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Algebraic Structures on Ordered Rooted Trees and Their Significance to Lie Group Integrators

by

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Abstract

Most Lie group integrators can be expanded in series indexed by the set of ordered rooted trees. To each tree one can associate two distinct higher order derivation operators, which we call frozen and unfrozen operators. Composition of frozen operators induces a concatenation product on the trees, whereas composition of unfrozen operators induces a somewhat more complicated product known as the Grossman–Larson product. Both of these algebra structures can be supplemented by the same coalgebra structure and an antipode, the result being two distinct cocommutative graded Hopf algebras. We discuss the use of these structures and characterize subsets of the Hopf algebras corresponding to vector fields and mappings on manifolds. This is further relevant for deriving order conditions for a general class of Lie group integrators and for deriving the modified vector field in backward error analysis for these integrators.

1 Introduction

The derivation of high order Runge–Kutta methods was revolutionized by Butcher's discovery of the beautiful connection between their series expansion in terms of the stepsize and the set T of rooted trees [2]. Virtually overnight, long and tedious calculations were replaced by elegant recursion formulas expressed in terms of trees. Later on, in 1972 Butcher published a paper [3] where he showed that Runge–Kutta methods form a group under composition, and derived explicit expressions for the group operations as induced on the trees. Hairer and Wanner named it the Butcher group and contributed substantially to the theory in [10]. The group is defined on the dual of the tree space by using a bialgebra structure on the space of rooted trees.

More recently, Kreimer [13] used a Hopf algebra of rooted trees to deal with the combinatorics of renormalization in quantum field theory, the connection to the work of Butcher was nicely presented in [1].

In the last few years, new classes of integrators have been subjected to order analysis by means of trees. In [19] order conditions for composition methods are studied by means of so called ∞-trees, see also [8]. Another class of novel schemes is the one based on Lie group actions on manifolds. Such integrators, which generalize classical Runge–Kutta methods, are now commonly referred to as Lie group integrators. Early contributors to this class of schemes include Crouch and Grossman [6] as well as Lewis and Simo [14, 15]. The Lie group schemes were later subjected to a more systematic treatment by many authors, see the survey [12]. In [16] Munthe-Kaas showed how a certain subclass of the Lie group integrators could be expanded in a series for the purpose of order analysis, but his approach was not pursued any further at that time since he discovered in [17] that a suitable change of variable would allow him to use the classical Butcher theory for deriving the order conditions. But the schemes of Crouch and Grossman [6] did not fit into this framework, and so Owren and Marthinsen [21] developed a slightly different framework based on *ordered rooted trees* for deriving the general order conditions for such schemes.

In this note, we will see how the algebraic structure introduced by Butcher can be extended to the set of ordered rooted trees. In particular we will present two different Hopf algebras on rooted trees, the first one was introduced by Grossman and Larson in [7] and the second is related to the one presented by Reutenauer in the text [22]. We will discuss their relevance to order conditions and backward error analysis for a general class of Lie group integrators.

2 Lie group integrators

An ordinary differential equation on a manifold has various different formulations,

$$y' = F(y) = f(y) \cdot y = \sum_i f^i(y)\, E_i(y). \tag{1}$$

F is here a smooth vector field on $\mathcal{M}$. The second equality tacitly refers to a transitive action on $\mathcal{M}$ by a Lie group G, and $f : \mathcal{M} \to \mathcal{V} \subset \mathfrak{g}$ where $\mathfrak{g}$ is the Lie algebra of G, and $\mathcal{V}$ is a subspace of $\mathfrak{g}$. The notation $v \cdot p$, $v \in \mathfrak{g}$, $p \in \mathcal{M}$ signifies the derivative of the group action in the sense that

$$v \cdot p = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \exp(tv) \cdot p.$$

In the last equality of (1), we have used a set of frame vector fields $E_1, \ldots, E_d$ that may be defined as $E_i(p) = e_i \cdot p$ for some basis $e_1, \ldots, e_d$ of $\mathfrak{g}$ (or $\mathcal{V}$). The functions $f^i \colon \mathcal{M} \to k$ are then given such that $f(y) = \sum f^i(y)\, e_i \cdot y$. To the end of this note, we shall always assume that the field k is either $\mathbf{R}$ or $\mathbf{C}$. Note that the action is usually not assumed to be free. For our purposes, the language of actions and frames can be used interchangeably, but for this present exposition we find it slightly advantageous to use frames. By a minor abuse of notation, we shall therefore denote by $\mathcal{V}$ also the linear span of the frame vector fields

$$\mathcal{V} = \operatorname{span}\{E_1(y), \dots, E_d(y)\}.$$

We will as usual interpret vector fields as derivations acting on functions $\psi : \mathcal{M} \to k$, and denote this action by $F[\psi]$ for any $F \in \mathfrak{X}(\mathcal{M})$.

In order to develop numerical integrators, we approximate the vector field by the *freeze* map $\mathrm{Fr}\colon \mathcal{M} \times \mathfrak{X}(\mathcal{M}) \to \mathcal{V}$, in which the vector fields E_i are assumed to be simpler to integrate than F,

$$\left(p, \sum_i f^i(y) E_i(y)\right) \mapsto \sum_i f^i(p) E_i(y). \tag{2}$$

We propose a scheme for Lie group integrators which generalizes both Crouch–Grossman (CG) type of schemes [6, 21], and the Runge–Kutta–Munthe-Kaas (RKMK) type [16, 17]. The scheme uses the point $p \in \mathcal{M}$ as input, together with a stepsize $h \in \mathbf{R}$ and produces as output a point $y_1 \in \mathcal{M}$ such that $y_1 \approx \exp(hF)\, p$.

$$g_i = \exp\left(\sum_r \alpha^r_{i,J} K_r\right) \cdots \exp\left(\sum_r \alpha^r_{i,1} K_r\right) p \tag{3}$$

$$\bar{K}_i = h\, \mathrm{Fr}(g_i, F) = h\, \sum_\ell f^\ell(g_i) E_\ell \tag{4}$$

$$K_i = P_i\left(\bar{K}_1, \dots, \bar{K}_s\right) \quad \text{(Lie polynomial)} \tag{5}$$

$$y_1 = \exp\left(\sum_r \beta^r_J K_r\right) \cdots \exp\left(\sum_r \beta^r_1 K_r\right) p \tag{6}$$

In (3) to (5) the index i runs from 1 to s, where s is the number of stages in the step.

This scheme belongs to the RKMK class if $J = 1$ in (3) and (6) (only one exponential used for g_i and y_1). If $\alpha^r_{i,j} = 0$ when $r \neq j$ in (3), $\beta^r_j = 0$ when $r \neq j$ in (6), and $K_i = \bar{K}_i$ for all i, then this is a Crouch–Grossman scheme. Requiring only $\bar{K}_i = K_i$ for all i, one obtains a commutator-free Lie group scheme [4].

The scheme is explicit if P_i in (5) depends only on $\bar{K}_1, \dots, \bar{K}_i$ and $\alpha^r_{i,j} = 0$ when $r \geq i,\ 1 \leq j \leq J$.

3 Algebraic structures on trees

In this section we shall impose algebraic structures on the space of ordered rooted trees. We will define two distinct associative products and a unit element and thereby introduce two different algebra structures. We next define a coassociative coproduct with counit to obtain one coalgebra which can be used with each of the two algebras to form two distinct bialgebras. Each of these can be equipped with an antipode, the result being two distinct cocommutative graded Hopf algebras. A good reference for the theory of Hopf algebras is Sweedler's book [23], to which we will refer frequently.

The set of all ordered rooted trees is denoted T_O, see e.g. [5] for a rigorous treatment of such trees and their combinatorial properties. We shall work recursively with trees, and our notation is based on the fact that a tree $t \in T_O$ is either the one-node tree $\bullet \in T_O$ (the identity tree), or obtained by connecting the roots of an ordered set of subtrees $t_1, \dots, t_\mu$ to a new common root, where each $t_i \in T_O$. We use the notation $t = B_+(t_1, \dots, t_\mu)$ for this operation. Conversely, $B_-(t)$ will denote the (ordered) set of subtrees obtained by deleting the root of t. Let $\sigma(t)$ be the underlying set of nodes of t. The number of nodes in a tree t is denoted $|t|$, and we let the grading be $\nu(t) = |t| - 1$. So $\nu(\bullet) = 0$, and for any other tree $t = B_+(t_1, \dots, t_\mu)$ one has $\nu(t) = \mu - 1 + \sum_{i=1}^{\mu} \nu(t_i)$. It is well known, see e.g. [5], that the number ν_r of trees such that $\nu(t) = r$ is given by the Catalan number

$$\nu_r = \frac{1}{r+1}\binom{2r}{r}. \tag{7}$$

The linear space kT_O is obtained by forming finite linear combinations of trees over the field k.

We shall later make use of the subset of T_O consisting of trees with only one subtree at the first level, we denote this subset by T_O^1, and let kT_O^1 be the corresponding subspace of kT_O.

$$T_O^1 = \left\{ t \in T_O : \ t = B_+(t'), \quad t' \in T_O \right\}.$$

3.1 Grossmann–Larson product on trees

An *attachment map* is a map which associates to any element of an ordered finite subset S of T_O a unique element of another set M, which will typically be the nodes of a tree, $\sigma(t)$. We write $d \colon S \longrightarrow \sigma(t)$ for this map. By the notation

$$v \leftharpoonup_d S \tag{8}$$

we mean an augmented tree w where each element $s \in S$ has been attached to the node $d(s)$ of v by adding an edge from the root of s to $d(s)$. Thus, s becomes a subtree of the tree which is rooted at $d(s)$. This subtree will be ordered *before* any of the existing subtrees at $d(s)$. Moreover, if $d(s) = d(s')$ where $s < s'$ then s will be ordered before s' as subtrees of the new tree w. By convention, we depict this ordering by grafting elements of S to the left of the already existing subtrees in v. Sometimes we need to sum over all possible attachment maps d from S to $\sigma(v)$ in (8) in which case we simply omit the subscript on $\leftharpoondown$ and write

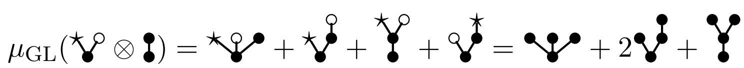
$$v \leftharpoondown S := \sum_d v \leftharpoondown_d S$$

Definition 3.1 (Grossman–Larson algebra). The identity element is the one-node tree $\bullet$, and the product of two trees is

$$\mu_{\mathrm{GL}}(v \otimes w) = w \leftharpoondown B_-(v), \quad v, w \in T_O$$

The unit in the algebra is $u\colon k \to kT_O$ given by $u(\alpha) = \alpha\bullet$ for $\alpha \in k$.

This product is non-commutative. An example is


(9)

where we have temporarily inserted a star and a circle for the grafted nodes to explicitly show the order-preservation.

Grossmann and Larson prove in [7, Section 3] that this product is indeed associative.

3.2 Concatenation algebra on trees

We continue to define a simpler product on the trees in T_O.

Definition 3.2 (Concatenation algebra). The concatenation product of two trees v and w results from joining all the subtrees of both v and w to a new common root,

$$\mu_{\mathrm{M}}(v \otimes w) = B_+(B_-(v) \cup B_-(w)), \quad v, w \in T_O$$

such that the order is preserved. The identity is the one-node tree $\bullet$.

Alternatively, if $v = B_+(v_1, \ldots, v_\mu)$ and $w = B_+(w_1, \ldots, w_\nu)$, then $\mu_{\mathrm{M}}(v \otimes w) = B_+(v_1, \ldots v_\mu, w_1, \ldots w_\nu)$.

Note that this product has a subset of the terms arising from the product in the Grossman–Larson algebra. We may write $\mu_M(v \otimes w) = w \leftharpoondown_{d_0} B_-(v)$ where d_0 is the map that sends all elements of the set $B_-(v)$ to the root $r \in \sigma(w)$.

3.3 Coalgebra on trees

The two Hopf algebras on trees we will present, share the same coproduct $\Delta : kT_O \to kT_O \otimes kT_O$. We here follow the presentation in [7], but we refer to [23] for the basic theory on algebras and coalgebras.

Definition 3.3 (Coalgebra). The coproduct on the trees in T_O is given by

$$\Delta(t) = \sum_{\mathcal{X} \subseteq B_-(t)} B_+(\mathcal{X}) \otimes B_+(\mathcal{X}^c)$$

which extends linearly to kT_O. The subsets $\mathcal{X}$ inherit the ordering from t as do the complements $\mathcal{X}^c$. We include the empty set $\emptyset$ as well as $B_-(t)$ in the sum, using the convention $B_+(\emptyset) = \bullet$. The counit is the linear map $\epsilon\colon kT_O \to k$ such that

$$\epsilon(\bullet) = 1 \quad \text{and} \quad \epsilon(t) = 0, \quad t \in T_O, t \neq \bullet.$$

We refer to [7] for a proof that the coproduct defined above is coassociative, meaning that $(I \otimes \Delta) \circ \Delta = (\Delta \otimes I) \circ \Delta$.

A bialgebra has both an algebra structure and a coalgebra structure which are compatible in the sense that the coproduct must be an algebra homomorphism (or equivalently, the product is a coalgebra homomorphism). That is

$$\Delta(\mu_{\mathrm{GL}}(v \otimes w)) = \mu_{\mathrm{GL}\otimes\mathrm{GL}}(\Delta(v) \otimes \Delta(w)). \tag{10}$$

We refer to Grossman and Larson [7, Section 3] for a proof of Equation (10). Note that the product structure $\mu_{\mathrm{GL}\otimes\mathrm{GL}}$ on $kT_O \otimes kT_O$ is naturally constructed using $\mu_{\mathrm{GL}\otimes\mathrm{GL}} = (\mu_{\mathrm{GL}} \otimes \mu_{\mathrm{GL}}) \circ (I \otimes T \otimes I)$ where $T\colon a \otimes b \mapsto b \otimes a$ is the twist map.

It is easier to prove that Δ is an algebra homomorphism with respect to the concatenation algebra.

Proposition 3.4. *The coproduct Δ given in Definition 3.3 is a concatenation algebra homomorphism, that is*

$$\Delta(\mu_{\mathrm{M}}(t_1 \otimes t_2)) = \mu_{\mathrm{M}\otimes\mathrm{M}}(\Delta(t_1) \otimes \Delta(t_2))$$

Proof. From the left we have

$$\begin{aligned}\Delta(\mu_{\mathrm{M}}(t_1 \otimes t_2)) &= \Delta(B_+(B_-(t_1) \cup B_-(t_2))) \\ &= \sum_{\mathcal{X} \subseteq B_-(t_1) \cup B_-(t_2)} B_+(\mathcal{X}) \otimes B_+(\mathcal{X}^c)\end{aligned}$$

and from the right, using $\mu_{\mathrm{M}\otimes\mathrm{M}} = (\mu_M \otimes \mu_M) \circ (I \circ T \circ I)$.

$$\begin{aligned}
\mu_{\mathrm{M}\otimes\mathrm{M}}(\Delta(t_1) \otimes \Delta(t_2)) &= \mu_{\mathrm{M}\otimes\mathrm{M}} \left(\sum_{\mathcal{X}_1,\mathcal{X}_2} B_+(\mathcal{X}_1) \otimes B_+(\mathcal{X}_1^c) \otimes B_+(\mathcal{X}_2) \otimes B_+(\mathcal{X}_2^c) \right) \\
&= (\mu_{\mathrm{M}} \otimes \mu_{\mathrm{M}}) \left(\sum_{\mathcal{X}_1,\mathcal{X}_2} B_+(\mathcal{X}_1) \otimes B_+(\mathcal{X}_2) \otimes B_+(\mathcal{X}_1^c) \otimes B_+(\mathcal{X}_2^c) \right) \\
&= \sum_{\mathcal{X}_1,\mathcal{X}_2} B_+(\mathcal{X}_1 \cup \mathcal{X}_2) \otimes B_+(\mathcal{X}_1^c \cup \mathcal{X}_2^c)
\end{aligned}$$

which is a sum equivalent to the one above. $\square$

It is also apparent from the definition of the coproduct that the coalgebra is cocommutative, that is $\Delta = \Delta \circ T$.

3.4 Grossmann–Larson Hopf algebra

A mapping $\mathcal{S}\colon kT_O \to kT_O$ in a bialgebra, is an antipode [23] if it satisfies

$$\mu \circ (\mathcal{S} \otimes \mathrm{Id}) \circ \Delta = u \circ \epsilon = \mu \circ (\mathrm{Id} \otimes \mathcal{S}) \circ \Delta \tag{11}$$

Note that $u \circ \epsilon$ is zero on all trees in T_O except from $\bullet$, one has $u \circ \epsilon(\bullet) = \bullet$. One may apply (11) with μ replaced by μ_{GL} recursively to obtain $\mathcal{S}_{\mathrm{GL}}(t)$ for any $t \in T_O$, noting that one gets $\mathcal{S}_{\mathrm{GL}}(\bullet) = \bullet$ as well as identities of the form

$$\mathcal{S}_{\mathrm{GL}}(t) = -t - \sum \mu_{\mathrm{GL}}(\mathcal{S}_{\mathrm{GL}}(t_{i_1}) \otimes t_{i_2}), \quad |t_{i_1}| < |t|.$$

An explicit formula for $\mathcal{S}_{\mathrm{GL}}(t)$ seems hard to derive or use in general. But there are some simple cases. For instance,

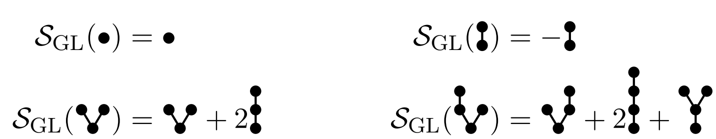
$$\mathcal{S}_{\mathrm{GL}}(t) = -t, \quad \text{for } t \in T_O^1. \tag{12}$$

For trees with exactly two branches emanating from the root, one has

$$\mathcal{S}_{\mathrm{GL}}(B_+(t_1, t_2)) = B_+(t_2, t_1) + B_+(t_1 \leftharpoonup t_2 + t_2 \leftharpoonup t_1).$$

where B_+ has been extended to a linear map.

Example 3.5 (Grossmann–Larson antipode).



3.5 Concatenation Hopf algebra

We define the antipode for the concatenation algebra in the same way, but the trivial product provides an easy factorization which facilitates a formula for the antipode.

The antipode of a tree $t = B_+(t_1, \dots t_\mu)$ in the concatenation algebra takes the form

$$\mathcal{S}(t) = (-1)^\mu B_+(t_\mu, \dots t_1)$$

which follows from the fact that the antipode of a Hopf algebra is an anti-automorphism [23, Proposition 4.0.1, page 74] and from Equation (12).

Because the coproduct for both Hopf algebras is cocommutative, the antipodes have the property that $\mathcal{S}^2$ is the identity map on kT_O [23, Proposition 4.0.1, page 74].

3.6 Infinite series and their subsets

We may define formal series on T_O as infinite sums

$$\sum_{t \in T_O} S_t \, t$$

where S_t is the coefficient of the tree t in the series S. The set of all such series is denoted $k_\infty T_O$ of which kT_O is clearly a subspace. We can extend the bialgebras to this space by setting the coefficients of the product of two series S and T to

$$(\mu(S \otimes T))_t = \sum_{\mu(v \otimes w) = t} S_v T_w \tag{13}$$

the sum being finite since the homogeneous components of kT_O are finite dimensional. The coproduct Δ is extended in a similar way. We may now define the commutator between two series in either algebra as

$$[S, T] = \mu(S \otimes T - T \otimes S).$$

The primitive elements of the extended Hopf algebras are those which satisfy

$$\Delta(S) = S \otimes \bullet + \bullet \otimes S. \tag{14}$$

The linear space of primitive elements is from now on denoted $\mathfrak{g}$, it is closed under the commutator and thus forms a Lie algebra. Later, we shall see that $\mathfrak{g}$ plays an important role as its members represent formal expansions of the vector fields used in the integration schemes. In particular, we observe from the definition of the coproduct that $k_\infty T_O^1 \subset \mathfrak{g}$. Moreover, it follows immediately from (14) and the general definition of the antipode that

$$\mathcal{S}(S) = -S, \quad S \in \mathfrak{g}.$$

The Milnor–Moore theorem ensures that the universal enveloping algebra of $\mathfrak{g}$ is isomorphic to $k_\infty T_O$.

The series $T \in k_\infty T_O$ with $\langle T, \bullet \rangle = 1$ form a group under the product in (13). Taking the formal exponential of all Lie series $\mathfrak{g}$, we obtain a subgroup $G = \exp(\mathfrak{g})$ with the property

$$\Delta(T) = T \otimes T. \tag{15}$$

if $T = \exp(S)$ for $S \in \mathfrak{g}$. The proof is simple, and can be found in [22, Thm. 3.2].

The group G is also invariant under the antipode, the antipode represents the group inverse, as we get

$$\mu(\mathcal{S}(T) \otimes T) = \bullet \tag{16}$$

from the defining equation (11) of the antipode. Later, we shall see that the elements of G represent expansions of maps defined as part of the integration schemes.

4 Elementary high order derivations

In this section we return to the Lie group integration schemes. Suppose that a frame set (action) is given together with the vector field F in (1). Letting vector fields be derivation operators acting on the functions on the manifold, we shall recursively define high order derivation operators which will feature in the expansions of the various quantities appearing in the Lie group integrators. The algebra obtained by composing these operators will be seen to coincide with the tree algebras of the previous section.

4.1 High order derivations

Definition 4.1 (Elementary High Order Derivation, EHOD). Let $F \in \mathfrak{X}(\mathcal{M})$ and $E_1, \ldots, E_d \in \mathfrak{X}(\mathcal{M})$ be given. We define $\mathbf{F}$ to be the k-linear map from $k_\infty T_O$ to the vector space of high order derivations on the manifold such that for $t \in T_O$

$$\mathbf{F}(t)\colon \psi \mapsto \mathbf{F}(t)[\psi]$$

where $\mathbf{F}(\bullet) = \mathrm{Id}$ and if $t = B_+(t_1, \ldots, t_\mu)$,

$$\mathbf{F}(t) = \sum_{i_1,\ldots,i_\mu} \mathbf{F}(t_1)[f^{i_1}] \cdots \mathbf{F}(t_\mu)[f^{i_\mu}] E_{i_1} \cdots E_{i_\mu}.$$

We now give some motivation for the above definition. Formally, one has the expansion of the flow of $F \in \mathfrak{X}(\mathcal{M})$ relative to the point $p \in \mathcal{M}$,

$$\psi(\exp(hF)p) = \psi(p) + F[\psi](p) + \frac{1}{2}F^2[\psi](p) + \cdots = \exp(hF)[\psi](p). \quad (17)$$

The powers of F are obtained by repeated application of F as a derivation operator. The expansion (17) is sometimes called a *pullback series.*

We may substitute Equation (1) ($F = f^i E_i$) into (17) and use Leibniz' rule repeatedly to generate terms that are EHODs. We use the convention that indices appearing more than once are summed over, and from [21] we find

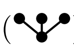
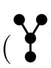
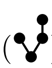
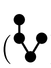
$F^1 = F = f^i E_i = \mathbf{F}($$)$

$F^2 = F[F] = f^i E_i[f^j E_j] = f^i E_i[f^j]E_j + f^i f^j E_i[E_j]$

$= \mathbf{F}($$) + \mathbf{F}($$)$

$F^3 = f^i f^j f^k E_i E_j E_k + f^i f^k E_i[f^j] E_j E_k + 2 f^i f^j E_i[f^k] E_j E_k +$ (18)

$f^i f^j E_i E_j [f^k] E_k + f^i E_i[f^j] E_j [f^k] E_k$

$= \mathbf{F}($$) + \mathbf{F}($$) + 2\mathbf{F}($$) + \mathbf{F}($$) + \mathbf{F}($$).$

Proposition 4.2. *The map* $\mathbf{F}$ *in Definition 4.1 is an algebra homomorphism from the Grossman–Larson algebra to the algebra of EHODs under composition,*

$$\mathbf{F}(\mu_{\mathrm{GL}}(v \otimes w)) = \mathbf{F}(v) \circ \mathbf{F}(w).$$

We first prove the following lemma.

Lemma 4.3. *Let* $v = B_+(t) \in T_O^1$, $t \in T_O$ *and* $w \in T_O$. *Then*

$$\mathbf{F}(v) \circ \mathbf{F}(w) = \mathbf{F}(w \leftharpoonup t)$$

Proof. The proof is by induction on $|w|$. Suppose first that $w = \bullet$, then $\mathbf{F}(v) \circ \mathbf{F}(\bullet) = \mathbf{F}(\bullet \leftharpoonup_{d_\bullet} \{t\}) = \mathbf{F}(v)$. Next suppose that the lemma holds for each w such that $|w| \leq k$ where $k \geq 1$. Any tree with $k+1$ nodes is of the form $w = B_+(w_1, \dots, w_\omega)$ where each $|w_i| \leq k$. We calculate

$$\mathbf{F}(v) \circ \mathbf{F}(w) = \sum_i \mathbf{F}(t)[f^i]E_i \left[\sum_{\mathbf{j}} \mathbf{F}(w_1)[f^{j_1}] \cdots \mathbf{F}(w_\omega)[f^{j_\omega}] E_{j_1} \cdots E_{j_\omega} \right]$$

We use Leibniz' rule and split the result in two parts, $\mathbf{F}(v) \circ \mathbf{F}(w) = T_1 + T_2$ where

$$T_1 = \mathbf{F}(B_+(t, w_1, \dots, w_\omega)) = \mathbf{F}(w \leftharpoonup_{d_r} \{t\})$$

where r is the root of w. T_1 is the part where E_i above acts as a derivation on the part $E_{j_1} \cdots E_{j_\omega}$. The second part is where E_i acts on the coefficient functions,

$$\begin{aligned}
T_2 &= \sum_{q=1}^{\omega} \sum_{i,\mathbf{j}} \mathbf{F}(t)[f^i]E_i \left[\mathbf{F}(w_q)[f^{j_q}] \right] \prod_{k \neq q} \mathbf{F}(w_k)[f^{j_k}] E_{j_1} \cdots E_{j_\omega} \\
&= \sum_{q=1}^{\omega} \sum_{\mathbf{j}} \mathbf{F}(v) \circ \mathbf{F}(w_q)[f^{j_q}] \prod_{k \neq q} \mathbf{F}(w_k)[f^{j_k}] E_{j_1} \cdots E_{j_\omega} \\
&= \sum_{\mathbf{j}} \sum_{q=1}^{\omega} \sum_{x_q \in \sigma(w_q)} \mathbf{F}(w_q \leftharpoonup_{d_{x_q}} \{t\})[f^{j_q}] \prod_{k \neq q} \mathbf{F}(w_k)[f^{j_k}] E_{j_1} \cdots E_{j_\omega} \\
&= \sum_{x \in \sigma(w) \setminus \{r\}} \mathbf{F}(w \leftharpoonup_{d_x} \{t\})
\end{aligned}$$

□

Proof of Proposition 4.2. If v is the unit tree $\bullet$, the result is obvious. Suppose that $v = B_+(v_1, \dots, v_\nu)$, each $v_i \in T_O$, and let y be the independent variable for the EHODs. Then

$$\begin{aligned}
\mathbf{F}(v) \circ \mathbf{F}(w) &= \sum_{\mathbf{i}} \mathbf{F}_s(v_1)[f^{i_1}] \cdots \mathbf{F}_s(v_1)[f^{i_\nu}] \Big|_{s=y} E_{i_1} \cdots E_{i_\nu}[\mathbf{F}(w)] \\
&= \sum_{\mathbf{i}} (\mathbf{F}_s(B_+(v_1))[f^{i_1}]E_{i_1}) \cdots (\mathbf{F}_s(B_+(v_\nu))[f^{i_\nu}]E_{i_\nu})[\mathbf{F}(w)] \Big|_{s=y}
\end{aligned}$$

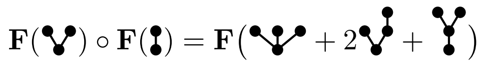
Each of the ν trees $B_+(v_i)$ are of the form $v = B_+(t)$ required by Lemma 4.3. The trees are all attached only to the nodes of w, there is no accumulation since the coefficient functions of the attached subtrees do not depend on y.

We get according to the lemma that

$$\mathbf{F}(v) \circ \mathbf{F}(w) = \sum_{k=1}^{\nu} \sum_{x \in \sigma(w)} \mathbf{F}(w \leftharpoonup_{d_x} \{v_k\}) = \sum_{d} \mathbf{F}(w \leftharpoonup_{d} B_-(v))$$

$\square$

Example 4.4. We use the same trees as in the example in Equation (9)



The corresponding EHODs composed with each other results in

$$\begin{aligned} f^i f^j E_i E_j \circ f^k E_k &= f^i f^j E_i E_j [f^k E_k] \\ &= f^i f^j E_i E_j [f^k] E_k + f^i f^j E_j [f^k] E_i E_k + \\ &\quad f^i f^j E_i [f^k] E_j E_k + f^i f^j f^k E_i E_j E_k \end{aligned}$$

which we see correspond to the correct trees as in Equation (18).

4.2 Frozen Elementary High Order Derivations

In (2) we introduced the freeze map which assigns to a pair (F, p) the vector field $F_p \in \text{span}\{E_1, \ldots, E_d\}$ which coincides with F at p, $F|_p = F_p|_p$. This amounts to freezing the coefficient functions f^i at the point p in the representation $F = f^i E_i$ in terms of the frame.

Definition 4.5 (Frozen Elementary High Order Derivation, FEHOD). Let $F \in \mathfrak{X}(\mathcal{M})$, $p \in \mathcal{M}$ and $E_1, \ldots, E_d \in \mathfrak{X}(\mathcal{M})$ be given. We define $\mathbf{F}_p$ to be the k-linear map from $k_\infty T_O$ to the vector space of high order derivations on the manifold such that for $t \in T_O$, one has: $\mathbf{F}_p(\bullet) = \text{Id}$, and if $t = B_+(t_1, \ldots, t_\mu)$, then

$$\mathbf{F}_p(t) = \sum_{i_1, \ldots, i_\mu} \mathbf{F}(t_1)[f^{i_1}](p) \cdots \mathbf{F}(t_\mu)[f^{i_\mu}](p)\, E_{i_1} \cdots E_{i_\mu}$$

Proposition 4.6. *The map $\mathbf{F}_p$ is an algebra homomorphism from the concatenation algebra to the algebra of FEHODs under composition,*

$$\mathbf{F}_p(\mu_{\mathrm{M}}(v \otimes w)) = \mathbf{F}_p(v) \circ \mathbf{F}_p(w).$$

Proof. Let $v = B_+(t_1, \dots, t_\mu)$ and $w = B_+(t_{\mu+1}, \dots, t_\nu)$, then

$$\begin{aligned}\mathbf{F}_p(v) \circ \mathbf{F}_p(w) &= \sum_{i_1,\dots,i_\mu} \mathbf{F}(t_1)[f^{i_1}](p) \cdots \mathbf{F}(t_\mu)[f^{i_\mu}](p)\, E_{i_1} \cdots E_{i_\mu} \circ \\ &\qquad \left(\sum_{i_{\mu+1},\dots,i_\nu} \mathbf{F}(t_{\mu+1})[f^{i_{\mu+1}}](p) \cdots \mathbf{F}(t_\nu)[f^{i_\nu}](p)\, E_{i_{\mu+1}} \cdots E_{i_\nu} \right) \\ &= \sum_{i_1,\dots,i_\nu} \mathbf{F}(t_1)[f^{i_1}](p) \cdots \mathbf{F}(t_\nu)[f^{i_\nu}](p)\, E_{i_1} \cdots E_{i_\nu} \\ &= \mathbf{F}_p(\mu_{\mathrm{M}}(v \otimes w))\end{aligned}$$

as each of the $\mathbf{F}(t_j)[f^{i_j}](p)$ is just a constant and thereby unaffected by the E_i's. □

5 B-series

Let kT_O^* be the algebraic dual of the space kT_O. For any $\mathbf{a} \in kT_O^*, p \in \mathcal{M}$ we associate a formal series of operators

$$B_p(\mathbf{a}) = \sum_{t \in T_O} h^{|t|-1} \langle \mathbf{a}, t \rangle \; \mathbf{F}_p(t) \tag{19}$$

where $\langle \cdot, \cdot \rangle$ is the duality pairing. We can think of (19) as a generalization of the B-series discussed in [9]. Some authors include symmetry coefficients $\sigma(t)$, and then take $\langle \mathbf{a}', t \rangle = \langle \mathbf{a}, t \rangle / \sigma(t)$ instead of $\langle \mathbf{a}, t \rangle$ in the definition.

Keeping the algebra homomorphism $\mathbf{F}_p$ from Definition 4.5 in mind, we employ the shorthand notation

$$\sum_{t \in T_O} \langle \mathbf{a}, t \rangle t \tag{20}$$

for the B-series (19) and this is now a series in $k_\infty T_O$. This formula also shows the natural identification of kT_O^* with $k_\infty T_O$.

Suppose that a map $\phi_{\mathbf{a}}$ has a B-series expansion with coefficients from $\mathbf{a} \in kT_O^*$ and relative to the point $p \in \mathcal{M}$. This means that formally

$$\psi(\phi_{\mathbf{a}}(y)) = B_p(\mathbf{a})[\psi](y) \tag{21}$$

for any function $\psi \in C^\infty(\mathcal{M}, k)$ and $y \in \mathcal{M}$. Suppose that we freeze the vector field F at the point $\phi_{\mathbf{a}}(p) \in \mathcal{M}$, we then compute the series of $hF_{\phi_{\mathbf{a}}(p)}$

using (21)

$$\begin{aligned} h\sum_i f^i(\phi_{\mathbf{a}}(p))E_i &= h\sum_i \sum_{t\in T_O} h^{|t|-1}\langle \mathbf{a}, t\rangle\, \mathbf{F}_p(t)[f^i](p)E_i \\ &= h\sum_{t\in T_O} h^{|t|-1}\langle \mathbf{a}, t\rangle \mathbf{F}_p(B_+(t)) = \sum_{t\in T_O^1} h^{|t|-1}\langle \mathbf{a}, B_-(t)\rangle \mathbf{F}_p(t). \end{aligned}$$

In other words, the B-series of a frozen vector field is associated to the space $k_\infty T_O^1$. In Section 3.6 we defined the Lie algebra $\mathfrak{g} \subset k_\infty T_O$, that is, those $S \in \mathfrak{g}$ which satisfy $\Delta(S) = S \otimes \bullet + \bullet \otimes S$. This Lie algebra contains $k_\infty T_O^1$. We may therefore conclude that the commuted vector fields $K_i = P_i(\bar{K}_1, \ldots, \bar{K}_s)$ for each of the Lie polynomials P_i in (5) belongs to $\mathfrak{g}$. Now, the quantities g_i (3) and y_1 (6) are, owing to the Baker–Campbell–Hausdorff (BCH) formula, exponentials of elements in $\mathfrak{g}$ and therefore belong to the group G. Note that the BCH formula can also be used in a formal way here so that no convergence criterion is needed.

The fact that series in $\mathfrak{g}$ satisfy (14), imposes restrictions on the dual elements $\mathbf{a}$ which represent such series. From [22, Theorem 3.1] we find that $\langle \mathbf{a}, v \sqcup\!\sqcup w\rangle = 0$ for all $v, w \in T_O$ where $v \sqcup\!\sqcup w$ is the shuffle product denoting the sum of all possible ordered insertions of w into v on the first subtree level [22, p. 23-24].

Similarly, (15) can now be used to characterize the coefficient forms in kT_O^* of a series which belongs to G. Suppose that such a $\mathbf{b} \in kT_O^*$ is representing a series in G. We find that $\langle \mathbf{b}, \bullet\rangle = 1$ and that $\langle \mathbf{b}, v \sqcup\!\sqcup w\rangle = \langle \mathbf{b}, v\rangle\langle \mathbf{b}, w\rangle$, which is called a shuffle relation. These relations were derived in a different way in [21], see also [24].

From [21] we find that the exact flow $\psi(\exp(hF)y)$ of the differential equation $\dot{y} = F(y)$ can be expressed in a B-series $B_p(\mathbf{a})$ where $\langle \mathbf{a}, t\rangle = \alpha(t)/(|t|-1)!$ and where $\alpha(t)$ is defined recursively as

$$\alpha(\bullet) = 1 \qquad \text{and} \qquad \alpha(B_+(t_1, \ldots t_\mu)) = \prod_{\ell=1}^{\mu} \binom{\sum_{i=1}^{\ell} |t_i| - 1}{|t_\ell| - 1} \alpha(t_\ell). \tag{22}$$

The linear form $\mathbf{a} \in kT_O^*$ obeys the shuffle relation $(\mathbf{a}, v \sqcup\!\sqcup w) = (\mathbf{a}, v)(\mathbf{a}, w)$.

As argued above, the numerical integration schemes presented in Section 2 admit a B-series expansion as well. Thus, for each such scheme, there exists a $\mathbf{b} \in kT_O^*$ with which (19) holds formally. In [20] one can find the details of how the B-series is obtained for commutator-free schemes.

Given two mappings on a manifold, say $\phi_{\mathbf{a}}, \phi_{\mathbf{b}} \colon \mathcal{M} \to \mathcal{M}$ with corresponding B-series $B(\mathbf{a})$ and $B(\mathbf{b})$ in $k_\infty T_O$. The composition $\phi_{\mathbf{c}} = \phi_{\mathbf{b}} \circ \phi_{\mathbf{a}}$

also has a B-series, with coefficients from $\mathbf{c}$. By applying (21) twice we get that $B_p(\mathbf{c}) = B_p(\mathbf{a}) \circ B_p(\mathbf{b})$ (note the usual reversal of order, passing from composition of mappings to composition of operators). The concatenation product on $k_\infty T_O$ now yields

$$\begin{aligned}\mu_{\mathrm{M}}\left(\sum_{v\in T_O}\langle \mathbf{a}, v\rangle\, v \otimes \sum_{w\in T_O}\langle \mathbf{b}, w\rangle\, w\right) &= \sum_{v,w\in T_O}\langle \mathbf{a}, v\rangle\,\langle \mathbf{b}, w\rangle\,\mu_{\mathrm{M}}(v\otimes w)\\ &= \sum_{t\in T_O}\sum_{\mu_{\mathrm{M}}(v\otimes w)=t}\langle \mathbf{a}, v\rangle\,\langle \mathbf{b}, w\rangle\, t = \sum_{t\in T_O}\langle \mathbf{c}, t\rangle\, t\end{aligned} \tag{23}$$

The resulting B-series has coefficients $\langle \mathbf{c}, \bullet\rangle = 1$ and for $t = B_+(t_1, \ldots, t_\mu)$,

$$\langle \mathbf{c}, t\rangle = \sum_{k=0}^{\mu}\langle \mathbf{a}, B_+(t_1, \ldots, t_k)\rangle\,\langle \mathbf{b}, B_+(t_{k+1}, \ldots, t_\mu)\rangle \tag{24}$$

In view of the identification of $k_\infty T_O$ with kT_O^*, we can think of μ_{M} as a product on kT_O^* and simply write

$$\mathbf{c} = \mu_{\mathrm{M}}(\mathbf{a}\otimes\mathbf{b}).$$

Taking the adjoint operator $\Delta_M := \mu_{\mathrm{M}}^* : kT_O \to kT_O \otimes kT_O$ (using the usual identification of $(kT_O^* \otimes kT_O^*)^*$ with $kT_O \otimes kT_O$) we obtain

$$\Delta_M(B_+(t_1, \ldots, t_\mu)) = \sum_{k=0}^{\mu} B_+(t_1, \ldots, t_k) \otimes B_+(t_{k+1}, \ldots, t_\mu),$$

and $\langle \mathbf{c}, t\rangle = \langle \mu_{\mathrm{M}}(\mathbf{a}\otimes\mathbf{b}), t\rangle = \langle \mathbf{a}\otimes\mathbf{b}, \Delta_M(t)\rangle$ which is precisely what (24) says.

The antipode in the concatenation algebra $\mathcal{S}_{\mathrm{M}}$ has an immediate application to the B-series $B_p(\mathbf{a})$ of maps $\phi_{\mathbf{a}}$ on the manifold. The antipode of a series $T \in G = \exp(\mathfrak{g})$ is the corresponding series of the inverse map $\phi_{\mathbf{a}}^{-1}$. This is evident from Equation (16) and from the fact that the B-series for the identity map on $\mathcal{M}$ has its coefficients from the counit $\epsilon \in kT_O^*$ where $\langle \epsilon, \bullet\rangle = 1$, $\langle \epsilon, t\rangle = 0$ for all other trees $t \neq \bullet$.

6 Applications

6.1 Order conditions for integration schemes

The paper [20] presents the order conditions for a subclass of the schemes introduced in Section 2. We will show here how one can use the algebra on trees to count the order conditions for any order of the numerical method.

The algebra kT_O is graded by $\nu(t) = |t| - 1$ as in the introduction to Section 3. We can decompose the algebra kT_O and the Lie algebra $\mathfrak{g}$ of primitive elements in kT_O into their respective graded components

$$kT_O = \sum_{k=0}^{\infty} \mathcal{B}_k \quad \text{and} \quad \mathfrak{g} = \sum_{k=0}^{\infty} \mathfrak{g}_k$$

The dimensions of each graded component in $\mathfrak{g}$ up to grade q are added to yield the number of order conditions for a q'th-order integration scheme. From (7) we have that $\dim \mathcal{B}_k = C_k = \frac{1}{k+1}\binom{2k}{k}$. It is well known [25, Theorem 3.2.8] that

$$kT_O = \mathrm{UEA}(\mathfrak{g})$$

where $\mathrm{UEA}(\mathfrak{g})$ is the universal enveloping algebra of $\mathfrak{g}$. Comparing generating functions for the dimensions of kT_O and $\mathrm{UEA}(\mathfrak{g})$ we get

$$\prod_{n=1}^{\infty} (1 - T^n)^{-\dim \mathfrak{g}_n} = \sum_{k=0}^{\infty} C_k T^k$$

When solved for $\dim \mathfrak{g}_k$ one obtains

$$\dim \mathfrak{g}_k = \frac{1}{2k} \sum_{d|k} \mu(k) \binom{2k/d}{k/d} \tag{25}$$

where $\mu(k)$ is the Möbius function defined for any positive integer as $\mu(1) = 1$, $\mu(k) = (-1)^p$ when k is the product of p distinct primes, and $\mu(k) = 0$ otherwise. The sum is over all positive integers d which divide k, including 1 and k.

The number of order conditions of an integration scheme of order of consistency q is then

$$N_q = \sum_{k=1}^{q} \dim \mathfrak{g}_k.$$

and the first ten numbers are

$$1, 1, 3, 8, 25, 75, 245, 800, 2700, 9225.$$

The formula (25) is well-known in the literature. For example, it counts the number of balanced Lyndon words [18] and also has an application to double bracket flows [11].

6.2 Backward error analysis

Suppose a numerical method applied to the differential equation

$$y' = F(y) \tag{26}$$

is the map $\phi_{h,F} \colon \mathcal{M} \to \mathcal{M}$. If there exists an h-dependent vector field $\tilde{F}$ such that

$$\phi_{h,F} = \exp(h\tilde{F}),$$

then the numerical method for Equation (26) solves the differential equation $y' = \tilde{F}(y)$ exactly. We call $\tilde{F}$ the *modified vector field* for $\phi_{h,F}$.

One may follow for example Hairer, Lubich and Wanner [8] and formally expand the modified vector field in powers of h

$$\tilde{F} = F + hF_2 + h^2 F_3 + \cdots . \tag{27}$$

The numerical method $\phi_{h,F}$ as a mapping on the manifold has an expansion in a B-series, say $B(\mathbf{a})$. Then we require that our modified vector field $\tilde{F}$ must obey

$$\psi(\phi_{h,F}(p)) = \psi(\exp(h\tilde{F})p) = B(\mathbf{a})[\psi](p).$$

where $B(\mathbf{a})$ is the series defined in (19).

We calculate $\exp(h\tilde{F})$ according to the expansion in (27) and get

$$\exp(h\tilde{F}) = I + hF + h^2(F_2 + \tfrac{1}{2}F^2) + h^3(F_3 + \tfrac{1}{2}(FF_2 + F_2F) + \tfrac{1}{6}F^3) + \cdots$$

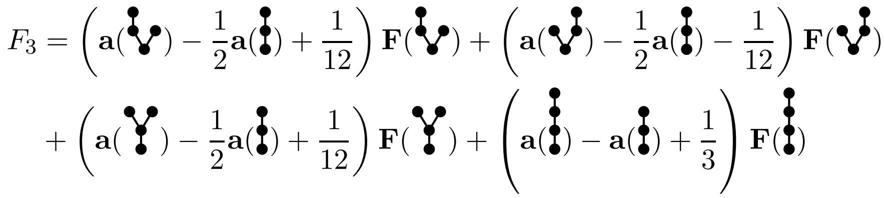
To calculate F_2 we compare coefficients of h^2 in the equation above and in $B(\mathbf{a})$. We get

$$\begin{aligned} \mathbf{a}([[\bullet]])\mathbf{F}([[\bullet]]) + \mathbf{a}([\bullet,\bullet])\mathbf{F}([\bullet,\bullet]) &= F_2 + \tfrac{1}{2}F^2 = F_2 + \tfrac{1}{2}\mathbf{F}([\bullet])^2 \\ &= F_2 + \frac{1}{2}\left(\mathbf{F}([[\bullet]]) + \mathbf{F}([\bullet,\bullet])\right) \end{aligned}$$

where we have used consistency of the method, $F = \mathbf{F}([\bullet])$ and the Grossman–Larson product of $[\bullet]$ and $[\bullet]$. Consistency of the numerical method requires $\mathbf{a}([\bullet]) = 1$, and by a shuffle relation we also have that $\mathbf{a}([\bullet,\bullet]) = \frac{1}{2}\mathbf{a}([\bullet])^2 = \frac{1}{2}$. In the end we solve for F_2 and get

$$F_2 = \left(\mathbf{a}([[\bullet]]) - \frac{1}{2}\right)\mathbf{F}([[\bullet]]) \tag{28}$$

The same approach will for the h^3 coefficients lead to



(29)

Again, putting this in a more general perspective, let $\epsilon + \mathbf{a} \in kT_O^*$ represent the B-series of the numerical method, where ϵ is the counit in the Grossman–Larson Hopf algebra, and $\langle \mathbf{a}, \bullet \rangle = 0$. We now find that the modified vector field $\tilde{F}$ has a B-series in $\mathfrak{g}$ associated to $\mathbf{b} \in kT_O^*$ such that

$$\mathbf{b} = \log_{\mathrm{GL}}(\epsilon + \mathbf{a}) = \mathbf{a} - \frac{1}{2}\mu_{\mathrm{GL}}(\mathbf{a} \otimes \mathbf{a}) + \cdots$$

Here, μ_{GL} is induced on kT_O^* from its identification with $k_\infty T_O$.

The expression for the vector fields F_k are obtained by projecting $\mathbf{b}$ onto the kth graded component of $k_\infty T_O$. One obtains that the series associated to $\mathbf{b}$ belongs to $\mathfrak{g}$.

7 Conclusion

We have discussed Hopf algebra structures on the space of ordered rooted trees, and shown how these structures are related to the expansions of Lie group integration schemes for ordinary differential equations on manifolds. The theory presented here is fairly general, in the sense that it accounts for most of the known Lie group integrators which are based on exponentials. It also allows for the analysis of schemes that are hybrids between for instance the RKMK methods [17] and the commutator-free schemes [4]. Although we have emphasized the algebraic aspects of the theory, we believe that there is a potential for using these aspects in developing integration schemes with high accuracy and good long-time behaviour.

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