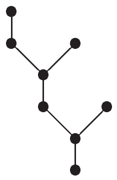
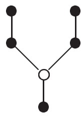
Tree	Integral $I(h)$, polytope $\mathcal{S}$ and multilinear form $\mathcal{L}(\boldsymbol{Z})$
	$I(h) = \int_0^h A(\xi)\mathrm{d}\xi$ $\mathcal{S} = \{\boldsymbol{\xi} \in \mathbb{R}^1 : 0 \le \xi_1 \le 1\}$ $\mathcal{L} = Z_1$
	$I(h) = \int_0^h \int_0^{\xi_1} [A(\xi_2), A(\xi_1)]\mathrm{d}\boldsymbol{\xi}$ $\mathcal{S} = \{\boldsymbol{\xi} \in \mathbb{R}^2 : 0 \le \xi_2 \le \xi_1 \le 1\}$ $\mathcal{L} = [Z_2, Z_1]$
	$I(h) = \int_0^h \int_0^{\xi_1} \int_0^{\xi_2} [[A(\xi_3), A(\xi_2)], A(\xi_1)]\mathrm{d}\boldsymbol{\xi}$ $\mathcal{S} = \{\boldsymbol{\xi} \in \mathbb{R}^3 : 0 \le \xi_3 \le \xi_2 \le \xi_1 \le 1\}$ $\mathcal{L} = [[Z_3, Z_2], Z_1]$
	$I(h) = \int_0^h \int_0^{\xi_1} \int_0^{\xi_1} A(\xi_2)A(\xi_1)A(\xi_3)\mathrm{d}\boldsymbol{\xi}$ $\mathcal{S} = \{\boldsymbol{\xi} \in \mathbb{R}^3 : 0 \le \xi_2, \xi_3 \le \xi_1 \le 1\}$ $\mathcal{L} = Z_2 Z_1 Z_3$

Table 2: Polytopes and multivariate forms for terms with trees in $\mathbb{T}_m$, $m = 1, 2, 3$.

An effective method to approximate (3.1) by quadrature has been introduced by Iserles & Nørsett (1999) and further elaborated in (Munthe-Kaas & Owren 1999) and (Iserles et al. 1998). Given integer $\nu \ge 1$ and distinct points $c_1, c_2, \ldots, c_\nu \in [0, 1]$, we let $A_k = A(t_N + c_k h)$, $k = 1, 2, \ldots, \nu$, where t_N and $t_{N+1} = t_N + h$ are the current and the next step, respectively. Let $\ell_k \in \mathbb{P}_{\nu-1}$ be the kth *cardinal function of Lagrange's interpolation:* $\ell_k(c_k) = 1$ and $\ell_k(c_j) = 0$, $j \ne k$. We approximate the integral (3.1) by the quadrature formula

$$Q(h) := h^r \sum_{\boldsymbol{k} \in \mathrm{C}_r^\nu} b_{\boldsymbol{k}} \mathcal{L}(A_{k_1}, A_{k_2}, \ldots, A_{k_r}), \tag{3.2}$$

where C_r^ν is the set of all r-tuples with elements in $\{1, 2, \ldots, \nu\}$ and

$$b_{\boldsymbol{k}} = \int_{\mathcal{S}} \prod_{i=1}^{r} \ell_{k_i}(\xi_i)\, \mathrm{d}\xi_r \mathrm{d}\xi_{r-1} \cdots \mathrm{d}\xi_1, \qquad \boldsymbol{k} \in \mathrm{C}_r^\nu.$$

Note that the quadrature formula (3.2) uses just ν function values, which are recycled at all possible positions in the multilinear function $\mathcal{L}$. Moreover, the very same function values are used time and again in *all* the integrals in the Cayley expansion! Its importance is further underscored by the following theorem.

Theorem 6 (Iserles & Nørsett (1999)) *The order of the quadrature (3.2) is $\nu+s$, where $s \geq 0$ is the maximal integer such that*

$$\int_0^1 \xi^{j-1} \prod_{i=1}^{\nu} (\xi - c_j) \mathrm{d}\xi = 0, \qquad j = 1, 2, \ldots, s.$$

In particular, the order is 2ν when $c_1, c_2, \ldots, c_\nu$ are the nodes of the (univariate) Gauss–Legendre quadrature in $[0, 1]$.

The formula (3.2) trades function evaluations off for the computation of commutators and matrix products. Although linear algebra is relatively cheap on modern computers, this nonetheless may result in substantial computational cost. Yet, exploiting further the structure of the underlying problem – specifically, the range of symmetries and linear dependencies in the Lie algebra – it is possible to represent most commutators as linear combinations of other commutators, thereby reducing the complexity by a large factor (Munthe-Kaas & Owren 1999). To this end we replace $A_1, A_2, \ldots, A_\nu$ by the matrices $B_0, B_1, \ldots, B_{\nu-1}$ which solve the Vandermonde linear system

$$\sum_{l=0}^{\nu-1} \frac{1}{l!} (c_k - \tfrac{1}{2})^l B_l = A_k, \qquad k = 1, 2, \ldots, \nu.$$

Note that $B_l = h^l A^{(l)}(t_N + \frac{1}{2}h) + \mathcal{O}\big(h^{l+1}\big)$, $l = 0, 1, \ldots, \nu - 1$. In particular, the order of magnitude of each B_l (as a function of the step size h) is known and it is transparent when different terms are composed in the multilinear form,

$$\mathcal{L}(B_{k_1}, B_{k_2}, \ldots, B_{k_r}) = \mathcal{O}\left(h^{|\boldsymbol{k}|}\right), \qquad \text{where} \qquad |\boldsymbol{k}| = \sum_{i=1}^{r} k_i.$$

For simplicity, let us assume that $c_1, c_2, \ldots, c_\nu$ are Gauss–Legendre points in $[0, 1]$. We replace (3.2) with the quadrature formula

$$\tilde{Q}(h) = h^r \sum_{|\boldsymbol{k}| \leq 2\nu - r} \tilde{b}_{\boldsymbol{k}} \mathcal{L}(B_{k_1}, B_{k_2}, \ldots, B_{k_r}), \tag{3.3}$$

where

$$\tilde{b}_{\boldsymbol{k}} = \frac{1}{k_1! k_2! \cdots k_r!} \int_{\mathcal{S}} \prod_{i=1}^{r} (\xi_i - \tfrac{1}{2})^{k_i} \, \mathrm{d}\xi_r \mathrm{d}\xi_{r-1} \cdots \mathrm{d}\xi_1. \tag{3.4}$$

The advantage of using (3.3), rather than (3.2), is threefold. Firstly, many terms can be thrown out without damaging the accuracy, since they are $\mathcal{O}(h^q)$ for some $q \geq 2\nu + 1$. Secondly, it is possible to prove that for Magnus expansions appropriate sums of terms vanish for all $\boldsymbol{k}$ such that $|\boldsymbol{k}| + r$ is even (Munthe-Kaas & Owren 1999). (Similar statement will be proved for Cayley expansions in Section 4.) Thirdly, and most importantly, it is possible to show that all terms $\mathcal{L}(B_{k_1}, B_{k_2}, \ldots, B_{k_r})$ for $|\boldsymbol{k}| \leq 2\nu - r$ are spanned by a low-dimensional basis which can be identified explicitly in the case of Magnus expansions (Munthe-Kaas & Owren 1999). Generalising the results of Munthe-Kaas & Owren (1999) to the realm of Cayley expansions is surprisingly intricate and forms the theme of a forthcoming publication (Iserles & Zanna 1999).

3.2 Examples of quadrature formulae

In this section we derive explicitly the formulae corresponding to the integrals from Table 2. Recall that $c_1, c_2, \ldots, c_\nu$ are Gauss–Legendre points in $[0,1]$.

Integral 1: , $r=1$. We deduce from (3.4) that

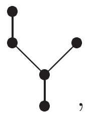
$$\tilde{b}_k = \frac{1}{k!}\int_0^1 (\xi - \tfrac{1}{2})^k \mathrm{d}\xi = \frac{1+(-1)^k}{(k+1)!}\cdot\frac{1}{2^{k+1}},$$

whereby we obtain the (2ν)-order quadrature

$$h\sum_{k=0}^{\lfloor \nu/2 \rfloor} \frac{1}{4^k(2k+1)!} B_{2k},$$

which is nothing else but the standard Gauss–Legendre quadrature, expressed in the basis $\{B_0, B_1, \ldots, B_{\nu-1}\}$. An alternative interpretation of this formula is that the *exact* integral can be expanded in the form

$$I(h) = h(B_0 + \tfrac{1}{24}B_2 + \tfrac{1}{1920}B_4 + \tfrac{1}{322560}B_6 + \tfrac{1}{92897280}B_8 + \cdots).$$

Integral 2: , $r=2$. For every $k_1, k_2 \geq 0$, $k_1+k_2 \leq 2\nu-2$, we have

$$\begin{aligned}\tilde{b}_{k_1,k_2} &= \frac{1}{k_1!k_2!}\int_0^1\int_0^{\xi_1} (\xi_2 - \tfrac{1}{2})^{k_2}(\xi_1 - \tfrac{1}{2})^{\xi_1}\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ &= \frac{1}{2^{k_1+k_2+2}}\cdot\frac{1}{k_1!(k_2+1)!}\left[\frac{1-(-1)^{k_1+k_2}}{k_1+k_2+2} + \frac{(-1)^{k_2}+(-1)^{k_1+k_2}}{k_1+1}\right].\end{aligned}$$

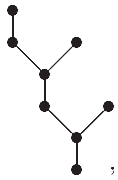
Since $[B_k, B_l] = -[B_l.B_k]$, we obtain after some manipulation the quadrature formula

$$h^2 \sum_{\substack{k_1 \leq k_2,\ k_1+k_2 \leq 2\nu-1 \\ k_1+k_2 \text{ odd}}} \frac{1}{4^{(k_1+k_2+1)/2}}\cdot\frac{(k_2-k_1)+(-1)^{k_1}(k_1+k_2+2)}{(k_1+1)!(k_2+1)!(k_1+k_2+2)}[B_{k_1}, B_{k_2}].$$

This corresponds to the expansion

$$\begin{aligned}I(h) = h^2\{&\tfrac{1}{6}[B_1,B_0] - \tfrac{1}{240}[B_2,B_1] + (\tfrac{1}{8064}[B_3,B_2] - \tfrac{1}{26880}[B_4,B_1]) \\ &+ (-\tfrac{1}{829440}[B_4,B_3] + \tfrac{1}{829440}[B_5,B_2] - \tfrac{1}{5806080}[B_6,B_1]) + \cdots\},\end{aligned}$$

where we have grouped in round brackets terms of the same order of magnitude.

Integral 3: , $r=3$. We now have

$$\tilde{b}_{k_1,k_2,k_3} = \frac{1}{k_1!k_2!k_3!}\int_0^1\int_0^{\xi_1}\int_0^{\xi_2} (\xi_3 - \tfrac{1}{2})^{k_3}(\xi_2 - \tfrac{1}{2})^{k_2}(\xi_1 - \tfrac{1}{2})^{k_1}\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1$$

$$= \frac{1}{2^{k_1+k_2+k_3+3}} \cdot \frac{1}{k_1!k_2!(k_3+1)!} \left[\frac{1+(-1)^{k_1+k_2+k_3}}{(k_2+k_3+2)(k_1+k_2+k_3+3)} \right.$$
$$- (-1)^{k_2+k_3} \frac{1+(-1)^{k_1}}{(k_1+1)(k_2+k_3+2)} + (-1)^{k_3} \frac{1-(-1)^{k_1+k_2}}{(k_2+1)(k_1+k_2+2)}$$
$$\left. + (-1)^{k_2+k_3} \frac{1+(-1)^{k_1}}{(k_1+1)(k_2+1)} \right].$$

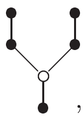
We deduce the expansion

$$\begin{aligned} I(h) = h^3\{ & -\tfrac{1}{24}[[B_1,B_0],B_0] + (-\tfrac{1}{80}[[B_1,B_0],B_1] + \tfrac{1}{240}[[B_2,B_0],B_0]) \\ & + (-\tfrac{7}{2880}[[B_1,B_0],B_2] + \tfrac{1}{1440}[[B_2,B_0],B_1] + \tfrac{1}{2880}[[B_2,B_1],B_0] \\ & - \tfrac{1}{960}[[B_3,B_0],B_0]) + \cdots\}. \end{aligned}$$

The above expansion can be further simplified by using the *Jacobi identity,* e.g.

$$[[B_2,B_1],B_0] = [[B_2,B_0],B_1] - [[B_1,B_0],B_2].$$

A systematic algorithm for Magnus expansions (and other methods for general Lie algebras) features in (Munthe-Kaas & Owren 1999), while Iserles & Zanna (1999) address themselves to the savings taking place within the context of quadratic Lie groups. Note that the expansion is no longer in odd powers of h, but this does not contradict our former statement. It is the *sum* of all terms in $\mathbb{F}_m$ (for any $m \geq 1$), rather than any particular term, that possesses this feature (Munthe-Kaas & Owren 1999).

Integral 4:  , $r = 3$. The explicit formula for the weights is

$$\tilde{b}_{k_1,k_2,k_3} = \frac{1}{k_1!k_2!k_3!} \int_0^1 \int_0^{\xi_1} \int_0^{\xi_1} (\xi_2 - \tfrac{1}{2})^{k_2} (\xi_1 - \tfrac{1}{2})^{k_1} (\xi_3 - \tfrac{1}{2})^{k_3} \mathrm{d}\xi_3 \mathrm{d}\xi_2 \mathrm{d}\xi_1$$
$$= \frac{1}{2^{k_1+k_2+k_3+3}} \cdot \frac{1}{k_1!(k_2+1)!(k_3+1)!} \left[\frac{1+(-1)^{k_1+k_2+k_3}}{k_1+k_2+k_3+3} \right.$$
$$\left. + (-1)^{k_2} \frac{1-(-1)^{k_1+k_3}}{k_1+k_3+2} + (-1)^{k_3} \frac{1-(-1)^{k_1+k_2}}{k_1+k_2+2} + (-1)^{k_2+k_3} \frac{1+(-1)^{k_1}}{k_1+1} \right].$$

In other words, we have the expansion

$$\begin{aligned} I(h) = {} & \tfrac{1}{3}h^3 B_0^3 + h^3\{\tfrac{1}{12}B_0B_1B_0 - \tfrac{1}{24}(B_1B_0^2 + B_0^2B_1)\} \\ & + h^3\{\tfrac{1}{60}B_0B_2B_0 + \tfrac{1}{80}(B_2B_0^2 + B_0^2B_2) + \tfrac{1}{120}B_1B_0B_1 - \tfrac{1}{240}(B_1^2B_0 + B_0B_1^2)\} \\ & + h^3\{\tfrac{1}{480}B_0B_3B_0 - \tfrac{1}{960}(B_3^2B_0 + B_0^2B_3 - \tfrac{1}{960}(B_1B_2B_0 + B_0B_2B_1) \\ & \quad + \tfrac{1}{360}(B_2B_1B_0 + B_0B_1B_2) - \tfrac{1}{576}(B_2B_0B_1 + B_1B_2B_2)\} \\ & + h^3\{\tfrac{1}{4480}B_0B_4B_0 + \tfrac{1}{6720}(B_4B_0^2 + B_0^2B_4) + \tfrac{1}{6720}B_1B_2B_1 \\ & \quad - \tfrac{1}{13440}(B_2B_1^2 + B_1^2B_2) - \tfrac{1}{13440}(B_1B_3B_0 + B_0B_3B_1) \\ & \quad - \tfrac{1}{8064}(B_3B_1B_0 + B_0B_1B_3) + \tfrac{1}{5040}(B_3B_0B_1 + B_1B_0B_3)\} + \cdots. \end{aligned}$$

In the expansion above we have grouped adjoint terms inside round brackets and enclosed terms of the same order of magnitude with curly brackets.

The expansion above can be converted to the language of commutators and 'symmetric products' $B_iB_jB_i$ by repeatedly employing the identity

$$B_i^2B_j + B_jB_i^2 - 2B_iB_jB_i = [[B_j, B_i], B_i].$$

The reader is urged to not to succumb to this temptation: as is proved in (Iserles & Zanna 1999), the best approach is exactly the opposite, expanding commutators as symmetric products.

Although it is tempting by this stage to illustrate our ideas by a specific example of a truncated Cayley expansion, with integrals replaced by quadrature, we defer this to the next section. The reason is that we need first to introduce another mechanism that enhances the quality of approximation.

4 Time symmetry under discretization

4.1 Time symmetry and a truncated Cayley expansion

We say that the flow $\psi_t X_0 = X(t)$, where t is in an open neighbourhood of the origin, is *time symmetric* if $\psi_t \circ \psi_{-t} = \mathrm{Id}$. Clearly, every exact solution of a differential equation is time-symmetric, but this is not necessarily true for its discretizations.

The importance of time symmetry is underscored by the well-known observation that it implies $\psi_t = \mathrm{e}^{\varphi_t}$, where φ_t can be expanded in *odd* powers of t. This means, in particular, that a time-symmetric truncated expansion is necessarily of an even order $2s$, say, even if we impose only order conditions up to $2s-1$. It has been indeed proved in (Iserles et al. 1998) that truncation of the Magnus expansion by power (similarly to (2.11)) is time symmetric and that this feature is preserved intact when integrals are replaced by quadrature (3.2), provided that the nodes $c_1, c_2, \ldots, c_\nu$ are symmetric with respect to the point $\frac{1}{2}$.

We prove in this section that this is not the case for a truncated Cayley expansion. In particular, imposing an order-3 requirement we obtain an order-3 method. Yet, amazingly, the order of this method is increased to four when integrals are replaced by appropriate quadrature!

It is usual to expand the solution of a differential equation about the initial point of an integration interval. Yet, within the Lie-algebraic formalism it is often advantageous to expand about the *centre* of an interval (Iserles et al. 1998, Zanna, Engø & Munthe-Kaas 1999). It is worthwhile to illustrate this with the trivial example of a scalar linear ordinary differential equation $y' = a(t)y$, $y_0 = 1$, assuming without loss of generality that $N = 0$. The exact solution is

$$y(t) = \exp\left[\int_0^t a(\xi)\mathrm{d}\xi\right] = \mathrm{cay}(\omega(t)),$$

where

$$\omega(t) = \frac{\mathrm{e}^{\int_0^t a(\xi)\mathrm{d}\xi} - 1}{\mathrm{e}^{\int_0^t a(\xi)\mathrm{d}\xi} + 1} = -2\left[\frac{1}{\mathrm{e}^{\int_0^t a(\xi)\mathrm{d}\xi} + 1} - 1\right] = -2\sum_{m=1}^{\infty} \frac{\mathrm{E}_m(0)}{m!}\left[\int_0^t a(\xi)\mathrm{d}\xi\right]^m,$$

$\{\mathrm{E}_m(x)\}_{m\geq 0}$ being *Euler polynomials* (Abramowitz & Stegun 1965). Since $\mathrm{E}_{2m}(0) = 0$, $m \geq 1$, we obtain

$$\omega(t) = -2\sum_{m=1}^{\infty} \frac{\mathrm{E}_{2m+1}(0)}{(2m+1)!}\left[\int_0^t a(\xi)\mathrm{d}\xi\right]^{2m+1}. \tag{4.1}$$

Substituting

$$\int_0^t a(\xi)\mathrm{d}\xi = \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} a^{(2k)}(\tfrac{1}{2}h)(\tfrac{1}{2}h)^{2k+1}$$

into (4.1) verifies that there exist functions c_m, $m \geq 1$, such that

$$\omega(t) = \sum_{m=0}^{\infty} c_m(\tfrac{1}{2}h)(\tfrac{1}{2}h)^{2m+1}.$$

The expansion in odd powers of h about the centre of the interval can be generalized to all linear equations.

Lemma 7 *The solution of the linear equation $Y' = A(t)Y$, $Y(0) = Y_0$, where A is an analytic matrix function, can be expanded in the form*

$$Y(h) = \mathrm{cay}(\Omega(h))Y_0,$$

where

$$\Omega(h) = \sum_{m=0}^{\infty} C_m(\tfrac{1}{2}h)(\tfrac{1}{2}h)^{2m+1}, \tag{4.2}$$

and $C_m(t) = \Omega^{(2m+1)}(\frac{1}{2}t)/(2m+1)!$, $m \geq 0$.

Proof For the sake of simplicity we shift the interval of integration from $[0, h]$ to $[-\frac{1}{2}h, \frac{1}{2}h]$. Therefore, Y is the solution of $Y' = \tilde{A}(t)Y$, $Y(-\frac{1}{2}h) = Y_0$, where $\tilde{A}(t) = A(t + \frac{1}{2}h)$.

Let X be the solution of the equation $X' = -\tilde{A}(-t)X$, $X(\frac{1}{2}h) = Y(\frac{1}{2}h)$ – in other words, we integrate $Y' = \tilde{A}(t)Y$ *backward in time.* Clearly, $X(-\frac{1}{2}h) = Y_0$. Therefore, letting $X(-t) = \mathrm{cay}(\Phi(t))Y(\frac{1}{2}h)$, we obtain

$$[I - \tfrac{1}{2}h\Phi(h)]^{-1} \cdot [I + \tfrac{1}{2}h\Phi(h)] \cdot [I - \tfrac{1}{2}h\Omega(h)]^{-1} \cdot [I + \tfrac{1}{2}h\Omega(h)] = I.$$

This is equivalent to

$$[I + \tfrac{1}{2}h\Phi(h)] \cdot [I + \tfrac{1}{2}h\Omega(h)] = [I - \tfrac{1}{2}h\Phi(h)] \cdot [I + \tfrac{1}{2}h\Omega(h)]$$

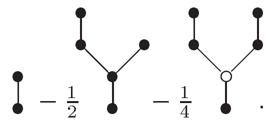
and we readily deduce that $\Phi(h) + \Omega(h) \equiv O$.

On the other hand, it follows from (1.7) that

$$\Omega'(t) = \tilde{A}(t) - \tfrac{1}{2}[\Omega(t), \tilde{A}(t)] - \tfrac{1}{4}\Omega(t)\tilde{A}(t)\Omega(t), \qquad t \geq 0,$$
$$\Phi'(t) = -\tilde{A}(-t) + \tfrac{1}{2}[\Phi(t), \tilde{A}(-t)] - \tfrac{1}{4}\Phi(t)\tilde{A}(-t)\Phi(t), \qquad t \geq 0.$$

This, in tandem with $\Omega(0) = \Phi(0) = O$, implies that $\Phi(-t) = \Omega(t)$. We therefore deduce that $\Omega(h) + \Omega(-h) = O$ and Ω is an odd function of h. The formula (4.2) follows by restoring the interval of integration to $[0, h]$. $\square$

Although Ω can be expanded in odd powers of h, *this is not the case for a truncated expansion.* The simplest nontrivial case is $\Omega_{[3]}$, which corresponds to



We have

$$\begin{aligned}\Omega_{[3]}(h) = & \int_0^h A(\xi)\mathrm{d}\xi - \tfrac{1}{2}\int_0^h\int_0^{\xi_1}[A(\xi_2), A(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ & - \tfrac{1}{4}\int_0^h\int_0^{\xi_1}\int_0^{\xi_1} A(\xi_2)A(\xi_1)A(\xi_3)\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1.\end{aligned} \tag{4.3}$$

Letting $\Phi_{[3]}(t) = \Omega_{[3]}(h-t)$, we have

$$\begin{aligned}\Phi_{[3]}(h) = & -\int_0^h A(h-\xi)\mathrm{d}\xi - \tfrac{1}{2}\int_0^h\int_0^{\xi_1}[A(h-\xi_2), A(h-\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ & + \tfrac{1}{4}\int_0^h\int_0^{\xi_1}\int_0^{\xi_1} A(h-\xi_2)A(h-\xi_1)A(h-\xi_3)\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ = & -\int_0^h A(\xi)\mathrm{d}\xi - \tfrac{1}{2}\int_0^h\int_{\xi_1}^h[A(\xi_2), A(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ & + \tfrac{1}{4}\int_0^h\int_{\xi_1}^h\int_{\xi_1}^h A(\xi_2)A(\xi_1)A(\xi_3)\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1.\end{aligned}$$

Therefore,

$$\begin{aligned}\Omega_{[3]}(h) + \Phi_{[3]}(h) = & -\tfrac{1}{2}\left\{\int_0^h\int_0^{\xi_1}[A(\xi_2), A(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 + \int_0^h\int_{\xi_1}^h[A(\xi_2), A(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1\right\} \\ & - \tfrac{1}{4}\left\{\int_0^h\int_0^{\xi_1}\int_0^{\xi_1} A(\xi_2)A(\xi_1)A(\xi_3)\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1\right. \\ & \left. - \int_0^h\int_{\xi_1}^h\int_{\xi_1}^h A(\xi_2)A(\xi_1)A(\xi_3)\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1\right\}.\end{aligned}$$

Since

$$\begin{aligned}& \int_0^h\int_0^{\xi_1}[A(\xi_2), A(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 + \int_0^h\int_{\xi_1}^h[A(\xi_2), A(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ = & \left[\int_0^h A(\xi)\mathrm{d}\xi, \int_0^h A(\xi)\mathrm{d}\xi\right] = O,\end{aligned}$$

we deduce that

$$\begin{aligned}
&\Omega_{[3]}(h) + \Phi_{[3]}(h) \\
&= -\tfrac{1}{4}\left\{\int_0^h F(\xi)A(\xi)F(\xi)\mathrm{d}\xi - \int_0^h [F(h) - F(\xi)]A(\xi)[F(h) - F(\xi)]\mathrm{d}\xi\right\} \\
&= -\tfrac{1}{4}\left\{F(h)\int_0 A(\xi)F(\xi)\mathrm{d}\xi + \int_0^h A(\xi)F(\xi)\mathrm{d}\xi F(h) - [F(h)]^3\right\},
\end{aligned}$$

where $F(t) = \int_0^t A(\xi)\mathrm{d}\xi$. Substituting $A(t) = A_0 + A_1 t + \mathcal{O}(t^2)$, we verify after long, yet trivial algebra that

$$\Omega_{[3]}(h) + \Phi_{[3]}(h) = \tfrac{1}{48}h^4[[A_1, A_0], A_0] + \mathcal{O}(h^5). \tag{4.4}$$

Therefore for general matrix functions $\Omega_{[3]}(h) + \Phi_{[3]}(h) \neq 0$ and there is no time symmetry.

On the face of it, this is a disappointing outcome. Unlike Magnus expansions, truncated Cayley expansions do not enjoy the benefits associated with time symmetry. This pessimistic outlook is unjustified: as soon as integrals are replaced by appropriate quadrature, we gain time symmetry. This will be proved in the next subsection.

4.2 Time symmetry and quadrature

Evaluating the integrals exactly, the method (4.3) is of order three, the reason being that the order of the method cannot exceed the order of time-symmetry error (4.4). Nonetheless, let us discretise the integrals with the fourth-order Gauss–Legendre quadrature. In other words, consistently with the analysis in Section 3, we evaluate

$$A_1 = A(t_N + (\tfrac{1}{2} - \tfrac{\sqrt{3}}{6})h), \qquad A_2 = A(t_N + (\tfrac{1}{2} + \tfrac{\sqrt{3}}{6})h)$$

and let

$$B_0 = \tfrac{1}{2}(A_1 + A_2), \qquad B_1 = \sqrt{3}(A_2 - A_1).$$

Thus, in line with Subsection 3.2, discarding $\mathcal{O}(h^4)$ terms and assuming without loss of generality that $t_N = 0$ yields the following approximants:

$$\begin{aligned}
\int_0^h A(\xi)\mathrm{d}\xi &\approx hB_0, \\
\int_0^h\int_0^{\xi_1} [A(\xi_2), A(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 &\approx -\tfrac{1}{6}h^2[B_1, B_0], \\
\int_0^h\int_0^{\xi_1}\int_0^{\xi_1} A(\xi_2)A(\xi_1)A(\xi_3)\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1 &\approx \tfrac{1}{3}h^3 B_0^3.
\end{aligned}$$

Assembling this together, we obtain

$$\tilde{\Omega}_{[3]}(h) = hB_0 + \tfrac{1}{12}h^2[B_1, B_0] - \tfrac{1}{12}h^3 B_0^3. \tag{4.5}$$

(We denote by $\tilde{\Omega}_{[p]}(h)$ our discretization of $\Omega_{[p]}(h)$.) The construction guarantees order three, but we claim that, as a matter of fact, this is a *fourth-order method.* Although it is possible to prove this by discretising all the terms corresponding to trees in $\mathbb{F}_m$, $m = 1, 2, 3, 4$ (which are precisely the four trees in Table 2), we pursue a different route, which lends itself to generalisation. We thus observe that $\tilde{\Omega}_{[3]}(h)+\tilde{\Omega}_{[3]}(-h) = 0$, hence time symmetry and increase in order. The immediate reason is that

$$B_0 = \sum_{l=0}^{\infty} \frac{1}{12^l(2l)!} A^{(2l)}(\tfrac{1}{2}h)(\tfrac{1}{2}h)^{2l},$$
$$B_1 = \sum_{l=0}^{\infty} \frac{1}{12^l(2l+1)!} A^{(2l+1)}(\tfrac{1}{2}h)(\tfrac{1}{2}h)^{2l+1}$$

and substitution in (4.5) confirms that $\tilde{\Omega}_{[3]}(h)$ is an odd function.

The observation that (4.5) is a fourth-order method is indicative of a more general pattern. Thus, let $\nu \geq 1$ be a given integer and $\tau \in \mathbb{F}_m$ for $1 \leq m \leq 2\nu - 1$. We denote by $Q_\tau^{[\nu]}(h)$ the quadrature (3.3) of $V_\tau(h)$, except that we throw away all $\mathcal{O}(h^{2\nu})$ terms. In other words, we throw away all terms such that $|\boldsymbol{k}| \geq 2\nu - r$ where $\tau \in \mathbb{T}_r$. Note that

$$Q_\tau^{[\nu]}(h) = V_\tau(h) + \mathcal{O}(h^{2\nu})$$

and (for the time being) we sacrifice order. We approximate (2.11) by letting

$$\tilde{\Omega}_{[2\nu-1]}(h) = \sum_{m=1}^{2\nu-1} \sum_{\tau\in\mathbb{F}_m} \alpha(\tau) Q_\tau^{[\nu]}(h). \tag{4.6}$$

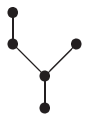
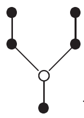
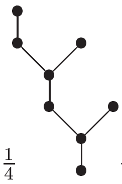
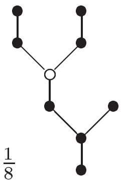
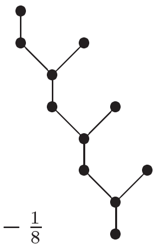
Theorem 8 *The method (4.6) approximates $\Omega(h)$ to order 2ν.*

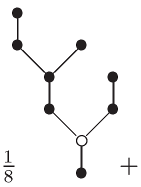
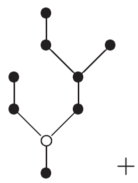
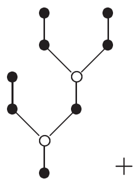
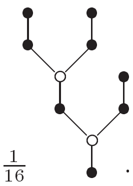
Proof It follows from our construction that $\tilde{\Omega}_{[2\nu-1]}(h) - \Omega(h) = \mathcal{O}(h^{2\nu})$ and the order is at least $2\nu - 1$. However, recall that, according to (4.2), $\Omega(h)$ can be expanded about $\frac{1}{2}h$ in odd powers of h. On the other hand, because of our construction of $Q_\tau^{[\nu]}(h)$, the latter contains no $\mathcal{O}(h^{2\nu})$ terms in its expansion about $\frac{1}{2}h$. We deduce that the first nonzero term in the expansion of the error $\tilde{\Omega}_{[2\nu-1]}(h) - \Omega(h)$ is $\mathcal{O}(h^{2\nu+1})$ and this proves that the order of the method (4.6) is indeed 2ν. □

Several observations are in order. Firstly, as often in mathematics, the derivation of the special case $\nu = 2$ is substantially more complicated than the proof of the general statement, valid for all $\nu \geq 1$. Secondly, a perfectly valid interpretation of the phenomenon displayed above is that the sum total of quadrature errors exactly annihilates the leading error term in the exact Cayley expansion (2.11). Thirdly, and most importantly, *the discretized approximant $\tilde{\Omega}_{[2\nu-1]}(h)$ is superior to the 'exact' approximant $\Omega_{[2\nu-1]}$!* It is often possible to evaluate multivariate integrals exactly, e.g. when A has polynomial or trigonometric entries. It is crucial to emphasise that even in this case it is better (at least insofar as the numerical error is concerned) to discretise the integral with the right quadrature formula, rather than evaluating it exactly.

4.3 A sixth-order Cayley expansion

According to Table 1, there are ten trees in $\mathbb{F}_m$, $m \leq 5$, and, according to (2.7), $\Omega_{[5]}$ corresponds to

 $-\frac{1}{2}$  $-\frac{1}{4}$  $+\frac{1}{4}$  $+\frac{1}{8}$  $-\frac{1}{8}$  (4.7)

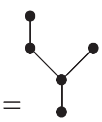
$+\frac{1}{8}$  $+\frac{1}{8}$  $+\frac{1}{16}$  $+\frac{1}{16}$  .

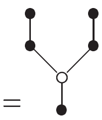
We evaluate $A_k = A(t_N + c_k h)$ at $c_1 = \frac{1}{2} - \frac{\sqrt{15}}{10}$, $c_2 = \frac{1}{2}$, $c_3 = \frac{1}{2} + \frac{\sqrt{15}}{10}$ and let

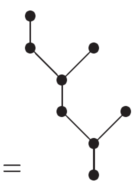
$$\begin{aligned} B_0 &= A_2, \\ B_1 &= \tfrac{\sqrt{15}}{3}(A_3 - A_1), \\ B_2 &= \tfrac{20}{3}(A_3 - 2A_2 + A_1). \end{aligned}$$

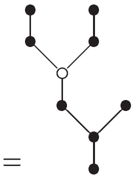
The following are sixth-order quadrature formulae corresponding to the terms in (4.7), with $\mathcal{O}(h^6)$ terms truncated. We have grouped adjoint terms together and 'massaged' expressions for a more succinct form. The adjoint of the tree τ is denoted by τ^*.

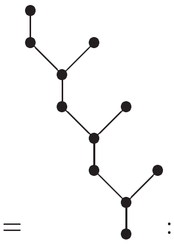
$\tau =$  : $Q_\tau^{[3]} = h(B_0 + \frac{1}{24}B_2)$,

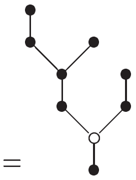
$\tau =$  : $Q_\tau^{[3]} = h^2(-\frac{1}{6}[B_1, B_0] + \frac{1}{240}[B_2, B_1])$,

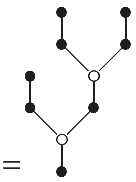
$\tau =$  : $Q_\tau^{[3]} = h^3(\frac{1}{3}B_0^3 - \frac{1}{24}[[B_1, B_0], B_0] + \frac{1}{80}[[B_2, B_0], B_0] + \frac{1}{240}[[B_1, B_0], B_1] + \frac{1}{24}B_0 B_2 B_0)$,

$\tau =$  : $Q_\tau^{[3]} = h^3(-\frac{1}{24}[[B_1, B_0], B_0] - \frac{1}{80}[[B_1, B_0], B_1])$,

$\tau =$  : $Q_\tau^{[3]} = -\frac{1}{24}h^4[B_1, B_0^3]$,

$\tau =$  : $Q_\tau^{[3]} = -\frac{1}{120}h^4[[[B_1, B_0], B_0], B_0]$,

$\tau =$  : $Q_\tau^{[3]} + Q_{\tau^*}^{[3]} = \frac{1}{30}h^4(B_0[B_1, B_0]B_0 - [B_1, B_0^3])$,

$\tau =$  : $Q_\tau^{[3]} + Q_{\tau^*}^{[3]} = \frac{2}{15}h^5 B_0^5$.

Substituting all this into (4.7) we obtain the sixth-order method

$$\begin{aligned}\tilde{\Omega}_{[5]}(h) = hB_0 &+ (\tfrac{1}{24}hB_2 + \tfrac{1}{12}h^2[B_1, B_0] - \tfrac{1}{12}h^3B_0^3)\\ &+ (-\tfrac{1}{480}h^2[B_2, B_1] - \tfrac{1}{320}h^3[[B_2, B_0], B_0] - \tfrac{1}{240}h^3[[B_1, B_0], B_1]\\ &- \tfrac{1}{96}h^3B_0B_2B_0 - \tfrac{3}{320}h^4[B_1, B_0^3] + \tfrac{1}{240}h^4B_0[B_1, B_0]B_0\\ &+ \tfrac{1}{960}h^4[[[B_1, B_0], B_0], B_0] + \tfrac{1}{120}h^5B_0^5).\end{aligned} \tag{4.8}$$

We have again grouped terms of the same order of magnitude in round brackets. Note that, as we have already proved, $\tilde{\Omega}_{[5]}(h)$ is an odd function of h (expanded about $\frac{1}{2}h$), thereby corresponding to a time-symmetric Cayley expansion. This is definitely *false* with regard to quadratures of individual terms. Specifically, the two trees in $\mathbb{T}_3$ result in quadratures which are not odd. However, the single term inconsistent with oddness is annihilated by linear combination.

We mention in passing that (4.8) does not represent the most economical means of evaluating $\tilde{\Omega}_{[5]}(h)$, since it is possible to take advantage of redundancies which are specific to Lie algebras corresponding to quadratic Lie groups. Systematic theory is developed in (Iserles & Zanna 1999), while a forthcoming paper of Blanes will address itself to the construction of most economical Cayley expansions for moderate orders.

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