An algebraic theory of order

P. Chartier[1] and A. Murua[2]

[1] *INRIA Rennes and Ecole Normale Supérieure de Cachan, Antenne de Bretagne,*
Avenue Robert Schumann, 35170 Bruz, France.
email: Philippe.Chartier@inria.fr
[2] *Konputazio Zientziak eta A. A. saila, Informatika Fakultatea, University of the Basque Country*
Donostia/San Sebastiàn, SPAIN.

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Abstract

In this paper, we present an abstract framework which describes algebraically the derivation of order conditions independently of the nature of differential equations considered or the type of integrators used to solve them. Our structure includes a Hopf algebra of functions, whose properties are used to answer several questions of prime interest in numerical analysis. In particular, we show that, under some mild assumptions, there exist integrators of arbitrarily high orders for arbitrary (modified) vector fields.

1 Introduction

When one needs to compute the numerical solution of a differential equation of a specific type (ordinary, differential-algebraic, linear...) with a method of a given class of one-step numerical integration schemes, a deciding criterion to pick up the right one is its order of convergence: the systematic determination of order conditions thus appears as a pivotal question in the numerical analysis of differential equations. Given a family of vector fields with some specific property (say for instance linear, additively split into a linear and a nonlinear part, scalar...) and a set of numerical schemes (rational approximations of the exponential, exponential integrators, Runge-Kutta methods...), a fairly general recipe consists in expanding into series both the exact solution of the problem and its numerical approximation: order conditions are then derived by comparing the two series term by term, once their independence has been established. Depending on the equation and on the numerical method, these series can be indexed by integers or trees, and can expressed in terms of elementary differentials or commutators of Lie-operators. Despite the great variety of situations encountered in practice and of ad-hoc techniques, the problems raised are strikingly similar and can be described as follows:

(Q1) is it possible to construct a set of algebraically independent order conditions?

(Q2) what are the order conditions corresponding to a scheme obtained by composition of two given methods?

(Q3) are there numerical schemes within the class considered of arbitrarily high order for arbitrary vector field?

(Q4) are there numerical schemes within the set of methods considered that approximate modified vector fields?

The Butcher group [But72], originally formulated to address these questions for Runge-Kutta methods, has a rich structure with (as first pointed out by [Dür86]) an underlying commutative Hopf algebra of rooted trees. In the past few years, such a Hopf algebra turned out to have far-reaching applications in several areas of mathematics and physics: they were rediscovered in non-commutative geometry by Connes and Moscovici [CM98] and they describe the combinatorics of re-normalization in quantum field theory as described by Kreimer [Kre98]. Hopf algebras on planar rooted trees have been recently considered and studied for generalizations of Runge-Kutta methods to Lie group integrators [MKW08, BO05]. The Hopf algebra of rooted trees associated to Butcher's group (as well as the Hopf algebras of planar rooted trees in [MKW08, BO05]) can be seen as a particular instance of a more general construction that we consider in the present work: given a group $\mathcal{G}$ of one-step integration schemes together with a map $\nu : \mathcal{G} \times \mathbb{R} \to \mathcal{G}$ (that corresponds to re-scaling the time-step) and a set $\mathcal{T}$ of functions on $\mathcal{G}$ (describing how close are two integration schemes to each other), we consider the algebra of functions $\mathcal{H}$ generated by $\mathcal{T}$, which under some natural assumptions gives rise to a commutative graded algebra of functions on $\mathcal{G}$ that turns out to have a Hopf algebra structure. Within this algebraic framework, we then address the questions listed above and provide answers that are relevant to many practical situations.

The paper is organized as follows: in Section 2, we present two simple situations aimed at introducing and motivating the main objects considered in the sequel. The first example is concerned with convergent approximations of the exponential, while the second one is concerned with approximations of two-by-two rotation matrices. In both cases, the set of integrators equipped with the composition law forms a group $\mathcal{G}$, while functions on $\mathcal{G}$ relevant to order conditions "naturally" form a graded algebra $\mathcal{H}$. Though several options exist to express the order conditions, the algebra $\mathcal{H}$ of functions they generate is the same. We also demonstrate in these two situations that the relation initiating the co-product in $\mathcal{H}$ can be derived easily.

Section 3 constitutes the core of the paper: it introduces an algebraic concept, that we call *group of abstract integration schemes*, composed of a group $\mathcal{G}$, an algebra $\mathcal{H}$ of functions on $\mathcal{G}$, and a scaling map ν whose existence is essential to the subsequent results. We begin by proving that, under some reasonable assumptions of a purely algebraic nature, the algebra $\mathcal{H}$ can be equipped with a co-product and an antipode, that give rise to a graded Hopf algebra structure. In particular, the co-product of $\mathcal{H}$ is per se the key to the second question in our list. It furthermore endows the linear dual $\mathcal{H}^*$ of $\mathcal{H}$ with an algebra structure, where a new group $\overline{\mathcal{G}}$ and a Lie-algebra $\mathfrak{g}$ can be defined and related through the exponential and logarithm maps. These two structures, standard in the theory of commutative Hopf algebras, are of prime interest in our context, since $\mathfrak{g}$ can be interpreted, in the more usual terminology of ODEs, as the set of "modified vector fields", while $\overline{\mathcal{G}}$ can be interpreted as a larger group of "integrators" containing $\mathcal{G}$. We then prove that all elements of $\overline{\mathcal{G}}$ can be "approximated" up to any order by elements of $\mathcal{G}$. With an appropriate topology for $\overline{\mathcal{G}}$, this can be interpreted by saying that $\mathcal{G}$ is dense in $\overline{\mathcal{G}}$: this answers the third and fourth questions in our list. The proof of this result also provides a positive answer to the first question of our list.

Section 4 considers the application of the results of previous sections to the case of composition integration methods. The group of abstract integration schemes is constructed explicitly leading to a new set of independent order conditions.

2 The derivation of order conditions in two simple situations

In this section, we consider two simple and hopefully enlightening examples and show how the derivation of order conditions naturally lead to some of the objects used in the sequel.

2.1 Approximation of the exponential by convergent series

Consider the class of integrators ψ for the linear equation

$$\dot{y} = \lambda y \tag{2.1}$$

which can be expanded in the parameter $z = \lambda h$ as a convergent series of the form

$$\psi(z) = 1 + \sum_{k=1}^{\infty} a_k z^k$$

on a disc $D(0, r_\psi) \subset \mathbb{C}$. For instance, one might think of explicit Runge-Kutta methods, for which $\psi(z)$ is a polynomial, or of implicit Runge-Kutta methods, for which $\psi(z)$ is a rational function. The set

$$\mathcal{G} = \{\psi;\, \exists\, r_\psi > 0,\ \forall z \in D(0, r_\psi),\ \psi(z) = 1 + \sum_{k=1}^{\infty} a_k z^k\}$$

is a group for the usual products of series. The scaling map $\nu : \mathcal{G} \times \mathbb{R} \to \mathcal{G}$ is defined as $(\psi)_\lambda = \nu(\psi, \lambda)$ where $(\psi)_\lambda(z) = \psi(\lambda z)$

Moreover, we can define a set of embedded equivalence relations $\overset{(n)}{\equiv}$ on $\mathcal{G}$ by saying that, given ψ and ϕ in $\mathcal{G}$,

$$\psi \overset{(n)}{\equiv} \phi \quad \Longleftrightarrow \quad \psi(z) = \phi(z) + \mathcal{O}(z^{n+1}) \quad \text{as} \quad z \to 0.$$

An integrator $\psi \in \mathcal{G}$ is then said to be of order $p \geq 1$ if and only if $\psi \overset{(p)}{\equiv} \varphi$, where $\varphi(z) = \exp(a_1 z)$ (with $a_1 = \psi'(0)$). Note that, owing to our definition, any $\psi \in \mathcal{G}$ is at least of order 1. Also, it is clear that if $\psi \in \mathcal{G}$ is of order n, then for all $\lambda \in \mathbb{R}$, $(\psi)_\lambda$ is also of order n.

2.1.1 Two different sets of functions generating the order conditions

In this part, we introduce two different sets of functions that both generate the order conditions. Each is based upon one of the following equivalent definitions of order

$$\psi(z) \overset{(p)}{\equiv} \exp(a_1 z) \Longleftrightarrow 1 + \log(\psi(z)) \overset{(p)}{\equiv} 1 + a_1 z,$$

and are thus expected to generate the same algebras. However, some of the questions in introduction are more conveniently answered using one set rather than the other.

We define the functions u_i, $i = 0, \ldots, \infty$ of $\mathbb{R}^{\mathcal{G}}$, i.e. functions from $\mathcal{G}$ into $\mathbb{R}$, as follows: for all $\psi \in \mathcal{G}$,

$$u_0(\psi) = 1 \text{ and } u_i(\psi) = a_i \text{ for } i \geq 1.$$

An integrator $\psi \in \mathcal{G}$ is then of order $p \geq 1$ if and only if

$$\forall\, 1 \leq i \leq p,\ u_i(\psi) = \frac{(u_1(\psi))^i}{i!}. \tag{2.2}$$

Notice that, for each $\lambda \in \mathbb{R}$, $\psi \in \mathcal{G}$, $u_i((\psi)_\lambda) = \lambda^i u_i(\psi)$. The functions u_i generate a graded algebra $\mathcal{H} \subset \mathbb{R}^{\mathcal{G}}$ obtained by considering :

$$\mathcal{H} = \bigoplus_{n \in \mathbb{N}} \mathcal{H}_n,$$

where

$$\mathcal{H}_n = \text{Span}\Big\{ \prod_{i=1}^{k} u_{n_i};\ n_1 + n_2 + \ldots n_k = n \Big\}.$$

We see that the functions u_i are convenient to express order conditions. However, their expression does not allow for an easy answer to Question (Q2) of the introduction: if ψ and ϕ are two integrators of order p, the value of u_i on $\psi \circ \phi$ can be expressed as follows

$$u_i(\psi \circ \phi) = u_i(\psi) + u_i(\phi) + \sum_{j=1}^{i-1} u_j(\psi) u_{i-j}(\phi),$$

so that checking conditions (2.2) requires some combinatorial manipulations, which, though evidently tractable, are not immediate. Alternatively, we can define another set of functions w_i as follows (computed from the Taylor series of $\log(1+x)$):

$$w_0(\psi) = 1 \text{ and } w_i(\psi) = \sum_{\mathbf{j}/S(\mathbf{j})=i} \frac{(-1)^{\#\mathbf{j}+1}}{\#\mathbf{j}} a_{\mathbf{j}}$$

where $\mathbf{j} = (j_1, \ldots, j_k)$ is an ordered multi-index of positive integers, $\#\mathbf{j} = k$, $S(\mathbf{j}) = j_1 + \ldots + j_k$ and $a_{\mathbf{j}} = \prod_{l=1}^{k} a_{j_l}$. In this case, $\psi \in \mathcal{G}$ is of order $p \geq 2$ if and only if

$$\forall\, p,\ 2 \leq i \leq p,\ w_i(\psi) = 0. \tag{2.3}$$

Note that the functions w_i can also be defined recursively, as this was the case for functions u_i. We have indeed

$$w_i(\psi) \quad = \quad a_i - \sum_{\mathbf{j}/S(\mathbf{j})=i, \#\mathbf{j}>1} \frac{1}{\sigma(\mathbf{j})} w_{\mathbf{j}}(\psi) \tag{2.4}$$

where $\mathbf{j} = [j_1^{r_1}, \ldots, j_k^{r_k}]$ is now an *unordered* multi-index of **pairwise distinct** non-zero-integers j_1, ..., j_k, each j_l being repeated $r_l > 0$ times, $\#\mathbf{j} = r_1 + \ldots + r_k$, $S(\mathbf{j}) = r_1 j_1 + \ldots + r_k j_k$, $\sigma(\mathbf{j}) = r_1! \cdots r_k!$ and $w_{\mathbf{j}}(\psi) = \prod_{l=1}^{k} (w_{j_l}(\psi))^{r_l}$. The values of functions w_i on the composed integrator $\psi \circ \phi$ have extremely simple expressions

$$w_i(\psi \circ \phi) = w_i(\psi) + w_i(\phi) \text{ for } i \geq 1,$$

so that checking the order conditions is obvious if both ψ and ϕ are of order p. We see that the functions w_i again generate the same sub-algebra of $\mathbb{R}^{\mathcal{G}}$ since they can be easily expressed in terms of functions u_i.

2.2 Approximation of rotation matrices

Let us assume that we want to approximate the rotation matrix

$$\begin{pmatrix} \cos(x) & \sin(x) \\ -\sin(x) & \cos(x) \end{pmatrix} \tag{2.5}$$

with products of the form

$$\begin{pmatrix} 1 & 0 \\ -a_{2s+1}x & 1 \end{pmatrix} \begin{pmatrix} 1 & a_{2s}x \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ -a_3 x & 1 \end{pmatrix} \begin{pmatrix} 1 & a_2 x \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -a_1 x & 1 \end{pmatrix}, \tag{2.6}$$

where $s \geq 1$ and $a_j \in \mathbb{R}$ for each $j \geq 1$. Clearly, (2.6) is a 2×2 matrix with polynomial entries, and determinant one.

Each different matrix of the form (2.6) can be identified with a finite sequence $\psi = (a_1, a_2, \ldots, a_{2s+1})$ of real numbers satisfying that $a_j \neq 0$ for $2 \leq j \leq 2s$. Let us consider the set $\mathcal{G}$ of such sequences (including the zero sequence $\epsilon = (0)$, with $s = 0$). For each sequence $\psi = (a_1, a_2, \ldots, a_{2s+1})$ of $\mathcal{G}$, we denote by $\psi(x)$ the product of matrices (2.6). Notice that, for the zero sequence $\epsilon = (0)$, $\epsilon(x)$ is the 2×2 identity matrix.

The set $\mathcal{G}$ can be endowed with a group structure with neutral element ϵ and the group law $\circ : \mathcal{G} \times \mathcal{G} \to \mathcal{G}$ defined as follows

$$(a_1, \ldots, a_{2s+1}) \circ (b_1, \ldots, b_{2m+1}) = (a_1, \ldots, a_{2s}, a_{2s+1} + b_1, b_2, \ldots, b_{2m+1}). \tag{2.7}$$

When $a_{2s+1} + b_1 = 0$, (2.7) must be interpreted by identifying sequences of the form $(a_1, \ldots, a_m, 0, a_{m+2}, \ldots, a_{2s+1})$ with $(a_1, \ldots, a_{m-1}, a_m + a_{m+2}, a_{m+3}, \ldots, a_{2s+1})$. Clearly, we have that the product of matrices $\psi(x)\phi(x)$ with $\psi, \phi \in \mathcal{G}$ is precisely $(\phi \circ \psi)(x)$.

We define for each $n \geq 0$, the equivalence relation $\overset{(n)}{\equiv}$ on $\mathcal{G}$ as follows: Given $\psi, \phi \in G$, we write $\psi \overset{(n)}{\equiv} \phi$ if $\psi(x) = \phi(x) + \mathcal{O}(x^{2n+1})$ as $x \to 0$.

We now address the problem of characterizing the equivalence relations $\overset{(n)}{\equiv}$ in terms of the sequence $\psi = (a_1, \ldots, a_{2s+1})$. It is straightforward to check that there exist functions $u_n : \mathcal{G} \to \mathbb{R}$ and $v_n : \mathcal{G} \to \mathbb{R}$ for $n \geq 1$ such that

$$\psi(x) = \begin{pmatrix} 1 + u_2(\psi)x^2 + u_4(\psi)x^4 + \cdots & u_1(\psi)x + u_3(\psi)x^3 + \cdots \\ v_1(\psi)x + v_3(\psi)x^3 + \cdots & 1 + v_2(\psi)x^2 + v_4(\psi)x^4 + \cdots \end{pmatrix}.$$

where

$$u_1(\psi) = \sum_{1 \leq i \leq s} a_{2i}, \quad u_2(\psi) = \sum_{1 \leq j \leq i \leq s} a_{2j-1}a_{2i}, \quad u_3(\psi) = \sum_{i \leq k \leq j \leq i \leq s-1} a_{2k}a_{2j+1}a_{2i+2},$$

$$v_1(\psi) = \sum_{1 \leq i \leq s+1} a_{2i-1}, \quad v_2(\psi) = \sum_{1 \leq j \leq i \leq s} a_{2j}a_{2i+1}, \quad v_3(\psi) = \sum_{1 \leq k \leq j \leq i \leq s} a_{2k-1}a_{2j}a_{2i+1},$$

and so on. In particular, $v_{2s+1}(\psi) = a_1 \cdots a_{2s+1}$, and if $a_1 = 0$, then $v_{2s}(\psi) = a_2 \cdots a_{2s+1}$. Similarly, $u_{2s}(\psi) = a_1 \cdots a_{2s}$ if $a_{2s+1} = 0$, and $u_{2s-1}(\psi) = a_1 \cdots a_{2s-1}$ if $a_1 = a_{2s+1} = 0$. This shows that

$$\psi = \epsilon \quad \Longleftrightarrow \quad \forall n \in \mathbb{N}/\{0\}, \quad u_n(\psi) = v_n(\psi) = 0. \tag{2.8}$$

We clearly have that $\psi \overset{(n)}{\equiv} \phi$ if and only if

$$u_i(\psi) = u_i(\phi), \quad v_i(\psi) = v_i(\phi), \ \text{ for } i = 1, \ldots, n. \tag{2.9}$$

However, the set of conditions (2.9) that characterizes $\psi \overset{(n)}{\equiv} \phi$ has the inconvenience of not being algebraically independent, due to the fact that $\det(\psi(x)) = 1$, which implies that

$$u_{2i} + \sum_{j=1}^{2i-1} (-1)^j v_j u_{2i-j} + v_{2i} = 0, \text{ for } i \geq 1.$$

Actually, a set of independent conditions that characterizes $\psi \overset{(n)}{\equiv} \phi$ can be obtained by considering (2.9) for odd indices i and either $u_i(\psi) = u_i(\phi)$ or $v_i(\psi) = v_i(\phi)$ for even values of the indices $i \le n$.

Some straightforward algebra leads to the following identities that relate the values of the functions u_n, v_n for the composition $\psi \circ \phi$ to the values for ψ and ϕ:

$$\begin{aligned}
u_{2k}(\psi \circ \phi) &= u_{2k}(\psi) + u_{2k}(\phi) + \sum_{i+j=k} (u_{2i}(\psi) u_{2j}(\phi) + u_{2i-1}(\psi) v_{2j+1}(\phi)), \\
v_{2k}(\psi \circ \phi) &= v_{2k}(\psi) + v_{2k}(\phi) + \sum_{i+j=k} (v_{2i}(\psi) v_{2j}(\phi) + v_{2i-1}(\psi) u_{2j+1}(\phi)), \\
u_{2k-1}(\psi \circ \phi) &= u_{2k-1}(\psi) + u_{2k-1}(\phi) + \sum_{i+j=k} (u_{2i}(\psi) u_{2j-1}(\phi) + u_{2i-1}(\psi) v_{2j}(\phi)), \\
v_{2k-1}(\psi \circ \phi) &= v_{2k-1}(\psi) + v_{2k-1}(\phi) + \sum_{i+j=k} (v_{2i}(\psi) v_{2j-1}(\phi) + v_{2i-1}(\psi) u_{2j}(\phi)).
\end{aligned}$$

It is easy to check that, for each $n \geq 1$ and each $s \geq 1$, $u_n(a_1, \dots, a_{2s+1})$ and $v_n(a_1, \dots, a_{2s+1})$ are polynomials of homogeneous degree n in the variables $a_1, \dots, a_{2s+1}$. Equivalently, if for each $\psi = (a_1, \dots, a_{2s+1}) \in \mathcal{G}$ and each $\lambda \in \mathbb{R}$ we denote by $(\psi)_\lambda$ the scaled element $(\psi)_\lambda = (\lambda a_1, \dots, \lambda a_{2s+1})$, then

$$u_n((\psi)_\lambda) = \lambda^n u_n(\psi), \quad v_n((\psi)_\lambda) = \lambda^n v_n(\psi).$$

3 Groups of abstract integration schemes

Motivated by the examples in Section 2, we will consider a group $\mathcal{G}$ with neutral element ϵ, an algebra $\mathcal{H}$ of functions on $\mathcal{G}$ and a map ν

$$\begin{aligned} \nu : \mathcal{G} \times \mathbb{R} &\to \mathcal{G} \\ (\psi, \lambda) &\mapsto \psi_\lambda \end{aligned} \tag{3.1}$$

satisfying the following assumptions:

(H_1) : For each $u \in \mathcal{H}$, there exist $v_1, w_1, \dots, v_m, w_m \in \mathcal{H}$ such that

$$u(\psi \circ \phi) = \sum_{j=1}^{m} v_j(\psi) w_j(\phi), \quad \forall (\psi, \phi) \in \mathcal{G} \times \mathcal{G}. \tag{3.2}$$

(H_2) : Given $\psi, \phi \in \mathcal{G}$, $(\psi \circ \phi)_\lambda = (\psi)_\lambda \circ (\phi)_\lambda$ for all $\lambda \in \mathbb{R}$, and $\psi_0 = \epsilon$.

(H_3) : The set

$$\mathcal{H}_n = \{u \in \mathcal{H} : u(\psi_\lambda) = \lambda^n u(\psi) \text{ for all } \lambda \in \mathbb{R}\} \tag{3.3}$$

where, by convention, $0^0 = 1$, is a finite-dimensional vector space and

$$\mathcal{H} = \bigoplus_{n \geq 0} \mathcal{H}_n.$$

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(H_4) : Given $\psi, \phi \in \mathcal{G}$, if $u(\psi) = u(\phi)$ for all $u \in \mathcal{H}$, then $\psi = \phi$.

We will say that a function $u \in \mathcal{H}$ is homogeneous if $u \in \mathcal{H}_n$ for some positive integer n, and we will say that n is the (homogeneous) degree of u and write $|u| = n$ in that case. From assumptions $(H_1 - H_4)$, one can draw some immediate consequences:

- By Assumption (H_3), $\mathcal{H} = \bigoplus_{n \geq 0} \mathcal{H}_n$ is a graded algebra: given two functions $u \in \mathcal{H}_n$ and $v \in \mathcal{H}_m$, $uv \in \mathcal{H}_{m+n}$.

- For any $\psi \in \mathcal{G}$, we have the identification $\psi_1 = \psi$. This follows from assumptions (H_3) and (H_4): for any $u \in \mathcal{H}_n$, $u(\psi_1) = 1^n u(\psi) = u(\psi)$.

- The statement of Assumption (H_1) holds with $|v_j| + |w_j| = |u|$: consider $u \in \mathcal{H}_n$ and $v_1, w_1, \ldots, v_m, w_m \in \mathcal{H}$ the functions of Assumption (H_1). By Assumption (H_3), we can suppose that all v_j 's and w_j 's are homogeneous functions, otherwise a similar equality would hold with another set of homogeneous functions. Then, for all real λ, we have

$$\lambda^n u(\psi \circ \phi) = u((\psi \circ \phi)_\lambda) = u(\psi_\lambda \circ \phi_\lambda) = \sum_{j=1}^{m} \lambda^{|v_j|+|w_j|} v_j(\psi) w_j(\phi) \tag{3.4}$$

  for all $\psi, \phi \in \mathcal{G}$. This implies that, for each $n' \neq n$,

$$\sum_{|v_j|+|w_j|=n'} v_j(\psi) w_j(\phi) = 0 \quad \forall (\psi, \phi) \in \mathcal{G} \times \mathcal{G},$$

  so that all terms with powers of λ different from n can be omitted from (3.4).

- For all $u \in \mathcal{H}_n$ with $n > 0$, one has $u(\epsilon) = 0$. By Assumption (H_2), $\psi_0 = \epsilon$ for each $\psi \in \mathcal{G}$, so that for $u \in \mathcal{H}_n$, $n \geq 1$, $u(\epsilon) = u(\psi_0) = 0^n u(\psi) = 0$.

- $\mathcal{H}_0$ is isomorphic to $\mathbb{R}$, i.e. $\mathcal{H}_0 = \mathbb{R}\mathbb{1}$, where $\mathbb{1}$ is the unity function (i.e., $\mathbb{1}(\psi) = 1$ for all $\psi \in \mathcal{G}$). Indeed, if $u \in \mathcal{H}_0$, then $u(\psi) = u(\psi_1) = u(\psi_0) = u(\epsilon)$ for all $\psi \in \mathcal{G}$, and thus

$$u = u(\epsilon)\,\mathbb{1} \quad \forall u \in \mathcal{H}_0. \tag{3.5}$$

Definition 3.1 *We say that the triplet* $(\mathcal{G}, \mathcal{H}, \nu)$ *satisfying assumptions (* H_1 *)–(* H_4 *) is a* group of abstract integration schemes *and call accordingly each element* ψ *of* $\mathcal{G}$ *an abstract integration scheme.*

Definition 3.2 *Given two elements* ψ *and* ϕ *of* $\mathcal{G}$ *, we say that* $\psi \overset{(n)}{\equiv} \phi$ *if*

$$\forall u \in \bigoplus_{k=0}^{n} \mathcal{H}_k, \quad u(\psi) = u(\phi).$$

It is clear that $\psi \overset{(0)}{\equiv} \phi$ and that $\psi \overset{(n+1)}{\equiv} \phi$ implies $\psi \overset{(n)}{\equiv} \phi$. In addition, given $\psi, \hat{\psi}, \phi, \hat{\phi} \in \mathcal{G}$ and $n \geq 1$, if $\psi \overset{(n)}{\equiv} \phi$ and $\hat{\psi} \overset{(n)}{\equiv} \hat{\phi}$, then $\psi \circ \hat{\psi} \overset{(n)}{\equiv} \phi \circ \hat{\phi}$.

It is easy to check that the example in Subsection 2.1 is a group of abstract integration schemes. This is also the case for the example in Subsection 2.2, where conditions (H_1), (H_2) and (H_3) are trivially checked, and condition (H_4) is a consequence of (2.8).

In Subsection 3.1 we describe how $\mathcal{H}$ can be endowed with a graded Hopf algebra structure. In Subsections 3.2 and 3.3 we present some standard results on commutative Hopf algebras in detail. In particular, we show that the exponential and logarithm maps are bijections between an extension $\overline{\mathcal{G}}$ of the group $\mathcal{G}$ and a Lie-algebra $\mathfrak{g}$. Finally, in Subsection 3.4, we prove the main result of this paper on the approximation properties of $\mathcal{G}$.

3.1 The graded Hopf algebra structure of $\mathcal{H}$

We now consider the tensor product algebra $\mathcal{H} \otimes \mathcal{H}$ of $\mathcal{H}$ by itself, which can be identified with a sub-algebra of the algebra of functions $\mathbb{R}^{\mathcal{G}\times\mathcal{G}}$ as follows: $\forall (u, v) \in \mathcal{H} \times \mathcal{H}$, define $(u \otimes v) : \mathcal{G} \times \mathcal{G} \to \mathbb{R}$ as

$$\forall (\phi, \psi) \in \mathcal{G} \times \mathcal{G}, \quad (u \otimes v)(\phi, \psi) = u(\phi)v(\psi).$$

Then, $\mathcal{H} \otimes \mathcal{H}$ can be defined as the linear span of $\{u \otimes v \ : \ (u, v) \in \mathcal{H} \times \mathcal{H}\}$.

Definition 3.3 *Let* $(\mathcal{G}, \mathcal{H}, \nu)$ *be a group of abstract integration schemes (satisfying Assumptions* (H_1) *to* (H_4)*). We define the map* $\Delta : \mathcal{H} \longrightarrow \mathbb{R}^{\mathcal{G}\times\mathcal{G}}$ *as follows*

$$\forall (\phi, \psi) \in \mathcal{G} \times \mathcal{G}, \quad \Delta(u)(\phi, \psi) = u(\phi \circ \psi).$$

By Definition, Δ is linear, $\Delta(\mathbb{1}) = \mathbb{1} \otimes \mathbb{1}$, and $\Delta(uv) = \Delta(u)\Delta(v)$ for all $(u, v) \in \mathcal{H} \times \mathcal{H}$, so that Δ is an algebra morphism from $\mathcal{H}$ to the algebra $\mathbb{R}^{\mathcal{G}\times\mathcal{G}}$ of functions on $\mathcal{G} \times \mathcal{G}$.

Lemma 3.4 *Given* $u \in \mathcal{H}_n$ *with* $n \geq 1$ *, there exists a finite (and* **possibly empty***) sequence of homogeneous functions* $\{v_1, w_1, \ldots, v_m, w_m\} \subset \mathcal{H}$ *such that* $|v_j| + |w_j| = n$ *,* $|v_j| \neq 0$ *,* $|w_j| \neq 0$ *and*

$$\Delta(u) = u \otimes \mathbb{1} + \mathbb{1} \otimes u + \sum_{j=1}^{m} v_j \otimes w_j. \tag{3.6}$$

Proof: We already have that the statement of Assumption (H_1) holds with $|v_j| + |w_j| = |u|$, which implies by Definition 3.3 that there exist $m > 1$ and $\{v_1, w_1, \ldots, v_m, w_m\} \subset \mathcal{H}$ with $|v_j| + |w_j| = n$ such that

$$\Delta(u) = \sum_{j=1}^{m} v_j \otimes w_j.$$

Considering successively $\Delta(u)(\psi, \epsilon) = u(\psi \circ \epsilon) = u(\psi)$ and $\Delta(u)(\epsilon, \psi) = u(\epsilon \circ \psi) = u(\psi)$ for arbitrary $\psi \in \mathcal{G}$, one immediately checks that

$$\sum_{j/|v_j|=n,\ |w_j|=0} w_j(\epsilon)\, v_j = \sum_{j/|v_j|=0,\ |w_j|=n} v_j(\epsilon)\, w_j = u,$$

and thus, by virtue of (3.5),

$$\begin{aligned} \sum_{j/|v_j|=n,\ |w_j|=0} v_j \otimes w_j &= \sum_{j/|v_j|=n,\ |w_j|=0} w_j(\epsilon)\, v_j \otimes \mathbb{1} = u \otimes \mathbb{1}, \\ \sum_{j/|v_j|=0,\ |w_j|=n} v_j \otimes w_j &= \sum_{j/|v_j|=0,\ |w_j|=n} v_j(\epsilon)\, \mathbb{1} \otimes w_j = \mathbb{1} \otimes u. \end{aligned}$$

All other terms in the sum then satisfy $|v_j| \neq 0$ and $|w_j| \neq 0$. □

Lemma 3.4 shows in particular that the image of Δ is in $\mathcal{H} \otimes \mathcal{H} \subset \mathbb{R}^{\mathcal{G} \times \mathcal{G}}$, and that Δ is a graded algebra morphism from $\mathcal{H}$ to $\mathcal{H} \otimes \mathcal{H}$:

$$\Delta(\mathcal{H}_n) \subset \bigoplus_{k=0}^{n} \mathcal{H}_k \otimes \mathcal{H}_{n-k}.$$

In what follows, it will be convenient to identify $\epsilon \in \mathcal{G}$ to the linear form $\epsilon : \mathcal{H} \to \mathbb{R}$ such that $\epsilon(u) = u(\epsilon)$, that is,

$$\epsilon(\mathbb{1}) = 1, \quad \epsilon(u) = 0 \quad \text{if} \quad |u| \geq 1. \tag{3.7}$$

Clearly, ϵ is an algebra morphism from $\mathcal{H}$ to $\mathbb{R}$. By Definition 3.3 and the group structure of $\mathcal{G}$, it immediately follows that the commutative graded algebra of functions $\mathcal{H}$ has a structure of graded bi-algebra with co-product Δ, and counit ϵ. In addition, given that $\mathcal{H}_0 = \mathbb{R}\mathbb{1}$ (i.e. $\mathcal{H}$ is graded connected), $\mathcal{H}$ is a graded connected bialgebra and as such has an antipode $S : \mathcal{H} \to \mathcal{H}$, that gives a structure of commutative graded connected Hopf algebra (see [Car07] for a general definition of a graded Hopf algebra) to $\mathcal{H}$ [1]. In our context, the antipode S is an algebra morphism $S : \mathcal{H} \to \mathcal{H}$ satisfying $S(u)(\psi) = u(\psi^{-1})$, which implies that $S(\mathbb{1}) = \mathbb{1}$ and, if (3.6) holds for $u \in \mathcal{H}_n$ with $n \geq 1$, then

$$0 = S(u) + u + \sum_{j=1}^{m} S(v_j)w_j, \quad 0 = u + S(u) + \sum_{j=1}^{m} v_j S(w_j). \tag{3.8}$$

Observe that any of the equalities in (3.8) can be used to obtain $S(u)$ recursively (in terms of the image by S of homogeneous functions of lower degree) starting from $S(\mathbb{1}) = \mathbb{1}$.

3.2 Exponential and logarithm maps

We first notice that the co-algebra structure of $\mathcal{H}$ endows the linear dual $\mathcal{H}^*$ of $\mathcal{H}$ with an algebra structure, where the product $\alpha\beta \in \mathcal{H}^*$ of two linear forms $\alpha, \beta \in \mathcal{H}^*$ is defined as

$$\alpha\beta(\mathbb{1}) = \alpha(\mathbb{1})\beta(\mathbb{1})$$

and for all $u \in \mathcal{H}_n$ with $n \geq 1$ satisfying (3.6),

$$\alpha\beta(u) = \alpha(u)\beta(\mathbb{1}) + \alpha(\mathbb{1})\beta(u) + \sum_{j=1}^{m} \alpha(v_j)\beta(w_j).$$

We can also write

$$\alpha\beta = \mu_{\mathbb{R}} \circ (\alpha \otimes \beta) \circ \Delta, \tag{3.9}$$

where $\mu_{\mathbb{R}}$ is the multiplication in the algebra $\mathbb{R}$. Clearly, the unity element in $\mathcal{H}^*$ is the counit $\epsilon : \mathcal{H} \to \mathbb{R}$ of $\mathcal{H}$.

Note that with respect to the trivial Lie-bracket commutator

$$\forall(\alpha, \beta) \in \mathcal{H}^* \times \mathcal{H}^*, \quad [\alpha, \beta] = \alpha\beta - \beta\alpha,$$

$\mathcal{H}^*$ can also be seen as a Lie-algebra.

Definition 3.5 *Consider the following Lie-sub-algebra $\mathcal{H}^*_{(1)}$ of $\mathcal{H}^*$*

$$\mathcal{H}^*_{(1)} = \{\beta \in \mathcal{H}^* : \beta(\mathbb{1}) = 0\}$$

[1] It may be of theoretical interest to observe that, $\mathcal{H}$ is a Hopf sub-algebra of the Hopf algebra of representative functions of the group $\mathcal{G}$.

and the group

$$\epsilon + \mathcal{H}^*_{(1)} = \{\alpha \in \mathcal{H}^* : \alpha(\mathbb{1}) = 1\}.$$

The exponential $\exp$ *is defined as a map from* $\mathcal{H}^*_{(1)}$ *to* $\epsilon + \mathcal{H}^*_{(1)}$ *satisfying*

$$\exp(\beta) = \sum_{n\geq 0} \frac{1}{n!}\beta^n \quad \textit{for all} \quad \beta \in \mathcal{H}^*_{(1)}.$$

Similarly, the logarithm $\log : \epsilon + \mathcal{H}^*_{(1)} \to \mathcal{H}^*_{(1)}$ *is defined as*

$$\log(\alpha) = \sum_{n\geq 1} \frac{(-1)^n}{n}(\alpha - \epsilon)^n \quad \textit{for all} \quad \alpha \in \epsilon + \mathcal{H}^*_{(1)}.$$

Though defined as infinite series, both maps are well defined, since

$$\beta^{n+1}(u) = 0 \text{ if } u \in \bigoplus_{k=0}^{n} \mathcal{H}_k$$

for all $\beta \in \mathcal{H}^*_{(1)}$. Indeed, this can be shown as follows: Consider for each $n \geq 0$ the subspace $\mathcal{H}^*_{(n)}$ of $\mathcal{H}^*$ defined as

$$\mathcal{H}^*_{(n)} = \{\beta \in \mathcal{H}^* \ : \ \beta(u) = 0 \text{ if } |u| < n\}.$$

Then, by definition (3.9) of the multiplication in $\mathcal{H}^*$, we have that, for $\beta \in \mathcal{H}^*_{(n)}$ and $\beta' \in \mathcal{H}^*_{(n')}$,

$$\forall\, u \in \bigoplus_{k=0}^{n+n'} \mathcal{H}_k, \quad (\beta\beta')(u) \quad = \quad \beta(\mathbb{1})\beta'(u) + \beta(u)\beta'(\mathbb{1}) + \sum_{j=1}^{m} \beta(v_j)\beta'(w_j)$$

where all pairs of homogeneous functions (v_j, w_j) are such that either $|v_j| < n$ or $|w_j| < n'$. As a consequence, it follows that

$$\forall\, (n,m) \ \in \ \mathbb{N}^2, \quad \mathcal{H}^*_{(n)}\mathcal{H}^*_{(m)} \subset \mathcal{H}^*_{(n+m)}. \tag{3.10}$$

In particular $\beta^{n+1} \in \mathcal{H}^*_{(n+1)}$ provided that $\beta \in \mathcal{H}^*_{(1)}$.

Note that, as a straightforward consequence of (3.10) and of the definition of $\exp$, we have the following result, which will be used later on.

Lemma 3.6 *Let* $(n,m) \in \mathbb{N}^2$ *and consider* $\beta \in \mathcal{H}^*_{(n)}$ *and* $\gamma \in \mathcal{H}^*_{(m)}$, *then*

$$\exp(\beta)\exp(\gamma) - \exp(\beta + \gamma) \in \mathcal{H}^*_{(n+m)}. \tag{3.11}$$

Proof. The series-expansion of $\exp(\beta)\exp(\gamma) - \exp(\beta+\gamma)$ is composed of products of the form $\beta^{i_1}\gamma^{j_1}\cdots\beta^{i_k}\gamma^{j_k}$ where at least one i and one j is non-zero. The statement thus follows from relation (3.10). ∎

Next result follows from the fact that the exponential and logarithm defined as power series are formally reciprocal to each other.

Lemma 3.7 *The maps* $\exp : \mathcal{H}^*_{(1)} \longrightarrow \epsilon + \mathcal{H}^*_{(1)}$ *and* $\log : \epsilon + \mathcal{H}^*_{(1)} \longrightarrow \mathcal{H}^*_{(1)}$ *are linear bijections that are reciprocal to each other, that is,*

$$\forall \beta \in \mathcal{H}^*_{(1)}, \quad (\log \circ \exp)(\beta) = \beta,$$
$$\forall \alpha \in \epsilon + \mathcal{H}^*_{(1)}, \quad (\exp \circ \log)(\alpha) = \alpha.$$

Remark 3.8 *In the sequel, the following relations will become useful: for* $\beta \in \mathcal{H}^*_{(1)}$ *and* $\lambda \in \mathbb{R}$, *consider* $\alpha^\lambda = \exp(\lambda\beta)$. *Then we have*

$$\frac{d}{d\lambda}\alpha^\lambda = \beta\alpha^\lambda = \alpha^\lambda\beta, \quad \alpha^0 = \epsilon \quad \textit{and} \quad \frac{d}{d\lambda}\alpha^\lambda\Big|_{\lambda=0} = \beta,$$

where $\frac{d}{d\lambda}\alpha^\lambda \in \mathcal{H}^*$ *and* $\frac{d}{d\lambda}\alpha^\lambda\big|_{\lambda=0} \in \mathcal{H}^*$ *are defined as follows:*

$$\forall u \in \mathcal{H}, \quad \Big(\frac{d}{d\lambda}\alpha^\lambda\Big)(u) = \frac{d}{d\lambda}\Big(\alpha^\lambda(u)\Big), \quad \Big(\frac{d}{d\lambda}\alpha^\lambda\Big|_0\Big)(u) = \frac{d}{d\lambda}\Big(\alpha^\lambda(u)\Big)\Big|_{\lambda=0}.$$

3.3 The group $\overline{\mathcal{G}}$ and its Lie algebra $\mathfrak{g}$

An important consequence of the Hopf algebra structure of $\mathcal{H}$ is that $\mathcal{G}$ can be viewed as the subgroup of a group[2] $\overline{\mathcal{G}} \subset \epsilon + \mathcal{H}^*_{(1)} \subset \mathcal{H}^*$, with associated Lie algebra[3] $\mathfrak{g}$. To this aim, we will eventually identify elements of $\mathcal{G}$ with elements of $\overline{\mathcal{G}} \subset \mathcal{H}^*$ through the relation

$$\forall \psi \in \mathcal{G},\ \forall u \in \mathcal{H},\ \psi(u) = u(\psi). \tag{3.12}$$

Recall that in particular, we identify the neutral element ϵ in $\mathcal{G}$ with the counit (3.7) of $\mathcal{H}$ (which is the unity element in $\mathcal{H}^*$).

Definition 3.9 *The group* $\overline{\mathcal{G}}$ *is defined as*

$$\overline{\mathcal{G}} = \Big\{\alpha \in \mathcal{H}^*; \forall (u,v) \in \mathcal{H}\times\mathcal{H},\ \alpha(uv) = \alpha(u)\alpha(v) \textit{ and } \alpha(\mathbb{1}) = 1\Big\}$$

i.e. the subset of $\mathcal{H}^*$ *of algebra morphisms from* $\mathcal{H}$ *to* $\mathbb{R}$.

[2] The group of characters of $\mathcal{H}$, or equivalently, the group of group-like elements of the dual Hopf algebra of $\mathcal{H}$.

[3] The Lie algebra of infinitesimal characters of $\mathcal{H}$, or equivalently, the Lie algebra of primitive elements of the dual Hopf algebra of $\mathcal{H}$.

It is rather straightforward to check that:

- Since Δ is an algebra morphism from $\mathcal{H}$ to $\mathcal{H}\otimes\mathcal{H}$, $\alpha\otimes\beta$ a morphism from $\mathcal{H}\otimes\mathcal{H}$ to $\mathbb{R}\otimes\mathbb{R}$ for $(\alpha,\beta)\in\overline{\mathcal{G}}^2$ and $\mu_{\mathbb{R}}$ a morphism from $\mathbb{R}\otimes\mathbb{R}$ to $\mathbb{R}$, formula (3.9) shows that $\alpha\beta$ is itself an algebra morphism and thus belongs to $\overline{\mathcal{G}}$.

- Any $\psi\in\mathcal{G}$ (and in particular, the neutral element $\psi=\epsilon$) belongs, through the identification (3.12), to $\overline{\mathcal{G}}$: Indeed, $\psi(\mathbb{1}) = \mathbb{1}(\psi) = 1$, and for any $(u,v)\in\mathcal{H}\times\mathcal{H}$, $\psi(uv)=uv(\psi)=u(\psi)v(\psi)=\psi(u)\psi(v)$. Thus, $\mathcal{G}$ can be seen as a subgroup of $\overline{\mathcal{G}}$.

- Any $\alpha\in\overline{\mathcal{G}}$ has an inverse defined in terms of the antipode S as $\alpha^{-1}=\alpha\circ S$: We have that $\alpha^{-1}\alpha(\mathbb{1})=\alpha(S(\mathbb{1}))\alpha(\mathbb{1})=\alpha(\mathbb{1})^2=1$, and similarly one gets that $\alpha\alpha^{-1}(\mathbb{1})=1$. For $u\in\mathcal{H}_n$ with $n\geq 1$, if (3.6) holds, then (3.8) implies, by taking into account that α is an algebra morphism, that $\alpha^{-1}\alpha(u)=\alpha\alpha^{-1}(u)=0$.

Eventually, the embedded equivalence relations $\overset{(n)}{\equiv}$ in $\mathcal{G}$ can be extended to $\overline{\mathcal{G}}$ as follows:

Definition 3.10 *Given $\alpha,\gamma\in\overline{\mathcal{G}}$ and $n\geq 0$, we write $\alpha\overset{(n)}{\equiv}\gamma$ if*

$$\alpha(u)=\gamma(u) \quad \textit{for all} \quad u\in\mathcal{H}_k,\ k\leq n.$$

Definition 3.11 *The Lie-algebra $\mathfrak{g}$ of infinitisimal characters of H is the Lie-sub-algebra of $\mathcal{H}^*$ defined by the set*

$$\mathfrak{g}=\{\beta\in\mathcal{H}^*:\forall(u,v)\in\mathcal{H}^2,\beta(uv)=\beta(u)\epsilon(v)+\epsilon(u)\beta(v)\}$$

Note that:

- For any $\beta\in\mathfrak{g}$, $\beta(\mathbb{1})=\beta(\mathbb{1}\cdot\mathbb{1})=2\beta(\mathbb{1})\epsilon(\mathbb{1})=2\beta(\mathbb{1})$, and thus $\beta(\mathbb{1})=0$. Hence, $\mathfrak{g}\subset\mathcal{H}^*_{(1)}$. Furthermore, given $u,u'\in\bigoplus_{n\geq1}\mathcal{H}_n$, $\beta(uu')=0$, since $\epsilon(u)=\epsilon(u')=0$.

- $\mathfrak{g}$ is clearly a subspace of $\mathcal{H}^*$.

Although this is standard in the literature, for the sake of clarity we prove here that $\mathfrak{g}$ is a Lie-algebra for the Lie-bracket $[\hat\beta,\beta]=\hat\beta\beta-\beta\hat\beta$: Given $u\in\mathcal{H}_n$ and $u'\in\mathcal{H}_{n'}$ with $n,n'>1$, let us assume (3.6) and an analogous expression for $\Delta(u')$ with $m'\geq 0$ and $|v'_j|+|w'_j|=n'$, then, since $\Delta(uu')=\Delta(u)\Delta(u')$, one gets

$$\begin{aligned}\Delta(uu') &= uu'\otimes\mathbb{1}+u\otimes u'+u'\otimes u+\mathbb{1}\otimes uu'+\sum_{i,j}v_iv'_j\otimes w_iw'_j \\ &\quad+\sum_j(uv'_j\otimes w'_j+v'_j\otimes uw'_j)+\sum_i(u'v_j\otimes w_j+v_j\otimes u'w_j),\end{aligned} \tag{3.13}$$

so that

$$(\hat{\beta}\beta)(uu') = \hat{\beta}(u)\beta(u') + \hat{\beta}(u')\beta(u),$$

and thus $[\hat{\beta}, \beta](u, u') = 0$.

The following result is standard for arbitrary commutative graded Hopf algebras [Car07].

Theorem 3.12 *The restriction of* $\exp$ *to* $\mathfrak{g}$ *is a bijection from* $\mathfrak{g}$ *to* $\overline{\mathcal{G}}$.

Proof. Consider $\beta \in \mathcal{H}^*_{(1)}$, $\alpha = \exp(\beta)$ and $\alpha^\lambda = \exp(\lambda\beta)$ in $\epsilon + \mathcal{H}^*_{(1)}$. We will prove by induction on n that, if $\beta \in \mathfrak{g}$ or $\alpha \in \overline{\mathcal{G}}$, then,

$$\alpha^\lambda(uu') = \alpha^\lambda(u)\alpha^\lambda(u') \quad \text{and} \quad \beta(uu') = 0 \tag{3.14}$$

for all $u, u' \in \cup_{k\geq 1}\mathcal{H}_k$ with $|u| + |u'| \leq n$. This trivially holds for $n = 1$ (the set of such pairs (u, u') with $|u| + |u'| \leq 1$ is empty). For $n \geq 2$, formula (3.13) and the induction hypothesis imply that

$$\begin{aligned} \frac{d}{d\lambda}(\alpha^\lambda(uu') - \alpha^\lambda(u)\alpha^\lambda(u')) &= (\beta\alpha^\lambda)(uu') - (\beta\alpha^\lambda)(u)\alpha^\lambda(u') - (\beta\alpha^\lambda)(u')\alpha^\lambda(u) \\ &= \beta(uu') \end{aligned}$$

or equivalently, after integration

$$\alpha^\lambda(uu') - \alpha^\lambda(u)\alpha^\lambda(u') = \lambda\beta(uu'),$$

and in particular $\alpha(uu') - \alpha(u)\alpha(u') = \beta(uu')$, so that (3.14) holds provided that $\alpha \in \overline{\mathcal{G}}$ or $\beta \in \mathfrak{g}$. This completes the proof. ■

Remark 3.13 *For any* $\alpha \in \overline{\mathcal{G}}$, *the map* $\lambda \mapsto \alpha^\lambda$ *defines a "near-to-identity" smooth curve in* $\overline{\mathcal{G}}$, *in the sense that* $\alpha^0 = \epsilon$ *and for any* $u \in \mathcal{H}$, $\lambda \mapsto \alpha^\lambda(u)$ *is a smooth function from* $\mathbb{R}$ *into itself. Clearly,* $\frac{d}{d\lambda}\alpha^\lambda\big|_{\lambda=0} = \log(\alpha) \in \mathfrak{g}$. *Actually, it is straightforward to check that, for any near-to-identity smooth curve* $c : \mathbb{R} \to \overline{\mathcal{G}}$, $\frac{d}{d\lambda}c(\lambda)\big|_{\lambda=0} \in \mathfrak{g}$. *Using the terminology of the theory of Lie-groups, we can loosely say that the Lie-algebra* $\mathfrak{g}$ *can then be seen as the "tangent space at identity" of* $\overline{\mathcal{G}}$.

In the sequel, it will be useful to consider, for each $n \geq 1$, the subspaces $\mathfrak{g}_n$ of the Lie algebra $\mathfrak{g}$ defined as

$$\mathfrak{g}_n = \{\beta \in \mathfrak{g} \ : \ \beta(u) = 0 \text{ if } u \in \mathcal{H}_k \text{ with } k \neq n\}. \tag{3.15}$$

Note that each $\mathfrak{g}_n$ is finite-dimensional since $\mathcal{H}_n$ is itself finite-dimensional. Clearly, each $\beta \in \mathfrak{g}$ can be written as

$$\beta = \sum_{n\geq 1} \beta_n, \quad \beta_n \in \mathfrak{g}_n,$$

where, for each $n \geq 1$, the "projected" linear form $\beta_n \in \mathfrak{g}_n$ is obtained as

$$\beta_n(u) = \begin{cases} \beta(u) \text{ if } |u| = n, \\ 0 \text{ if } |u| = k \neq n. \end{cases}$$

The commutative graded Hopf algebra $\mathcal{H}$ is connected (i.e., $\mathcal{H}_0 = \mathbb{R}\,\mathbb{1}$) and of finite type (i.e., each $\mathcal{H}_n$ is finite-dimensional), which implies that there exists a set $\mathcal{T} \subset \mathcal{H}$ of homogeneous functions that freely generates the algebra $\mathcal{H}$, that is, such that the set

$$\mathcal{F} = \Big\{ u_1 \dots u_m \ : \ u_1, \dots, u_m \in \mathcal{T} \Big\} \tag{3.16}$$

is a basis of the vector space $\mathcal{H}$. More specifically, the following can be proven from standard results[4]:

Theorem 3.14 *Given a group of abstract integration schemes $(\mathcal{G}, \mathcal{H}, \nu)$ and a basis $\{\delta_{n,i} : i = 1, \dots, l_n\}$ for each $\mathfrak{g}_n$, $n \geq 1$ defined in (3.15), there exist $u_{n,i} \in \mathcal{H}$, $n \geq 1$, $i = 1, \dots, l_n$ satisfying the following two conditions:*

- *The set $\mathcal{T} = \{u_{n,i} \in \mathcal{H},\ n \geq 1,\ i = 1, \dots, l_n\}$ freely generates the algebra $\mathcal{H}$.*
- *Given $\alpha \in \overline{\mathcal{G}}$, consider for each $n \geq 1$ the element $\alpha_n \in \overline{\mathcal{G}}$ defined as*

$$\alpha_n = \exp\Big(\alpha(u_{n,1})\delta_{n,1}\Big) \cdots \exp\Big(\alpha(u_{n,l_n})\delta_{n,l_n}\Big), \tag{3.17}$$

then,

$$\forall n \geq 1, \quad \alpha \overset{(n)}{\equiv} \alpha_1 \cdots \alpha_n. \tag{3.18}$$

3.4 The order of an abstract integration scheme

Recall that, given an element $\beta \in \mathfrak{g}$, one can write $\beta = \beta_1 + \beta_2 + \dots$, where $\beta_n \in \mathfrak{g}_n$ for each $n \geq 1$. We typically interpret, in the context of numerical integration of ODEs, β_1 as a *basic* vector field and β as a *modified* vector field. If ψ is an element of $\mathcal{G}$, then it is typically aimed at approximating $\exp(\beta_1)$ where β_1 can be obtained as the first term in the development of $\beta = \log(\psi)$ or alternatively as

$$\left.\frac{du(\psi_\lambda)}{d\lambda}\right|_{\lambda=0} = \begin{cases} u(\psi) & \text{if } |u| = 1 \\ 0 & \text{otherwise.} \end{cases} \tag{3.19}$$

[4] As a consequence of the application of the Milnor-Moore theorem [MM65], $\mathcal{H}$ is the graded dual Hopf algebra of the universal enveloping Hopf algebra of the Lie algebra $\bigoplus_{n\geq 1} \mathfrak{g}_n$. Then, a basis of $\mathcal{H}$ of the form (3.16) is obtained by considering the dual basis of a Poincaré-Witt-Birkhoff basis of the universal enveloping bi-algebra of a Lie algebra [Bou89].

It is straightforward to check that, if another element $\hat{\beta} \in \mathfrak{g}$ is decomposed in accordance with β, we have $(\beta_k \hat{\beta}_{n-k})(u) = 0$ unless $|u| = n$, and it follows that

$$\forall n \geq 1, \quad (\beta\hat{\beta})_n = \sum_{k=1}^{n-1} \beta_k \hat{\beta}_{n-k}.$$

For all $u \in \mathcal{H}_n$ and all $\lambda \in \mathbb{R}$, we thus have

$$u(\psi_\lambda) = \lambda^n \epsilon(u) + \sum_{k=1}^{n} \frac{\lambda^n}{k!} \sum_{i_1+\ldots+i_k=n} \Big(\beta_{i_1} \ldots \beta_{i_k}\Big)(u),$$

i.e.

$$\psi_\lambda = \exp(\lambda\beta_1 + \lambda^2\beta_2 + \ldots).$$

In particular, it becomes clear why

$$\beta_1 = \frac{d\psi_\lambda}{d\lambda}\bigg|_{\lambda=0},$$

and we are led to the following definition of order

Definition 3.15 *An integration scheme* $\psi \in \mathcal{G}$ *is said to be of order* $n \geq 1$ *if there exists* $\beta \in \mathfrak{g}$ *such that*

$$\forall\, \lambda \in \mathbb{R}, \quad \psi_\lambda \overset{(n)}{\equiv} \exp(\lambda\beta), \tag{3.20}$$

or, equivalently, if

$$\psi \overset{(n)}{\equiv} \exp\Big(\frac{d\psi_\lambda}{d\lambda}\bigg|_{\lambda=0} \Big). \tag{3.21}$$

Now, the question arises as to whether there exist abstract integration schemes of arbitrarily high order in $\mathcal{G}$. Theorem 3.17 provides an affirmative answer to that question. Before proving it, we first consider the following preliminary result:

Lemma 3.16 *Let* n *and* k *be two non-zero integers and consider* $\beta \in \mathfrak{g}_n$ *and* $\gamma \in \mathfrak{g}_{n+k}$. *Then it holds that*

$$\forall\, (\lambda, \bar{\lambda}, \mu, \bar{\mu}) \in \mathbb{R}^4, \;\; \exp(\lambda\beta + \mu\gamma)\exp(\bar{\lambda}\beta + \bar{\mu}\gamma) \overset{(n+k)}{\equiv} \exp((\lambda + \bar{\lambda})\beta + (\mu + \bar{\mu})\gamma). \tag{3.22}$$

Proof: Lemma 3.6 implies that $\exp(\lambda\beta+\mu\gamma)-\exp(\lambda\beta)\exp(\mu\gamma)\in\mathcal{H}^*_{(2n+k)}\subset\mathcal{H}^*_{(n+k+1)}$ so that

$$\exp(\lambda\beta+\mu\gamma)\ \overset{(n+k)}{\equiv}\ \exp(\lambda\beta)\exp(\mu\gamma),$$

and similarly

$$\begin{aligned}\exp(\bar\lambda\beta+\bar\mu\gamma)\ &\overset{(n+k)}{\equiv}\ \exp(\bar\lambda\beta)\exp(\bar\mu\gamma),\\ \exp(\mu\gamma)\exp(\bar\lambda\beta)\ &\overset{(n+k)}{\equiv}\ \exp(\mu\gamma+\bar\lambda\beta)\overset{(n+k)}{\equiv}\exp(\bar\lambda\beta)\exp(\mu\gamma).\end{aligned}$$

As a consequence, we have

$$\begin{aligned}\exp(\lambda\beta_n+\mu\gamma)\exp(\bar\lambda\beta_n+\bar\mu\gamma)\ &\overset{(n+k)}{\equiv}\ \exp(\lambda\beta)\exp(\mu\gamma)\exp(\bar\lambda\beta)\exp(\bar\mu\gamma)\\ &\overset{(n+k)}{\equiv}\ \exp(\lambda\beta)\exp(\bar\lambda\beta)\exp(\mu\gamma)\exp(\bar\mu\gamma)\\ &=\ \exp((\lambda+\bar\lambda)\beta)\exp((\mu+\bar\mu)\gamma)\\ &\overset{(n+k)}{\equiv}\ \exp((\lambda+\bar\lambda)\beta+(\mu+\bar\mu)\gamma).\end{aligned}$$

□

Theorem 3.17 *Assume that* $(\mathcal{G},\mathcal{H},\nu)$ *is a group of abstract integration schemes. Then, given arbitrary* $\psi\in\mathcal{G}$ *and* $n\geq 1$ *, there exists* $\phi\in\mathcal{G}$ *such that*

$$\phi\overset{(n)}{\equiv}\exp\Big(\left.\frac{d\psi_\lambda}{d\lambda}\right|_{\lambda=0}\Big).$$

Proof: Denote $\beta_1=\left.\frac{d\psi_\lambda}{d\lambda}\right|_{\lambda=0}$. Then, by definition, $\psi\overset{(1)}{\equiv}\exp(\beta_1)$ and more generally, for any $\lambda\in\mathbb{R}$, $\psi_\lambda\overset{(1)}{\equiv}\exp(\lambda\beta_1)$. Now, let $\beta=\log(\psi)$ and write

$$\beta=\beta_1+\beta_2+\ldots+\beta_k+\ldots$$

According to previous discussion, we have

$$\psi_\lambda=\exp(\lambda\beta_1+\lambda^2\beta_2+\ldots).$$

Then the "triple jump" composition (of elements in $\mathcal{G}$)

$$\phi=\psi_\lambda\psi_\mu^{-1}\psi_\lambda\in\mathcal{G},$$

where ψ_μ^{-1} denotes the inverse in $\mathcal{G}$ of ψ_μ, with Lemma 3.16 shows that

$$\phi \overset{(2)}{\equiv} \exp\Big((2\lambda-\mu)\beta_1 + (2\lambda^2-\mu^2)\beta_2\Big),$$

and thus $\phi \overset{(2)}{\equiv} \exp(\beta_1)$ provided $\mu = \sqrt{2}\lambda$ and $\lambda = (2-\sqrt{2})^{-1}$. Repeating recursively this procedure, starting from

$$\phi = \exp(\beta_1 + \widetilde{\beta}_3 + \ldots),$$

allows to prove the result. $\square$

3.5 Three fundamental results

In the present subsection we address three important related questions:

- Assume that, given $\alpha \in \overline{\mathcal{G}}$ and $n \geq 1$, we want to find $\psi \in \mathcal{G}$ such that

$$\psi \overset{(n)}{\equiv} \alpha. \tag{3.23}$$

  Does there exist a set $\mathcal{T} \subset \mathcal{H}$ of homogeneous functions such that the equalities

$$u(\psi) = \alpha(u) \quad \text{for all} \quad u \in \mathcal{T} \text{ with } |u| \leq n, \tag{3.24}$$

  provide a set of independent conditions that characterizes (3.23)?

- Is it possible to "approximate" any $\alpha \in \overline{\mathcal{G}}$ by $\psi \in \mathcal{G}$ in the sense that (3.23) holds for arbitrary n (this is question (Q4) of the introduction)?

- Given a group of abstract integration schemes $(\mathcal{G}, \mathcal{H}, \nu)$, does there exist $\tilde{H} \neq H$ such that $(\mathcal{G}, \tilde{\mathcal{H}}, \nu)$ is a group of abstract integration schemes giving rise, according to Definition 3.2, to the same family of equivalent relations $\overset{(n)}{\equiv}$?

The **first question** can be answered in two steps:

(i) According to Theorem 3.14, there exists a set $\mathcal{T}$ of homogeneous functions (i.e., $\mathcal{T} = \cup_{n\geq 1}\mathcal{T}_n$ with $\mathcal{T}_n \subset \mathcal{H}_n$) that freely generates the algebra $\mathcal{H}$, that is, such that the set $\mathcal{F}$ in (3.16) is a basis of the vector space $\mathcal{H}$. For this $\mathcal{T} \subset \mathcal{H}$, the set of conditions (3.24) characterizes (3.23), since for $\alpha \in \overline{\mathcal{G}}$, one has

$$\forall\, m \geq 2,\ \forall\, (u_1, \ldots, u_m) \in \mathcal{T}^m, \quad \alpha(u_1 \cdots u_m) = \alpha(u_1) \cdots \alpha(u_m).$$

(ii) Despite the fact that for $\mathcal{T}$, conditions (3.24) are algebraically independent, non-polynomial dependences among the functions in $\mathcal{T}$ could exist that would allow to reduce the number of conditions required to characterize (3.23). As a consequence of Theorem 3.20 given below, for any $n \geq 1$ and any map a from $\cup_{k=1}^{n} \mathcal{T}_k$ into $\mathbb{R}$, there exists $\psi \in \mathcal{G}$ such that

$$\forall u \in \cup_{k=1}^{n} \mathcal{T}_k, \quad u(\psi) = a(u).$$

This guarantees that conditions (3.24) are actually independent of each other.

The **second question** has an affirmative answer, stated in Theorem 3.20 below. Its proof requires the following technical results.

Lemma 3.18 *Assume that* $\psi \in \mathcal{G}$ *and* $\beta_n \in \mathfrak{g}_n$ *are such that*

$$\psi \overset{(n)}{\equiv} \exp(\beta_n).$$

Then, for each $k \geq 0$ *there exists* $\phi \in \mathcal{G}$ *such that*

$$\phi \overset{(n+k)}{\equiv} \exp(\beta_n). \tag{3.25}$$

Proof: If there exists $\phi \in \mathcal{G}$ for which (3.25) holds, then $\phi \overset{(n+k+1)}{\equiv} \exp(\beta_n + \beta_{n+k})$ for some $\beta_{n+k} \in \mathfrak{g}_{n+k}$, and thus:

$$\forall \lambda \in \mathbb{R}, \quad \phi_\lambda \overset{(n+k+1)}{\equiv} \exp(\lambda^n \beta_n + \lambda^{n+k} \beta_{n+k}).$$

Proceeding as in Theorem 3.17, we have that

$$\begin{aligned} \phi_\lambda \circ (\phi_\mu)^{-1} \circ \phi_\lambda &\overset{(n+k+1)}{\equiv} \exp((2\lambda^n - \mu^n)\beta_n + (2\lambda^{n+k} - \mu^{n+k})\beta_{n+k}), \\ &\overset{(n+k+1)}{\equiv} \exp(\beta_n) \text{ for } \lambda = \left(2 - 2^{\frac{n}{n+k}}\right)^{-1/n} \text{ and } \mu = 2^{\frac{1}{n+k}} \lambda. \end{aligned}$$

The result then follows by induction. □

Lemma 3.19 (Lemma 1.1 in [Hoc81]) *Given a set* $\mathcal{G}$ *and a finite-dimensional subspace* V *of the set of functions* $\mathbb{R}^{\mathcal{G}}$, *there exist a basis* $\{v_1, \ldots, v_m\}$ *of* V *and* ${}^1\psi, \ldots, {}^m\psi \in \mathcal{G}$ *such that* $v_i({}^j\psi) = 1$ *if* $i = j$ *and* $v_i({}^j\psi) = 0$ *otherwise, and thus*

$$u = \sum_{j=1}^{m} u({}^j\psi) v_j.$$

Theorem 3.20 *Given a group of abstract integration schemes* $(\mathcal{G},\mathcal{H},\nu)$ *, for arbitrary* $\alpha\in\overline{\mathcal{G}}$ *and* $n\geq 1$ *there exists* $\psi\in\mathcal{G}$ *such that*

$$\psi\overset{(n)}{\equiv}\alpha.$$

Proof: Consider the set

$$\mathcal{K}=\{\alpha\in\overline{\mathcal{G}};\ \forall n\ \in\ \mathbb{N}/\{0\},\ \exists\psi\in\mathcal{G},\ \psi\overset{(n)}{\equiv}\alpha\}$$

In order to prove that $\mathcal{K}=\overline{\mathcal{G}}$, as stated by the theorem, we first notice that $\mathcal{K}$ satisfies the following properties:

(P1) $\mathcal{K}$ is a subgroup of $\overline{\mathcal{G}}$

(P2) For $\alpha\in\mathcal{K}$, define α_λ by $\alpha_\lambda(u)=\lambda^n\alpha(u)$ for all $(\lambda,u)\in\mathbb{R}\times\mathcal{H}_n$. Then, $\alpha_\lambda\in\mathcal{K}$.

(P3) If $\alpha\in\mathcal{K}$ and $\alpha\overset{(n)}{\equiv}\exp(\beta_n)$ where $n\geq 1$ and $\beta_n\in\mathfrak{g}_n$, then $\exp(\beta_n)\in\mathcal{K}$. This follows from Lemma 3.18.

(P4) Let $n\geq 1$ and β_n and γ_n in $\mathfrak{g}_n$. If $\exp(\beta_n)$ and $\exp(\gamma_n)$ are in $\mathcal{K}$, then $\exp(\beta_n+\gamma_n)\in\mathcal{K}$. Indeed, by Lemma 3.6, $\exp(\beta_n)\exp(\gamma_n)\overset{(n)}{\equiv}\exp(\beta_n+\gamma_n)$, and then (P3) implies $\exp(\beta_n+\gamma_n)\in\mathcal{K}$.

(P5) Let $n\geq 1$, β_n in $\mathfrak{g}_n$ and $\mu\in\mathbb{R}$. If $\exp(\beta_n)\in\mathcal{K}$, then $\exp(\mu\beta_n)\in\mathcal{K}$. As a matter of fact, (P2) implies $\exp(\lambda^n\beta_n)\in\mathcal{K}$, while (P1) and (P2) imply $\exp(-\lambda^n\beta_n)\in\mathcal{K}$.

By virtue of Theorem 3.14, $\mathcal{K}=\overline{\mathcal{G}}$ if for each $n\geq 1$,

$$\forall\mu\in\mathbb{R},\quad i=1,\dots,l_n,\quad \exp\left(\mu\delta_{n,i}\right)\in\mathcal{K}. \tag{3.26}$$

We will prove (3.26) by induction on $n\geq 1$. Given $k\geq 1$, assume that (3.26) holds for all $n<k$.

Consider the subspace W_k of $\mathcal{H}_k$ having $\{u_{k,i}\ :\ i=1,\dots,l_k\}$ as a basis (the functions $u_{n,i}$ are linearly independent, as the set $\mathcal{T}$ in Theorem 3.14 freely generates the algebra $\mathcal{H}$). Lemma 3.19 applied for the subspace $W_k\subset\mathbb{R}^{\mathcal{G}}$ implies that there exist ${}^1\psi,\dots,{}^{l_k}\psi\in\mathcal{G}$ and a new basis $\{v_{k,i}\ :\ i=1,\dots,l_k\}$ of W_k such that, for each $i=1,\dots,l_k$,

$$u_{k,i}=\sum_{j=1}^{l_k}u_{k,i}({}^j\psi)v_{k,j}.$$

As the matrix $(u_{k,i}({}^j\psi))_{i,j=1}^{l_k}$ is invertible, and $\{\delta_{k,i} \ : \imath = 1,\ldots,l_k\}$ is a basis of $\mathfrak{g}_k$,

$$\{\bar{\delta}_{k,i} = \sum_{j=1}^{l_k} u_{k,j}({}^i\psi)\delta_{k,j} \ : \ i = 1,\ldots,l_k\} \tag{3.27}$$

is also a basis of $\mathfrak{g}_k$.

Now, Theorem 3.14 applied for $\alpha = {}^i\psi \in \mathcal{G}$, $i = 1,\ldots,l_k$, and the induction hypothesis, followed by repeated application of Lemma 3.6 implies that, for each $i = 1,\ldots,l_k$, there exists $\gamma \in \mathcal{K}$ such that

$$\gamma \overset{(k)}{\equiv} \exp\left(\sum_{i=1}^{l_k} u_{k,i}(\psi)\delta_{k,i}\right) = \exp(\bar{\delta}_{k,i}),$$

and by property P3, $\exp(\bar{\delta}_{k,i}) \in K$, and finally, (3.26) follows from properties P4 and P5 and the fact that (3.27) is a basis of g_k . □

As for the **third question**, we have the following:

Theorem 3.21 *Consider a group of abstract integration schemes* $(\mathcal{G},\mathcal{H},\nu)$ *giving rise (see Definition 3.2), to the family of equivalence relations* $\overset{(n)}{\equiv}$, $n \geq 1$. *If* $(\mathcal{G},\hat{\mathcal{H}},\nu)$ *is also a group of abs. int. schemes and gives rise to the* **same** *family of equivalence relations, then* $\hat{\mathcal{H}} = \mathcal{H}$.

Proof: Consider two *different* algebras $\tilde{\mathcal{H}},\hat{\mathcal{H}} \subset \mathbb{R}^{\mathcal{G}}$, such that $(\mathcal{G},\tilde{\mathcal{H}},\nu)$ and $(\mathcal{G},\hat{\mathcal{H}},\nu)$ are groups of abstract integration schemes and give rise to the same family of equivalence relations through Def. 3.2. Then, it is straightforward to check that this is also true for the algebra $\mathcal{H}$ generated by $\tilde{\mathcal{H}} \cup \hat{\mathcal{H}}$. Given a set $\hat{\mathcal{T}} = \cup_{n\geq 1}\hat{\mathcal{T}}_n$ of homogeneous functions that freely generates the algebra $\hat{\mathcal{H}}$, it is possible to construct a set $\mathcal{T} = \cup_{n\geq 1}\mathcal{T}_n$ of homogeneous functions that freely generates the algebra $\mathcal{H}$ and $\hat{\mathcal{T}}_n \subset \mathcal{T}_n$ for all $n \geq 1$. As $\mathcal{H} \neq \hat{\mathcal{H}}$ by assumption, $\hat{\mathcal{T}}_n \neq \mathcal{T}_n$ for some $n \geq 1$, and then there exist two *different* maps a and b from $\cup_{k=1}^n \mathcal{T}_k$ into $\mathbb{R}$, such that their restriction to $\cup_{k=1}^n \hat{\mathcal{T}}_k$ coincide. As in the second step (ii) above, there exist ψ and ϕ in $\mathcal{G}$ such that

$$\forall u \in \cup_{k=1}^n \hat{\mathcal{T}}_k \quad u(\psi) = u(\phi),$$

and $u(\psi) \neq u(\phi)$ for some $u \in \cup_{k=1}^n \mathcal{T}_k$. This implies $\psi \overset{(n)}{\equiv} \phi$ w.r.t. $(\mathcal{G},\hat{\mathcal{H}},\nu)$, while $\psi \overset{(n)}{\not\equiv} \phi$ w.r.t. $(\mathcal{G},\mathcal{H},\nu)$ in contradiction with the assumption of the theorem. □

4 The group of composition integration schemes

As a preamble to the discussion of order conditions for composition methods, we introduce the set $\mathcal{G}_c$ of finite sequences $\psi = (\mu_1,\ldots,\mu_{2s})$ of real numbers satisfying that $\mu_j \neq \mu_{j+1}$ for

$1 \leq j \leq 2s-1$, including the empty sequence $\epsilon = ()$. The set $\mathcal{G}_{\mathrm{c}}$ is a group, with neutral element ϵ and composition law defined, for $\psi, \phi \in \mathcal{G}/\{\epsilon\}$ as follows:

$$(\mu_1, \ldots, \mu_{2s}) \cdot (\nu_1, \ldots, \nu_{2k}) = (\mu_1, \mu_2) \cdots (\mu_{2s-1}, \mu_{2s}) \cdots (\nu_1, \nu_2) \cdots (\nu_{2k-1}, \nu_{2k})$$

where for $\lambda, \mu, \nu \in \mathbb{R}$,

$$(\lambda, \mu) \cdot (\mu, \nu) = \begin{cases} \epsilon & \text{if } \lambda = \nu, \\ (\lambda, \nu) & \text{otherwise,} \end{cases}$$

and, if $(\mu_1, \ldots, \mu_{2s}) \in \mathcal{G}$, then

$$(\mu_1, \mu_2) \cdots (\mu_{2s-1}, \mu_{2s}) = (\mu_1, \ldots, \mu_{2s}).$$

In particular, we have that $(\mu_1, \ldots, \mu_{2s}) \cdot (\mu_{2s}, \ldots, \mu_1) = \epsilon$.

Now, consider successively:

- a smooth system of ODEs
$$\dot{y} = f(y), \quad f : \mathbb{R}^d \to \mathbb{R}^d; \tag{4.1}$$
- its exact flow φ_h from $\mathbb{R}^d$ to itself (such that $\varphi_h(y(t)) \equiv y(t+h)$ for any solution $y(t)$ of (4.1)) and
- a consistent integrator χ_h for (4.1), that is to say a smooth map χ_h from $\mathbb{R}^d$ to itself which depends smoothly on the real parameter h and is such that
$$\chi_h(y) = y + hf(y) + \mathcal{O}(h^2) = \varphi_h(y) + \mathcal{O}(h^2)$$
as $h \to 0$.

Given $\psi = (\mu_1, \ldots, \mu_{2s}) \in \mathcal{G}_{\mathrm{c}}$, a new integrator ψ_h for the system (4.1) can then be obtained as

$$\psi_h \quad = \quad \chi_{\mu_{2s}h} \circ \chi^{-1}_{\mu_{2s-1}h} \circ \cdots \circ \chi_{\mu_2 h} \circ \chi^{-1}_{\mu_1 h}. \tag{4.2}$$

Definition 4.1 *Given $\psi \in \mathcal{G}_{\mathrm{c}}$ and $p \geq 1$, we say that ψ is a consistent integration scheme of order p if for arbitrary χ_h the integrator (4.2) satisfies*

$$\psi_h(y) = \varphi_h(y) + \mathcal{O}(h^{p+1}) \quad \text{as} \quad h \to 0 \tag{4.3}$$

for the h-flow φ_h of the system (4.1) with

$$f(y) = \frac{d}{dh}\chi_h(y)\bigg|_{h=0}. \tag{4.4}$$

Clearly, (4.3) is equivalent to the following: For all smooth real functions $g \in \mathrm{C}^\infty(\mathbb{R}^d;\mathbb{R})$, all $y \in \mathbb{R}^d$,

$$g(\psi_h(y)) = g(\varphi_h(y)) + \mathcal{O}(h^{p+1}) \quad \text{as} \quad h \to 0.$$

Motivated by that, we consider, for each $n \geq 0$ and each $\psi \in \mathcal{G}_\mathrm{c}$, the linear differential operator $\theta_n(\psi)$ acting on smooth functions $g \in \mathrm{C}^\infty(\mathbb{R}^d;\mathbb{R})$ as follows: $\theta_0(\psi)$ is the identity operator I, and for each $n \geq 1$

$$\theta_n(\psi)[g](y) = \frac{1}{n!}\frac{d^n}{dh^n}\, g(\psi_h(y))|_{h=0}\,, \tag{4.5}$$

so that formally,

$$g(\psi_h(y)) = \sum_{n\geq 0} h^n \theta_n(\psi)[g](y).$$

For arbitrary ψ and ϕ in $\mathcal{G}_\mathrm{c}$, we have

$$\begin{aligned}
\sum_{n\geq 0} h^n \theta_n(\phi\cdot\psi)[g](y) &= g(\psi_h \circ \phi_h(y)) = \sum_{n\geq 0} h^n \theta_n(\psi)[g](\phi_h(y)) \\
&= \sum_{n\geq 0} h^n \sum_{m\geq 0} h^m \theta_m(\phi)[\theta_n(\psi)[g]](y) \\
&= \Big(\sum_{n\geq 0}\sum_{m\geq 0} h^{n+m}\theta_m(\phi)\theta_n(\psi)\Big)[g](y),
\end{aligned}$$

and equating like powers of h, we get for each $n \geq 0$,

$$\theta_n(\phi\cdot\psi) = \sum_{k=0}^{n} \theta_k(\phi)\theta_{n-k}(\psi) = \theta_n(\phi) + \theta_n(\psi) + \sum_{k=1}^{n-1} \theta_k(\phi)\theta_{n-k}(\psi). \tag{4.6}$$

For the *scaling map*, as defined for a group of abstract integration schemes, we define ν by $\nu(\psi,\lambda) = (\psi)_\lambda$, where for each $\psi = (\mu_1,\ldots,\mu_{2s}) \in \mathcal{G}_\mathrm{c}$ and each $\lambda \in \mathbb{R}$,

$$\nu(\psi,\lambda) = (\psi)_\lambda = (\lambda\mu_1,\ldots,\lambda\mu_{2s}). \tag{4.7}$$

It clearly holds, for each $n \geq 0$, $\lambda \in \mathbb{R}$, $\psi \in \mathcal{G}_\mathrm{c}$, that

$$\theta_n((\psi)_\lambda) = \lambda^n \theta_n(\psi). \tag{4.8}$$

Obviously, the integrator ψ_h given by (4.2) for $(\mu_1,\ldots,\mu_{2s}) = (0,1) \in \mathcal{G}_\mathrm{c}$ is precisely the basic integrator χ_h. Let us denote, $\chi = (0,1) \in \mathcal{G}_\mathrm{c}$, so that each $\psi = (\mu_1,\ldots,\mu_{2s})$ can be written as

$$\psi = (\chi^{-1})_{\mu_1}\cdot(\chi)_{\mu_2}\cdots(\chi^{-1})_{\mu_{2s-1}}\cdot(\chi)_{\mu_{2s}}.$$

Let also denote, for each $n \geq 0$, $X_n = \theta_n(\chi)$. That is, X_n is the linear differential operator such that, for each $g \in \mathrm{C}^\infty(\mathbb{R}^d;\mathbb{R})$ and each $y \in \mathbb{R}^d$,

$$X_n[g](y) = \theta_n(\chi)[g](y) = \frac{1}{n!}\frac{d^n}{dh^n}\, g(\chi_h(y))|_{h=0}\,. \tag{4.9}$$

Then, each $\theta_n(\psi)$ for $\psi \in \mathcal{G}_\mathrm{c}$ and $n \geq 1$ is a linear combination of differential operators of the form $X_{i_1}\cdots X_{i_m}$ with $m \geq 1$ and $i_1 + \cdots + i_m = n$, more precisely,

$$\theta_n(\psi) = \sum_{m\geq 1}\sum_{i_1+\cdots+i_m=n} u_{i_1,\cdots,i_m}(\psi)\, X_{i_1}\cdots X_{i_m} \tag{4.10}$$

for suitable functions $u_{i_1,\cdots,i_m} \in \mathbb{R}^{\mathcal{G}_\mathrm{c}}$. Indeed, this is trivially so for $\psi = \chi$. By considering (4.6) with $\psi = \chi$ and $\phi = \chi^{-1}$, one can check by induction on n that (4.10) is also true for $\psi = \chi^{-1}$. If (4.10) holds for given $\psi \in \mathcal{G}_\mathrm{c}$, then by (4.8), it is also true for $(\psi)_\lambda$. If (4.10) holds for $\psi, \phi \in \mathcal{G}_\mathrm{c}$, then by virtue of (4.6), it is also true for $\phi \cdot \psi$.

Proposition 4.2 *Consider for* $m \geq 1$ *and* $(i_1,\ldots,i_m) \in (\mathbb{N}^+)^m$ *the functions* $u_{i_1,\ldots,i_m} \in \mathbb{R}^{\mathcal{G}_\mathrm{c}}$ *are recursively defined as follows. Given* $\psi = (\mu_1,\ldots,\mu_{2s}) \in \mathcal{G}_\mathrm{c}$,

$$u_i(\psi) = \sum_{j=1}^{s}(\mu_{2j}^i - \mu_{2j-1}^i), \quad u_{i_1,\ldots,i_m}(\psi) = \sum_{j=1}^{s}(\mu_{2j}^i - \mu_{2j-1}^i)\, u_{i_1,\ldots,i_{m-1}}({}^j\psi), \tag{4.11}$$

where ${}^j\psi \in \mathcal{G}$ *is defined for each* $j \geq 1$ *as*

$${}^j\psi = \begin{cases} (\mu_1,\ldots,\mu_{2j-2},\mu_{2j-1},0) & \text{if } \mu_{2j-1} \neq 0, \\ (\mu_1,\ldots,\mu_{2j-2}) & \text{if } \mu_{2j-1} = 0 \text{ and } j > 1, \\ \epsilon & \text{otherwise.} \end{cases}$$

Then, (4.10) holds for arbitrary basic integrators χ_h *and arbitrary* $\psi \in \mathcal{G}_\mathrm{c}$ *and* $n \geq 1$.

Proof: From (4.10) and (4.6) one gets that

$$u_{i_1,\ldots,i_m}(\psi\cdot(\chi)_\lambda) = u_{i_1,\ldots,i_m}(\psi) + \lambda^{i_m}\, u_{i_1,\ldots,i_{m-1}}(\psi),$$

which together with the equalities

$$\psi = {}^{2s}\psi\cdot(\chi)_{\mu_{2s}}, \quad {}^{j+1}\psi\cdot(\chi)_{\mu_{2j+1}} = {}^{j}\psi\cdot(\chi)_{\mu_{2j}}$$

lead to the recursion (4.11). □

As for the expansion of $g(\varphi_h(y))$ for the exact h-flow of the system (4.1), it formally holds that

$$g(\varphi_h(y)) = g(y) + \sum_{n\geq 1}\frac{1}{n!}F^n = \exp(hF),$$

where F is the Lie derivative of the ODE system (4.1), that is, the first order linear differential operator F acting on functions in $C^\infty(\mathbb{R}^d;\mathbb{R})$ as follows: For each $g \in C^\infty(\mathbb{R}^d;\mathbb{R})$ and each $y \in \mathbb{R}^d$

$$F[g](y) = \sum_{j=1}^{d} f^j(y) \frac{\partial g}{\partial y^j}(y). \tag{4.12}$$

Notice that, (4.4) and (4.9) imply that $F = X_1$. Thus, the composition integrator (4.2) associated to a given $\psi \in \mathcal{G}_c$ is consistent of order p if and only if

$$\forall n \leq p, \quad \theta_n(\psi) = \frac{1}{n!}(X_1)^n.$$

This, together with Proposition 4.2 implies the following: Let $\mathcal{F}_0 = \{\mathbb{1}\}$, and for each $n \geq 1$

$$\mathcal{F}_n = \{u_{i_1,\ldots,i_m} \ : \ m \geq 1, \ i_1, \ldots, i_m \geq 1, \ i_1 + \cdots + i_m = n\}. \tag{4.13}$$

Given $p \geq 1$, if

$$\forall u \in \bigcup_{n\geq 1} \mathcal{F}_n, \quad u(\psi) = \begin{cases} \frac{1}{m!} & \text{if} \quad \psi = \overbrace{(1, \ldots, 1)}^{m} \\ 0 & \text{otherwise,} \end{cases} \tag{4.14}$$

then ψ is consistent of order p. However, are all the conditions (4.14) necessary for the integration scheme ψ be of order p? The following lemma shows that they are actually necessary.

Lemma 4.3 *Given $d \geq 1$ and a multi-index $(i_1, \ldots, i_d) \in (\mathbb{N}^+)^d$ with $i_1 + \cdots + i_d = n \geq 1$, there exists $\chi_h : \mathbb{R}^d \to \mathbb{R}^d$ and $g \in C^\infty(\mathbb{R}^d;\mathbb{R})$ such that for $y = 0 \in \mathbb{R}^d$, $X_{j_1} \cdots X_{j_m}[g](0) \neq 0$ if and only if $(j_1, \ldots, j_m) = (i_1, \ldots, i_d)$.*

Proof: Consider the basic integrator $\chi_h : \mathbb{R}^d \to \mathbb{R}^d$ defined as $\chi_h(y) = y + (h^{i_1}, h^{i_2}y^1, \ldots, h^{i_d}y^{d-1})^T$ and $g(y) = y^1$ for $y = (y^1, \ldots, y^d) \in \mathbb{R}^d$. □

It is straightforward to check the following result.

Lemma 4.4 *Let us consider for each $u \in \mathbb{R}^{\mathcal{G}_c}$ and each $n \geq 1$, the new function $[u]_n \in \mathbb{R}^{\mathcal{G}_c}$ defined as follows. Given $\psi = (\mu_1, \ldots, \mu_{2s}) \in \mathcal{G}_c$,*

$$[u]_n(\psi) = \sum_{j=1}^{s} (\mu_{2j}^n - \mu_{2j-1}^n) u({}^j\psi), \tag{4.15}$$

where ${}^j\psi \in \mathcal{G}$ is defined for each $j \geq 1$ as in Proposition 4.2. Then, given $u, v \in \mathbb{R}^{\mathcal{G}_c}$ and $n, k \geq 1$,

$$[u]_n[v]_k = [u[v]_k]_n + [v[u]_n]_k + [uv]_{n+k}$$

This implies that the product of two functions of the form (4.11) is a linear combination of functions of that form, and in particular that

- the order conditions (4.14) are not independent of each other. For instance, we have that $(u_1)^2 = 2\,u_{1,1} + u_2$, and thus $u_1(\psi) = 1$ and $u_2(\psi) = 0$ imply $u_{1,1}(\psi) = 1/2$.
- the vector space $\mathcal{H}_{\rm c}$ spanned by the set $\mathcal{F} = \cup_{n\geq 0}\mathcal{F}_n$ is a subalgebra of $\mathbb{R}^{\mathcal{G}_{\rm c}}$.

However, how can we obtain from them a set of independent (necessary and sufficient) order conditions? How are different sets of independent order conditions of composition integrators related? In order to answer these questions, we will first show that, $(\mathcal{G}_{\rm c}, \mathcal{H}_{\rm c}, \nu)$ has (with the algebra $\mathcal{H}_{\rm c}$ spanned by the set of functions $\mathcal{F}$) a structure of a group of abstract integration schemes, and then interpret the algebraic results in precedent sections in the context of series of differential operators of the form (4.10).

Lemma 4.5 *Given $\psi \in \mathcal{G}_{\rm c}$, the composition integrator (4.2) corresponding to arbitrary basic integrators χ_h is the identity map if and only if $\psi = \epsilon$.*

Proof: The 'if' part trivially holds, and the 'only if' part can be proven by considering the symplectic Euler method applied to the harmonic oscillator as basic integrator $\chi_h : \mathbb{R}^2 \to \mathbb{R}^2$, that is,

$$\chi_h(y) = \begin{pmatrix} 1 & 0 \\ -h & 1 \end{pmatrix} \begin{pmatrix} 1 & h \\ 0 & 1 \end{pmatrix} y. \tag{4.16}$$

Then, given $\psi \in \mathcal{G}_{\rm c}/\{\epsilon\}$, that is, $\psi = (\mu_1, \ldots, \mu_{2s}) \in \mathcal{G}_{\rm c}$ with $s \geq 1$, the composition integrator (4.2) corresponding to the basic integrator χ_h is defined as the map $\psi_h : \mathbb{R}^2 \to \mathbb{R}^2$ given by

$$\psi_h(y) = \begin{pmatrix} 1 & 0 \\ -a_{2s+1}h & 1 \end{pmatrix} \begin{pmatrix} 1 & a_{2s}h \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ -a_3 h & 1 \end{pmatrix} \begin{pmatrix} 1 & a_2 h \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -a_1 h & 1 \end{pmatrix} y, \tag{4.17}$$

where $a_1 = -\mu_1$, $a_{2s+1} = \mu_{2s}$, and $a_j = (-1)^j(\mu_j - \mu_{j-1})$ for $j = 2, \ldots, 2s$, and thus $a_j \neq 0$ for all j . The required result then follows by showing that the map ψ_h given in (4.17) cannot be the identity map unless $a_j = 0$ for some $j \in \{2, \ldots, 2s\}$. Indeed, if $\psi_h(y) \equiv y$, then, with the notation in Subsection 2.2, for all $n \geq 1$, $u_n(\psi) = v_n(\psi) = 0$, and from (2.8), we conclude that $a_j = 0$ for some $j \in \{2, \ldots, 2s\}$. □

Theorem 4.6 *The triplet $(\mathcal{G}_{\rm c}, \mathcal{H}_{\rm c}, \nu)$, where $\mathcal{H}_{\rm c}$ is the algebra of functions on $\mathcal{G}_{\rm c}$ spanned by the set (4.13) and the scaling map ν given by (4.7), is a group of abstract integration schemes.*

Proof: From (4.6) and (4.10) and Lemma 4.3, one easily gets that, given a multi-index $(i_1, \dots, i_m)$ and $\psi, \phi \in \mathcal{G}_c$,

$$u_{i_1,\dots,i_m}(\psi \cdot \phi) = u_{i_1,\dots,i_m}(\psi) + u_{i_1,\dots,i_m}(\phi) + \sum_{j=1}^{m-1} u_{i_1,\dots,i_j}(\psi) u_{i_{j+1},\dots,i_m}(\phi). \tag{4.18}$$

We thus have that assumption (H_1) holds. It is straightforward to check Assumption (H_2). Assumption (H_3) trivially holds with $\mathcal{H}_n$ the linear span of (4.13). As for Assumption (H_4), it follows from (4.6) and (4.10) and Lemma 4.5. □

Proposition 4.7 *The set $\mathcal{F} = \cup_{n\geq 0}\mathcal{F}_n$ of homogeneous functions on $\mathcal{G}_c$ is a basis of the algebra $\mathcal{H}_c$.*

Proof: It is not difficult to check that, for each $\psi = (\mu_1, \dots, \mu_{2s}) \in \mathcal{G}_c$ satisfying $\mu_j = 0$ for odd j, then, for each multi-index $(i_1, \dots, i_m)$,

$$u_{i_1,\dots,i_m}(\psi) = \sum_{1\leq j_1 < \cdots < j_m \leq s} \mu_{2j_1}^{i_1} \cdots \mu_{2j_m}^{i_m},$$

so that $u_{i_1,\dots,i_m}(\psi) = 0$ if $s < m$ and otherwise, for each $k = 1, \dots, s$, the degree of $u_{i_1,\dots,i_m}(\psi)$ as a polynomial in the variables $\mu_{2(s-k+1)}, \dots, \mu_{2s}$ is $i_{s-k+1} + \cdots + i_s$. This implies the linear independence of the set $\mathcal{F}$. □

Proposition 4.7 together with Lemma 4.4 actually shows that $\mathcal{H}_c$ is the quasi-shuffle (Hopf) algebra of Hoffman [Hof00] (over the graded set $\{1, 2, 3, \dots, \}$ with grading $|n| = n$), and in particular, admits the set of Lyndon multi-indices as a set of free generators of the algebra $\mathcal{H}_c$, thus giving a set of (necessary and sufficient) independent order conditions for the group of composition integration schemes.

Definition 4.8 *Consider the lexicographical order $<$ on $\mathcal{F}$ (for $1 < 2 < 3 < \cdots$). Given $i_1, \dots, i_m \geq 1$, $(i_1, \dots, i_m)$ is a Lyndon multi-index if $(i_1, \dots, i_k) < (i_{k+1}, \dots, i_m)$ for each $1 \leq k < m$. We consider for each $n \geq 1$, the subset $\mathcal{L}_n \subset \mathcal{F}_n$ of functions $u_{i_1,\dots,i_m}$ such that $(i_1, \dots, i_m)$ is a Lyndon multi-index.*

The first subsets $\mathcal{L}_n = \{u \in \mathcal{L} : \ |u| = n\}$ are the following.

$$\begin{aligned}
\mathcal{L}_1 &= \{u_1\}, \quad \mathcal{L}_2 = \{u_2\}, \quad \mathcal{L}_3 = \{u_{12}, u_3\}, \quad \mathcal{L}_4 = \{u_{112}, u_{13}, u_4\}, \\
\mathcal{L}_5 &= \{u_{1112}, u_{113}, u_{122}, u_{14}, u_{23}, u_5\}.
\end{aligned}$$

Proposition 4.9 *The set $\mathcal{L} = \cup_{n\geq 1}\mathcal{L}_n$ freely generates the algebra $\mathcal{H}_c$.*

Notice that (4.18) implies that the coproduct Δ in $\mathcal{H}_c$ is defined as

$$\Delta(u_{i_1,\ldots,i_m}) = u_{i_1,\ldots,i_m} \otimes \mathbb{1} + \mathbb{1} \otimes u_{i_1,\ldots,i_m} + \sum_{j=1}^{m-1} u_{i_1,\ldots,i_j} \otimes u_{i_{j+1},\ldots,i_m}, \tag{4.19}$$

which endows the linear dual $\mathcal{H}_c^*$ with an algebra structure, where the multiplication has a useful interpretation in the context of series of linear differential operators: It is straightforward to check that, if we associate a formal series of the form

$$\sum_{m\geq 1} \sum_{i_1,\ldots,i_m \geq 1} h^{i_1+\cdots+i_m} \alpha(u_{i_1,\cdots,i_m})\, X_{i_1} \cdots X_{i_m} \tag{4.20}$$

to each $\alpha \in \mathcal{H}_c^*$, then the multiplication in $\mathcal{H}_c^*$ corresponds to the (formal) composition of the corresponding series of differential operators. This implies that, if $\beta \in \mathfrak{g}$, then

$$\exp\Big(\sum_{m\geq 1} \sum_{i_1,\ldots,i_m \geq 1} h^{i_1+\cdots+i_m} \beta(u_{i_1,\cdots,i_m})\, X_{i_1} \cdots X_{i_m}\Big)$$

formally coincides with (4.20) with $\alpha = \exp(\beta) \in \overline{\mathcal{G}_c}$. In particular, given $\psi \in \mathcal{G}_c$, $\beta = \frac{d\psi_\lambda}{d\lambda}\Big|_{\lambda=0} \in \mathfrak{g}$, where $\beta(u_1) = u_1(\psi)$ and $\beta(u_{i_1,\ldots,i_m}) = 0$ otherwise, so that

$$\sum_{m\geq 1} \sum_{i_1,\ldots,i_m \geq 1} h^{i_1+\cdots+i_m} \beta(u_{i_1,\cdots,i_m})\, X_{i_1} \cdots X_{i_m} = h u_1(\psi) X_1,$$

and thus

$$\exp\Big(\frac{d\psi_\lambda}{d\lambda}\Big|_{\lambda=0}\Big)(u_{i_1,\ldots,i_m}) = \begin{cases} \frac{u_1(\psi)^m}{m!} & \text{if} \quad (i_1,\ldots,i_m) = (1,\ldots,1), \\ 0 & \text{otherwise.} \end{cases}$$

Corollary 4.10 *A set of independent necessary and sufficient conditions for an arbitrary* $\psi \in \mathcal{G}_c$ *to be consistent of order* p *is the following:* $u_1(\psi) = 1$, *and*

$$\forall u \in \bigcup_{n\geq 1} \mathcal{L}_n, \quad u(\psi) = 0.$$

Remark 4.11 *A systematic construction of an independent set of necessary and sufficient order conditions for composition integrators was obtained in [MSS99] in terms of a certain set of functions* $\hat{\mathcal{T}} \subset \mathbb{R}^{\mathcal{G}_c}$ *indexed by certain subset of labeled rooted trees. According to Theorem 3.21, the algebra of functions generated by* $\hat{\mathcal{T}}$ *(which happens to satisfy, together with* $\mathcal{G}_c$ *and* ν, *the assumptions* (H_1)–(H_4)*)) must coincide with* $\mathcal{H}_c$. *With the notation introduced in Lemma 4.4, let* $\mathcal{F}_{n-1}$, $\mathcal{T}_n$ *(* $n \geq 1$ *) be sets of functions on* $\mathcal{G}_c$ *recursively defined as* *follows:* $\mathcal{F}_0 = \{\mathbb{1}\}$ *, and for each* $n \geq 1$ *,*

$$\mathcal{T}_n = \Big\{[u]_k \;:\; u \in \mathcal{F}_{n-k},\; k = 0, \ldots, n-1\Big\},$$
$$\mathcal{F}_n = \Big\{u_1 \ldots u_m \;:\; u_i \in \mathcal{T}_{n_i} \text{ and } \sum_{i=1}^{m} n_i = n\Big\}.$$

It is not difficult to see that the set $\mathcal{T} = \bigcup_{n\geq 1} \mathcal{T}_n$ *can be naturally indexed by rooted trees labeled by the set* $\{1, 2, 3, \ldots\}$ *. A subset* $\hat{\mathcal{T}} \subset \mathcal{T}$ *(in one-to-one correspondence with a Hall set [Bou89] on the alphabet* $\{1, 2, 3, \ldots\}$ *) is identified in [MSS99] that provides a set of necessary and sufficient order conditions for composition integrators (see also [HLW06]), which implies that* $\hat{\mathcal{T}}$ *freely generates the (quasi-shuffle) algebra* $\mathcal{H}_{\mathrm{c}}$ *. Actually, a different subset* $\hat{\mathcal{T}} \subset \mathcal{T}$ *that freely generates the quasi-shuffle algebra* $\mathcal{H}_{\mathrm{c}}$ *can be obtained associated to each generalized Hall set on the alphabet* $\{1, 2, 3, \ldots\}$ *(see [Mur06] for a closely related sets of free generators of the shuffle algebra indexed by subsets of labeled rooted trees).*

5 Conclusion

In this paper, we have introduced an algebraic structure, that we call group of abstract integration schemes, and composed of a group, an algebra of functions acting on this group and a scaling map. In Section 2, we have have considered two very simple examples of integrators, for respectively arbitrary linear differential equations and linear Schrödinger-like differential equations: these examples, though basic in comparison with the theory that follows, share essential characteristics with more involved situations and are of great help to get a grip on the general situation. From a set of four assumptions, of a purely algebraic nature, we exhibit step by step a structure of graded Hopf algebra. The richness of this structure enables us to prove several results that answer recurrent questions in numerical analysis (in particular, questions (Q1) to (Q4) of the introduction). An interesting aspect of this work, is, according to us, that it is independent of the specific differential equation considered and the specific type of integrators. On top of the two examples considered in the introduction, and composition methods, studied in [MSS99], receive much attention here: a new presentation of order conditions is revealed based only upon the theory developed here.

We note that, the case of Runge-Kutta methods, of much historic interest (see [But72]), can be easily treated within the present framework. The existence of an underlying group of abstract integration schemes for a given class of integration schemes can also be stated under very mild assumptions on the relevant series expansions of the integration methods. Moreover, the algebraic structure of the Hopf algebra introduced here is richer than this paper allows to show within a limited number of pages. In particular, the Hopf algebra structure of $\mathcal{H}$ can be interpreted (as in the case of composition methods in Section 4) in terms of formal series expansions of linear differential operators. This also applies for the Hopf algebra structure of

Runge-Kutta methods, which have very useful interpretations in terms of series expansion such as S-series (see [Mur99, Mur06]). Note that S-series, that generalize in a sense B-series, have proven very useful in a number of results in geometric integrations [CFM06, CM07]. It is thus the intention of the authors to pursue this work in a second article.

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