On post-Lie algebras, Lie–Butcher series and moving frames

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Abstract

Pre-Lie (or Vinberg) algebras arise from a flat and torsion free connection on a differential manifold. These algebras have been extensively studied in recent years, both from algebraic operadic points of view and through numerous applications in numerical analysis, control theory, stochastic differential equations and renormalization. Butcher series is an algebraic tool used to study geometric properties of flows on euclidean spaces, which is founded on pre-Lie algebras. Motivated by analysis of flows on manifolds and homogeneous spaces, we investigate algebras arising from flat connections with constant torsion, leading to the definition of *post-Lie* algebras, a generalization of pre-Lie algebras. Whereas pre-Lie algebras are intimately associated with euclidean geometry, post-Lie algebras occur naturally in the differential geometry of homogeneous spaces, and are also closely related to Cartan's method of moving frames. The generalized Lie–Butcher series combining Butcher series with Lie series are used to analyze flows on manifolds. In this paper we show that Lie–Butcher series are founded on post-Lie algebras. The functorial relations between post-Lie algebras and their enveloping algebras, called D-algebras, is explored. Furthermore, we develop new formulas for computations in free post-Lie algebras and D-algebras, based on recursions in a magma, and we show that Lie–Butcher series are related to invariants of curves described by moving frames.

1 Introduction

In 1857 Arthur Cayley published a remarkable paper [5] introducing the idea that differential operators can be described in terms of trees. This became a fundamental tool in the analysis of numerical flows through the seminal work of John Butcher [3, 4] in the 1960s, where he introduced the Butcher group, or, in modern language, the character group of the Butcher–Connes–Kreimer Hopf algebra. In 1963 *pre-Lie algebras* appeared simultaneously from two different investigations, Vinberg [40] from differential geometry (classification of homogeneous cones) and Gerstenhaber [13] from algebra (Hochschild cohomology). The free pre-Lie algebra [7], described in terms of trees, is the algebraic foundation of B-series [10]. B-series have evolved into algebraic tools that are suitable for studying a variety geometric properties of flows, such as symplecticity, preservation of first integrals and backward error analysis. In the late 1990s similar structures appeared in the renormalization theories of Connes and Kreimer [8]. Christian Brouder [2] pointed out connections between this theory and numerical analysis.

During the 1990s numerical integration was generalized from euclidean spaces to manifolds [9, 24, 25, 34]. In this work it was necessary to generalize B-series to manifolds, called Lie–Butcher series (LB-series). Inspired by the unexpected connections between numerical analysis and renormalization, the algebraic foundations of LB-series were investigated in several papers in the last decade [27, 1, 29, 22, 20]. Through this work it became clear that the foundations of LB-series are fundamental algebraic structures generalizing pre-Lie algebras, which may be important also in areas of mathematics outside of numerical analysis.

The motivation for the investigations of this paper was to establish the algebraic foundations of LB-series in a similar manner to the foundation of B-series in terms of pre-Lie algebras. This

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leads to the definition of *post-Lie* algebras, first found by Bruno Valette [39] in 2007 through the purely operadic technique of Koszul dualisation. In this paper we show that post-Lie algebras also arise naturally from the differential geometry of homogeneous spaces and Klein geometries, topics that are closely related to Cartan's method of *moving frames*. Applications of moving frames in computational mathematics have been pioneered by Peter Olver and his co-workers [32, 11, 12]. In this paper we will also show that post-Lie algebras and LB-series are related to moving frame theory and point to possible applications of moving frames in the design of numerical methods.

2 Post-Lie algebras in differential geometry

2.1 Algebras of connections

In this section we motivate the abstract definition of pre-Lie, post-Lie and Lie-admissible algebras by considering algebras of vector fields originating from constant connections on a manifold.

The most fundamental concept in differential geometry is *connections*, defining parallel transport and covariant derivations. Connections appear in various abstractions, e.g. Koszul, Ehresmann and Cartan connections. To motivate pre-Lie, post-Lie and Lie-admissible algebras, it is sufficient to consider the simplest definition, a Koszul connection on the tangent bundle.

Let $\mathcal{XM}$ denote the vector fields on a manifold $\mathcal{M}$. A *Koszul connection* [38] is defined as map $\nabla\colon \mathcal{XM}\times\mathcal{XM}\to\mathcal{XM}$ such that

$$\begin{aligned}\nabla_{fx}y &= f\nabla_x y\\ \nabla_x(fy) &= df(x)y + f\nabla_x y,\end{aligned}$$

for any $x, y \in \mathcal{XM}$ and scalar field f. The connection defines a (non-commutative and non-associative) $\mathbb{R}$-bilinear product on $\mathcal{XM}$, henceforth written as

$$x \rhd y := \nabla_x y.$$

The *torsion* of the connection is a skew-symmetric tensor $T\colon T\mathcal{M}\wedge T\mathcal{M}\to T\mathcal{M}$ defined as

$$T(x,y) = x\rhd y - y\rhd x - [\![x,y]\!], \tag{1}$$

where $[\![\cdot,\cdot]\!]$ denotes the Jacobi–Lie bracket of vector fields. The *curvature tensor* $R\colon T\mathcal{M}\wedge T\mathcal{M}\to \mathrm{End}(T\mathcal{M})$ is defined as

$$R(x,y)z = x\rhd(y\rhd z) - y\rhd(x\rhd z) - [\![x,y]\!]\rhd z = a(x,y,z) - a(y,x,z) + T(x,y)\rhd z, \tag{2}$$

where $a(x,y,z)$ is the (negative) *associator* of the product $\rhd$, defined for any algebra $\{\mathcal{A},\rhd\}$ as

$$a(x,y,z) := x\rhd(y\rhd z) - (x\rhd y)\rhd z. \tag{3}$$

The relationship between torsion and curvature is given by the Bianchi identities

$$\begin{aligned}\mathfrak{S}(T(T(x,y),z) + (\nabla_x T)(y,z)) &= \mathfrak{S}(R(x,y)z) &(4)\\ \mathfrak{S}((\nabla_x R)(y,z) + R(T(x,y),z)) &= 0, &(5)\end{aligned}$$

where $\mathfrak{S}$ denotes the sum over the three cyclic permutations of (x,y,z).

Torsion free connection $\Rightarrow$ Lie-admissible algebra. If $T=0$ then (2)-(4) imply

$$\mathfrak{S}(a(x,y,z) - a(y,x,z)) = 0. \tag{6}$$

A general algebra with a product $\rhd$ satisfying (6) is called a *Lie-admissible algebra*. Lie-admissible algebras are exactly those algebras which give rise to Lie algebras by skew-symmetrization of the product [14], i.e. a bracket defined as

$$[\![x,y]\!] := x\rhd y - y\rhd x,$$

is a Lie bracket if and only if $\{\mathcal{A},\rhd\}$ is Lie-admissible. For a torsion free connection on vector fields, $[\![\cdot,\cdot]\!]$ is the Jacobi–Lie bracket. Any associative algebra is clearly Lie-admissible. A more general example is pre-Lie algebras.

Flat and torsion free connection ⇒ Pre-Lie algebra. Consider a connection which is both flat $R = 0$ and torsion free $T = 0$. Equation (2) implies that

$$a(x, y, z) - a(y, x, z) = 0. \tag{7}$$

A general algebra with a product $\triangleright$ satisfying (7) is called a *pre-Lie algebra* or Vinberg algebra. Pre-Lie algebras appear in many applications. A fundamental algebraic result is that the free pre-Lie algebra is the set of rooted trees with grafting as the product [7]. This structure is the foundation of all classical B-series, and this was essentially known to Arthur Cayley already in 1857 [5].

Note that a Riemannian manifold with a flat, torsion free connection is locally isometric to a euclidean space $\mathbb{R}^n$ with the standard metric [38], hence pre-Lie algebras are tightly associated with the differential geometry of euclidean spaces. For Lie groups and homogeneous spaces (Klein geometries), pre-Lie algebras are not sufficiently general to capture the basic differential geometry algebraically.

Flat and constant torsion connection ⇒ Post-Lie algebra. Given a connection which is flat $R = 0$ and has constant torsion $\nabla T = 0$, then (4) reduces to a Jacobi identity $\mathfrak{S}(T(T(x, y), z)) = 0$ and hence the torsion defines a Lie bracket (see Remark 2.2 about the negative sign).

$$[x, y] := -T(x, y). \tag{8}$$

The covariant derivation formula $\nabla_x(T(y, z)) = (\nabla_x T)(y, z) + T(\nabla_x y, z) + T(y, \nabla_x z)$ together with $\nabla_x T = 0$ imply

$$x \triangleright [y, z] = [x \triangleright y, z] + [y, x \triangleright z]. \tag{9}$$

On the other side, (2) together with $R = 0$ imply

$$[x, y] \triangleright z = a(x, y, z) - a(y, x, z). \tag{10}$$

This leads to the general definition of a *post-Lie algebra*.

Definition 2.1. A post-Lie algebra $\{\mathcal{A}, [\cdot, \cdot], \triangleright\}$ is a Lie algebra $\{\mathcal{A}, [\cdot, \cdot]\}$ together with a product $\triangleright\colon \mathcal{A} \times \mathcal{A} \to \mathcal{A}$ such that (9)-(10) hold. We call $[\cdot, \cdot]$ the *torsion* and $\triangleright$ the *connection* of the post-Lie algebra.

Remark 2.2. In many applications one may naturally obtain (10) with opposite sign

$$[x, y] \triangleright z = a(y, x, z) - a(x, y, z).$$

We could have defined *left* and *right* post-Lie algebras according to these sign changes. This terminology would make sense e.g. in the case of the Maurer–Cartan form on a Lie group. However, the sign in (10) can always be absorbed into a change of the sign in the definition of the torsion bracket, since $\{\mathcal{A}, -[\cdot, \cdot]\}$ is also a Lie algebra and (9) is invariant under a sign change in the torsion. There is therefore no need to define both left- and right-versions of post-Lie algebras.

Remark 2.3. Post-Lie algebras were introduced around 2007 by B. Vallette [39], who found the structure in a purely operadic manner as the Koszul dual of a commutative trialgebra. The enveloping algebra of a post-Lie algebra was independently introduced about the same time under the name D-algebra in [29], and studied in the context of Lie–Butcher series. A basis for the free post-Lie algebra was presented in [27], before the post-Lie definition was formalised. Vallette defines a post-Lie operad and proves that post-Lie algebras have the important algebraic property of being Koszul. This property is shared by many other important algebras, such as Lie algebras, associative algebras, commutative algebras, pre-Lie algebras, dendriform algebras etc. He also defines the operadic homology of post-Lie algebras and computes this for the free post-Lie algebra.

Remark 2.4. The present differential geometric explanation of a post-Lie algebra is, as far as we are aware, new. Since condition (10) is expressing the flatness of the connection, while (9) derives from the constant torsion, we initially called this structure a FCT (flat, constant torsion) algebra, but will henceforth adhere to the name *post-Lie algebra*.

A pre-Lie algebra is a post-Lie algebra where $[\cdot,\cdot] = 0$, hence most results about post-Lie algebras also yield information about pre-Lie algebras. In particular, the D-algebra provides a definition for the enveloping algebra of a pre-Lie algebra. We return to this in the sequel.

2.1.1 Some basic results about post-Lie algebras.

Proposition 2.5. *If* $\{A, [\cdot,\cdot], \rhd\}$ *is post-Lie, then the bracket* $[\![x, y]\!]$ *defined as*

$$[\![x, y]\!] := x \rhd y - y \rhd x + [x, y]$$

is a Lie bracket.

Proof. Identifying A with $\mathrm{Der}(U(A))$, defined in Section 3.2, we get $[\![x, y]\!] = x \circ y - y \circ x$. Since $\circ$ is associative this is a Lie bracket. $\square$

In the case of a flat constant torsion connection on a manifold $\mathcal{M}$, the Lie bracket $[\![\cdot,\cdot]\!]$ is the Jacobi–Lie bracket of vector fields on $\mathcal{M}$.

By a modification of the product $\rhd$ in A, we obtain another post-Lie algebra.

Proposition 2.6. *Let* $\{A, [\cdot,\cdot], \rhd\}$ *be post-Lie. Define the product* $\blacktriangleright$ *as*

$$x \blacktriangleright y = x \rhd y + [x, y],$$

then $\{A, -[\cdot,\cdot], \blacktriangleright\}$ *is also post-Lie.*

Proof. Since both $x \rhd \cdot$ and $[x, \cdot]$ are derivations on the torsion bracket, $x \rhd \cdot + \alpha[x, \cdot]$ is also a derivation, for any α. A direct computation shows that (10) holds with a sign change, which is corrected by negating the torsion bracket. $\square$

Proposition 2.7. *Let* $\{A, [\cdot,\cdot], \rhd\}$ *be post-Lie. Define the product* $\succ$ *as*

$$x \succ y = x \rhd y + \frac{1}{2}[x, y],$$

then $\{A, \succ\}$ *is Lie-admissible, torsion free with constant curvature*

$$R(x, y)z := a_{\succ}(x, y, z) - a_{\succ}(y, x, z) = -\frac{1}{4}[[x, y], z].$$

Proof. Lie-admissible follows from $x \succ y - y \succ x = [\![x, y]\!]$. The curvature follows from a lengthy but straightforward computation. $\square$

Remark 2.8. In the case of vector fields on a Lie group, discussed below, $\rhd$ and $\blacktriangleright$ come from the right and left Maurer–Cartan form and $\succ$ is the Levi–Civita connection.

2.2 Lie groups, homogeneous spaces and moving frames

A more general view on torsion and curvature appears in the theory of G-structures and $\mathfrak{g}$-valued forms on a manifold. This is the foundation for Cartan's method of moving frames, which Peter Olver and his co-workers have developed into a powerful tool in applied and computational mathematics [33, 23].

2.2.1 Post-Lie algebras and numerical Lie group integrators

We will briefly review the fundamentals of numerical Lie group integration, as formulated in [26]. Let G be a Lie group with Lie algebra $\mathfrak{g}$, and let

$$\lambda\colon G\times\mathcal{M}\to\mathcal{M},\quad (g,u)\mapsto g\cdot u$$

be a transitive left action of G on a homogeneous space $\mathcal{M}$, with infinitesimal generator

$$\lambda_\star\colon \mathfrak{g}\times\mathcal{M}\to T\mathcal{M},\quad (v,u)\mapsto \left.\frac{\partial}{\partial t}\right|_{t=0}\exp(tv)\cdot u\in T_u\mathcal{M}. \tag{11}$$

Let $\Omega^k(\mathcal{M},\mathfrak{g})$ be the space of $\mathfrak{g}$-valued k-forms on $\mathcal{M}$, in particular $\Omega^0(\mathcal{M},\mathfrak{g})$ is the space of maps from $\mathcal{M}$ to $\mathfrak{g}$. Any $x\in\Omega^0(\mathcal{M},\mathfrak{g})$ generates a vector field $X\in\mathcal{X}\mathcal{M}$ as

$$X(u)=\lambda_\star(x(u),u), \tag{12}$$

which by abuse of notation is written compactly as $X=\lambda_\star(x)$, where $\lambda_*\colon\Omega^0(\mathcal{M},\mathfrak{g})\to\mathcal{X}\mathcal{M}$.

Remark 2.9. Most Lie group integrators for the differential equation $u'(t)=F(u(t))$, where $u(t)\in\mathcal{M}$ and $F\in\mathcal{X}\mathcal{M}$, are based on rewriting the equation as $u'(t)=\lambda_*f(u(t))$ for $f\in\Omega^0(\mathcal{M},\mathfrak{g})$. It is important to note that if the action of G is transitive but not free on $\mathcal{M}$, then $\lambda_*\colon\Omega^0(\mathcal{M},\mathfrak{g})\to\mathcal{X}\mathcal{M}$ is surjective but not injective. The freedom in choice of a f to represent F is given by the isotropy (stabiliser) subgroup of G at a point $u\in\mathcal{M}$. Different choice of isotropy can lead to significantly different numerical integrators. As pointed out by Lewis and Olver [18], moving frames is an important tool in the study of isotropy choice for Lie group integrators. We return to this in the sequel.

Numerical analysis of Lie group integrators is intimately related to post-Lie algebras, due to the following result.

Proposition 2.10. *Let $\mathcal{M}$ be acted upon from left by a Lie group G with Lie algebra $\{\mathfrak{g},[\cdot,\cdot]_\mathfrak{g}\}$. Let the Lie bracket $[\cdot,\cdot]\colon\Omega^0(\mathcal{M},\mathfrak{g})\times\Omega^0(\mathcal{M},\mathfrak{g})\to\Omega^0(\mathcal{M},\mathfrak{g})$ and the product $\rhd\colon\Omega^0(\mathcal{M},\mathfrak{g})\times\Omega^0(\mathcal{M},\mathfrak{g})\to\Omega^0(\mathcal{M},\mathfrak{g})$ be defined pointwise at $u\in\mathcal{M}$ as*

$$[x,y](u) = [x(u),y(u)]_\mathfrak{g} \tag{13}$$

$$x\rhd y = \lambda_*(x)(y)\quad \textit{(the Lie derivative of y along $\lambda_*(x)$)}, \tag{14}$$

then $\{\Omega^0(\mathcal{M},\mathfrak{g}),[\cdot,\cdot],\rhd\}$ is a post-Lie algebra.

Proof. This can be verified by a coordinate computation. Let $\{e_j\}$ be a basis for $\mathfrak{g}$ and $\partial_j=\lambda_*(e_j)$ the corresponding right invariant vector fields on $\mathcal{M}$. Note that $\lambda_*([e_j,e_k])=-[\![\partial_j,\partial_k]\!]$, where the right hand side is the Jacobi–Lie bracket of vector fields. Letting $x(p)=\sum_j x^j(p)e_j$ and $y(p)=\sum_k y^k(p)e_k$, where x^j and y^k are scalar functions on $\mathcal{M}$, we obtain

$$\begin{aligned}[x,y] &= \sum_{j,k} x^j y^k[e_j,e_k]\\ x\rhd y &= \sum_{j,k} x^j\partial_j(y^k)e_k.\end{aligned}$$

The post-Lie conditions follow by a straightforward computation. □

A similar result, formulated in the enveloping algebra, can be found in [29, Lemma 3].

The connection $\rhd$ leads to a parallel transport of vector fields $\phi^*x(p)=x(\phi(p))$ for $x\in\Omega^0(\mathcal{M},\mathfrak{g})$ and $\phi\in\mathrm{Diff}(\mathcal{M})$. This parallel transport is used in numerical Lie group integrators to collect tangent vectors to a common base point in order to compute the timestep of the algorithm. The parallel transport is clearly independent of paths, since the connection is flat, and it is given algebraically as the exponential of $\rhd$.

2.2.2 The Maurer–Cartan form

The (left) Maurer–Cartan (MC) form on a Lie group G is a $\mathfrak{g}$-valued one-form $\omega \in \Omega^1(G, \mathfrak{g})$, defined as the map $\omega\colon TG \to \mathfrak{g}$ moving $v \in T_g G$ to $\mathfrak{g}$ by left translation

$$\omega(v) = TL_{g^{-1}}v,$$

where $L_g h = gh$ is left multiplication in the group[1].

The Maurer–Cartan form defines a linear isomorphism $\omega_p\colon T_pG \to \mathfrak{g}$ and hence defines an isomorphism between $\Omega^0(G, \mathfrak{g})$ and vector fields $\mathcal{X}G$. For the *right* Maurer–Cartan form, this isomorphism is given by λ_* defined in (11)-(12), when $\mathcal{M} = G$. For the left MC form, the corresponding isomorphism $\rho_*\colon \Omega^0(G, \mathfrak{g}) \to \mathcal{X}G$ is given as the infinitesimal right action

$$\rho_*(x)(g) = \left.\frac{\partial}{\partial t}\right|_{t=0} g\exp(tx(g)). \tag{15}$$

The Maurer–Cartan form satisfies the structural equation

$$d\omega + \frac{1}{2}\omega \wedge \omega = 0. \tag{16}$$

On a general (connected, smooth) manifold $\mathcal{M}$, the existence of a $\mathfrak{g}$-valued one form which is an isomorphism on the fibre and satisfies (16) implies that $\mathcal{M}$ can be given the structure of a Lie group (up to a covering) [36, Theorem §8.8.7]. Thus the Maurer–Cartan form is fundamental in a differential geometric characterization of Lie groups.

The curvature of $\omega \in \Omega^1(G, \mathfrak{g})$ is given as $R = d\omega + \frac{1}{2}\omega \wedge \omega \in \Omega^2(G, \mathfrak{g})$, and (16) is therefore a flatness condition $R = 0$. Taking $\theta = -\omega$ as a solder form, we compute the torsion form $\Theta = d\theta + \omega \wedge \theta = -\frac{1}{2}\omega \wedge \omega \in \Omega^2(G, \mathfrak{g})$. This yields

$$\Theta(X, Y) = -[\omega(X), \omega(Y)]_{\mathfrak{g}}.$$

Therefore, the Maurer–Cartan form is flat with constant torsion.

Proposition 2.11. *Given a Lie group G and the inverse of the (left) MC form $\rho_*\colon \Omega^0(G, \mathfrak{g}) \to \mathcal{X}G$ in (15), then $\{\Omega^0(G, \mathfrak{g}), -[\cdot,\cdot], \blacktriangleright\}$ is a post-Lie algebra, where*

$$\begin{aligned} x \blacktriangleright y &:= \rho_*(x)(y) \\ [x, y](g) &:= [x(g), y(g)]_{\mathfrak{g}}. \end{aligned}$$

The product $x \blacktriangleright y$ is related to the connection of the right MC form $x \triangleright y$, see (14), as

$$x \blacktriangleright y = x \triangleright y + [x, y]. \tag{17}$$

Proof. From the right MC form we get the post-Lie algebra $\{\Omega^0(G, \mathfrak{g}), [\cdot,\cdot], \triangleright\}$ (Proposition 2.10). The correspondence between a right trivialized $\tilde{x}$ and the corresponting left trivialized x in $\in \Omega^0(G, \mathfrak{g})$ is given as $x(g) = \omega(\lambda_*\tilde{x})(g) = \mathrm{Ad}_g\tilde{x}(g)$, from which (17) follows by differentiation. Hence, by Proposition 2.6, $\{\Omega^0(G, \mathfrak{g}), -[\cdot,\cdot], \blacktriangleright\}$ is post-Lie. $\square$

Remark 2.12. Since $\rho_*\colon \Omega^0(G, \mathfrak{g}) \to \mathcal{X}G$ is an isomorphism, we can equivalently define $\blacktriangleright\colon \mathcal{X}G \times \mathcal{X}G \to \mathcal{X}G$ as $X \blacktriangleright Y = \rho_*\left(X(\omega(Y))\right)$. This is a flat Koszul connection on $\mathcal{X}G$ with torsion $[X, Y] = -\rho_*[\omega(X), \omega(Y)]_{\mathfrak{g}}$. The vector fields on a Lie group with this connection and torsion is a prime example of a post-Lie algebra.

[1] The MC form can also be defined by right translation, but the left form is more convenient for moving frames.

2.2.3 Homogeneous spaces, a leftist view

We recall some aspects of the Klein–Cartan geometry of a homogeneous space $\mathcal{M}$ from [36]. Given a transitive left action $\cdot \colon G \times \mathcal{M} \to \mathcal{M}$ and an arbitrary point $o \in \mathcal{M}$. Let $H = \{ h \in G \mid h{\cdot}o = o \}$ be the isotropy subgroup at o with Lie algebra $\mathfrak{h} < \mathfrak{g}$. Define

$$G \times_H \mathfrak{g} := (G \times \mathfrak{g}) \,/ \sim\, ,$$

where $(g, v) \sim (gh, \mathrm{Ad}_{h^{-1}} v)$ for all $h \in H$. Define the map

$$\rho_M \colon G \times_H \mathfrak{g} \to \mathcal{M}, \quad (g, v) \mapsto g \exp(v) \cdot o, \tag{18}$$

and its differential with respect to the second variable $\rho_{M*} \colon G \times_H \mathfrak{g} \to T\mathcal{M}$ as

$$\rho_{M*}(g, v) := \left.\frac{\partial}{\partial t}\right|_{t=0} g \exp(tv){\cdot}o \in T_{g\cdot o}\mathcal{M}. \tag{19}$$

Since $\rho_{M*}(g, v + v^{\perp}) = \rho_{M*}(g, v)$ for all $v^{\perp} \in \mathfrak{h}$, it follows that ρ_{M*} induces a smooth quotient mapping

$$\overline{\rho_M}_* \colon G \times_H \mathfrak{g}/\mathfrak{h} \to T\mathcal{M}, (g, v + \mathfrak{h}) \mapsto \rho_{M*}(g, v), \tag{20}$$

where $\mathfrak{g}/\mathfrak{h}$ denotes the quotient as vector spaces. In [36][Prop. 5.1] it is shown:

Proposition 2.13. *$\overline{\rho_M}_*$ defines an isomorphism $G \times_H \mathfrak{g}/\mathfrak{h} \simeq T\mathcal{M}$ as vector bundles over $\mathcal{M}$.*

Thus, tangents in $T_{g\cdot o}\mathcal{M}$ are uniquely represented as $(g, v) \in G \times_H \mathfrak{g}/\mathfrak{h}$, while finite motions are not invariant under change of isotropy; in general $\rho_M(g, v) \neq \rho_M(g, v + v^{\perp})$ for $v^{\perp} \in \mathfrak{h}$. In order to fix a choice of isotropy, it is useful to discuss the notion of *gauges*. This is essentially the same concept as gauges in field theories of theoretical physics.

A *Cartan gauge* is a local section of the principal H-bundle $\pi \colon G \to \mathcal{M}, g \mapsto g{\cdot}o$, i.e. a map $\sigma \colon U \subset \mathcal{M} \to G$ such that $\pi{\circ}\sigma = \mathrm{Id}$ on an open set U. We denote this (σ, U).

The *Darboux derivative* of a map $f \colon \mathcal{M} \to G$, denoted $\omega_f \colon T\mathcal{M} \to \mathfrak{g}$, is defined as the pullback of the Maurer–Cartan form ω on G along f,

$$\omega_f := f^*\omega = \omega{\circ}f_*, \tag{21}$$

where $f_* \colon T\mathcal{M} \to TG$ is the differential of f. This will always satisfy the Cartan condition

$$\omega_f + \frac{1}{2}\omega_f \wedge \omega_f = 0, \tag{22}$$

and thus it is a flat $\mathfrak{g}$-valued 1-form $\omega_f \in \Omega^1(\mathcal{M}, \mathfrak{g})$. We call f the *primitive* of ω_f. A generalization of the fundamental theorem of calculus [36] states that, *locally*, a one form $\theta \in \Omega^1(\mathcal{M}, \mathfrak{g})$ has a primitive $f \colon \mathcal{M} \to G$ if and only if θ is flat, i.e. iff θ satisfies (22). Furthermore, the primitive is determined uniquely up to left multiplication by a constant $c \in G$: if $\omega_f = \omega_{\tilde{f}}$ then $\tilde{f} = cf$ for some constant of integration $c \in G$.

The Darboux derivative of the Cartan gauge $\omega_\sigma \in \Omega^1(\mathcal{M}, \mathfrak{g})$ is called an *infinitesimal Cartan gauge*. Since ω_σ is flat, we can uniquely recover σ from ω_σ (the integration constant is found by the condition that σ is a section).

Proposition 2.14. *A Cartan gauge (σ, U) with derivative ω_σ, defines a map $\sigma_* \colon T\mathcal{M} \to G \times_H \mathfrak{g}$ as*

$$\sigma_*(v) = \sigma(\pi v) {\times_H} \omega_\sigma(v), \tag{23}$$

which extends to $\overline{\sigma}_* \colon T\mathcal{M} \to G \times_H \mathfrak{g}/\mathfrak{h}$ by composition with the projection $\mathfrak{g}/\mathfrak{h} \mapsto \mathfrak{h}$

$$\overline{\sigma}_* \colon T\mathcal{M} \xrightarrow{\sigma_*} G \times_H \mathfrak{g} \to G \times_H \mathfrak{g}/\mathfrak{h}. \tag{24}$$

The maps $\overline{\sigma}_*$ and $\overline{\rho_M}_*$ are locally inverse vector bundle isomorphisms, $\overline{\sigma}_*{\circ}\overline{\rho_M}_* = \mathrm{Id}$ and $\overline{\rho_M}_*{\circ}\overline{\sigma}_* = \mathrm{Id}$ on their domains of definition.

Proof. This is a straightforward computation. □

Infinitesimally all gauges are equivalent, but how does a change of gauge affect the finite motions induced by ρ_M? A *retraction map* is a smooth, locally defined map $\mathcal{R}\colon T\mathcal{M} \to \mathcal{M}$ such that:

- $\mathcal{R}(v) = \pi_M v$ if and only if v is a 0-tangent, where $\pi_M\colon T\mathcal{M} \to \mathcal{M}$.
- $\mathcal{R}'(0) = \mathrm{Id}$ (the identity on the tangent fibre).

Retractions provide a useful way of formulating numerical integration schemes [6]. For any Cartan gauge (σ, U) there corresponds a retraction map $\mathcal{R}_\sigma\colon TU \to \mathcal{M}$ defined as

$$\mathcal{R}_\sigma(v) = \rho_M \circ \sigma_*(v) = \sigma(\pi v)\exp(\omega_\sigma(v))\cdot o, \quad \text{for } v \in TU. \tag{25}$$

If (σ, U) and (σ', U) are two gauges on $U \subset \mathcal{M}$, then $\sigma'(u) = \sigma(u)h(u)$ for some smooth $h\colon U \to H$. The corresponding infinitesimal gauges ω_σ and $\omega_{\sigma'}$ are related as [36][p. 168]

$$\omega'_\sigma = \mathrm{Ad}_{h^{-1}}\omega_\sigma + \omega_h, \tag{26}$$

where $\omega_h \in \Omega^1(U, \mathfrak{h})$ is the Darboux derivative of h. Thus, the modified retraction is given as

$$\mathcal{R}_{\sigma'} = \sigma(\pi v)\exp\left(\omega_\sigma(v) + \omega_h(v)\right)\cdot o. \tag{27}$$

If h is constant then $\omega_h = 0$ and the two retractions are equal, but generally they differ. For numerical integration it is important to choose the gauge in a good manner. We return to this in the discussion of moving frames below.

Let $\Gamma(G \times_H \mathfrak{g})$ denote sections of the bundle $G \times_H \mathfrak{g} \to \mathcal{M}$. This space can be identified with the subspace $\Omega^0_H(G, \mathfrak{g}) \subset \Omega^0(G, \mathfrak{g})$ defined as

$$\Omega^0_H(G, \mathfrak{g}) := \left\{ x \in \Omega^0(G, \mathfrak{g}) \mid x(gh) = \mathrm{Ad}_{h^{-1}} x(g) \right\}. \tag{28}$$

Proposition 2.15. *There is a 1–1 correspondence between $x \in \Omega^0_H(G, \mathfrak{g})$ and $X \in \Gamma(G \times_H \mathfrak{g})$, defined locally by a Cartan gauge (σ, U) as*

$$X(u) = \sigma(u) \times_H x(\sigma(u)), \quad \text{for } u \in U \subset \mathcal{M}.$$

The map $x \mapsto X$ is independent of the choice of section σ.

Proof. $x \mapsto X$ is independent of σ since $\sigma(u)h \times x(\sigma(u)h) \sim \sigma(u) \times \mathrm{Ad}_h x(\sigma(u)h) = \sigma(u) \times x(\sigma(u))$. Given X we recover x on the section $\sigma(U) \subset G$, and reconstruct x on the fibres of $H \to G \to \mathcal{M}$ by $x(gh) = \mathrm{Ad}_{h^{-1}} x(g)$. □

Thus, to sum up, we have an identification $\Omega^0_H(G, \mathfrak{g}) \simeq \Gamma(G \times_H \mathfrak{g})$. An $X \in \Gamma(G \times_H \mathfrak{g})$ corresponds to a vector field $\rho_{M*} \circ X \in \mathcal{X}\mathcal{M}$ and a diffeomorphism $\rho_M \circ X \in \mathrm{Diff}(\mathcal{M})$. Furthermore, given a Cartan gauge (σ, U), we can map a vector field $Y \in \mathcal{X}\mathcal{M}$ to $\sigma_* Y \in \Gamma(G \times_H \mathfrak{g})$, but this map depends on the gauge σ. Finally, there is a post-Lie algebra also associated with this view of homogeneous spaces:

Proposition 2.16. *$\{\Omega^0_H(G, \mathfrak{g}), -[\cdot,\cdot], \blacktriangleright\}$, with $\blacktriangleright$ and $[\cdot,\cdot]$ defined in Prop. 2.11, is post-Lie.*

Proof. A straightforward computation reveals that $(x \blacktriangleright y)(gh) = \mathrm{Ad}_{h^{-1}}(x \blacktriangleright y)(g)$ and $[x(gh), y(gh)] = \mathrm{Ad}_{h^{-1}}[x(g), y(g)]$. Hence $\blacktriangleright$ and $[\cdot,\cdot]$ are well defined on the subspace $\Omega^0_H(G, \mathfrak{g})$. □

What is the parallel transport in this post-Lie algebra? Note that $x \in \Omega^0_H(G, \mathfrak{g})$ defines a vector field $\rho_* x \in \mathcal{X}G$ with a flow $\Phi_t\colon G \to G$ satisfying

$$\Phi_t(gh) = \Phi_t(g)h, \quad \text{for all } h \in H. \tag{29}$$

For such a diffeomorphism we define $\Phi^*\colon \Omega^0_H(G, \mathfrak{g}) \to \Omega^0_H(G, \mathfrak{g})$ as

$$\Phi^* y(g) := y(\Phi(g)). \tag{30}$$

Proposition 2.17. *For $x, y \in \Omega^0_H(G, \mathfrak{g})$ define the exponential series*

$$\exp(x\blacktriangleright)y := y + x \blacktriangleright y + \frac{1}{2}(x \blacktriangleright (x \blacktriangleright y)) + \frac{1}{6}(x \blacktriangleright (x \blacktriangleright (x \blacktriangleright y))) + \cdots . \tag{31}$$

Parallel transport in $\Omega^0_H(G, \mathfrak{g})$ is given as

$$\exp(x\blacktriangleright)y = \Phi^* y,$$

where $\Phi^* \colon G \to G$ is the $t = 1$ flow of $\rho_* x \in \mathcal{X}G$.

Remark 2.18. The post-Lie structure captures algebraically both infinitesimal aspects of homogeneous spaces and also finite motions such as flows and parallel transport. It is therefore clear that the post-Lie structure cannot carry over to the quotient space $\Gamma(G \times_H \mathfrak{g}/\mathfrak{h}) \simeq \mathcal{X}\mathcal{M}$, both $\blacktriangleright$ and $[\cdot, \cdot]$ change under an isotropy change $x \mapsto x + x^\perp$ where $x, x^\perp \in \Omega^0_H(G, \mathfrak{g})$ and $x^\perp(g) \in \mathfrak{h}$. Hence this post-Lie structure does not carry over to $\mathcal{X}\mathcal{M}$, except when the action is free.

Remark 2.19. In Section 2.2.1, we described a post-Lie algebra on a homogeneous space $\mathcal{M}$ derived from the right MC form. This has been the basis for almost all work on numerical integration schemes on homogeneous spaces since [30]. In the present section, we have detailed an alternative post-Lie structure on $\mathcal{M}$ derived from the left MC form. We believe that this formulation should lead to better geometric integration algorithms on symmetric spaces. Also, it seems as this formulation is better suited for combination of numerical Lie group integration with moving frame algorithms.

2.2.4 Moving frames

Moving frames provide an important tool for choosing gauges that are naturally derived from the geometry of e.g. a differential equation or other geometric objects such as curves and surfaces in a homogeneous space (Klein geometry). Let $\mathcal{M}$ be a manifold acted upon from left by a Lie group G with Lie algebra $\mathfrak{g}$. We do not require the action to be transitive, so $\mathcal{M}$ needs not be a homogeneous space.

Definition 2.20. A left moving frame is a map $\sigma \colon \mathcal{M} \to G$ such that

$$\sigma(g \cdot u) = g\sigma(u) \quad \text{for all } g \in G \text{ and } u \in \mathcal{M},$$

a right moving frame is a map $r \colon \mathcal{M} \to G$ such that

$$r(g \cdot u) = r(u)g^{-1} \quad \text{for all } g \in G \text{ and } u \in \mathcal{M}.$$

If r is a right moving frame then $\sigma(u) = r(u)^{-1}$ (inverse in G) is a left moving frame. Moving frames exist if and only if the G action on $\mathcal{M}$ is free and regular. In that case, moving frames can be constructed (locally) as follows [33]:

1. Choose a submanifold $\mathcal{K} \subset \mathcal{M}$ which is transverse to the G orbits and of the maximal dimension $p = \dim(M) - \dim(G)$. Locally, there is one point in $\mathcal{K}$ for each orbit, and each orbit intersect $\mathcal{K}$ in one point. In coordinates, $\mathcal{K}$ is often chosen by setting $d = \dim(G)$ of the coordinates to constant values.

2. A right moving frame r is found by solving the normalisation equations $r(u)u \in \mathcal{K}$ for $r(u)$.

3. A left moving frame is obtained by inverting r.

If the action is not free, there is a standard procedure of obtaining a free and regular action by *prolongation* of the group action, i.e. we extend $\mathcal{M}$ to a jet-space $J^k(\mathcal{M})$, which is the geometrical way of saying that we consider the space of all curves in $\mathcal{M}$ represented by Taylor expansions up to order k. The prolongation of the group action is the natural induced action of G on (Taylor expansions) of curves. Coordinates on the jet-space are given by the (higher order) derivatives of curves. We can always obtain a free regular action (and thus a moving frame) by prolongation. Thus, by this construction we find a left moving frame $\sigma\colon J^k(\mathcal{M}) \to G$.

Moving frames are closely related to Cartan gauges on a homogeneous space $\mathcal{M}$. Let G act transitively on $\mathcal{M}$ with an isotropy subgroup H, and let $\sigma\colon \mathcal{M} \to G$ be a local section of the bundle $\pi\colon G \to \mathcal{M}$. Note that σ is a section if and only if

$$\sigma(g\cdot u) = g\sigma(u)h(u) \quad \text{for } h\colon \mathcal{M} \to H. \tag{32}$$

Thus it is a left moving frame, up to isotropy. Such a map is also called a *partial* moving frame [17].

Thus, the theory of moving frames (full and partial) provides geometric ways of constructing sections (σ, U) of $G \to \mathcal{M}$, hence also geometric ways of fixing isotropy through the map $\sigma_*\colon T\mathcal{M} \to \Gamma(G \times_H \mathfrak{g}) \simeq \Omega^0_H(G, \mathfrak{g})$ in (23). On $\Omega^0_H(G, \mathfrak{g})$ we have all the tools we need to do numerical integration and analysis of numerical integration schemes. The details of such algorithms is subject to future research. We see at least two useful ways to proceed in choosing σ.

- By prolongation of the group action we can obtain a full moving frame $\sigma\colon J^k(\mathcal{M}) \to G$. To solve a differential equation $u' = F(u)$, $F \in \mathcal{X}\mathcal{M}$, we must prolong also F to the jet-bundle. This should be a very attractive numerical method in cases where we can compute the k-th derivatives of F, either by computer algebraic means, or by automatic differentiation.
- In the case where $\mathcal{M}$ is a symmetric space, there is a canonical choice of section $\sigma\colon \mathcal{M} \to G$. In this case there exists a canonical splitting $\mathfrak{g} = \mathfrak{h} \oplus \mathfrak{k}$, where $\mathfrak{h}$ is a sub algebra and $\mathfrak{k}$ is a Lie triple system (LTS). The infinitesimal gauge ω_σ takes values in $\mathfrak{k}$, and thus exponentials need only be computed on the LTS. Efficient algorithms for computing exponentials on an LTS are discussed in [41]. This theory opens up the possibility of new classes of numerical integration on symmetric spaces.

3 The algebraic structure of post-Lie and D-algebras

In this chapter we discuss the algebraic structure of general post-Lie algebras $\{\mathcal{A}, [\cdot,\cdot], \rhd\}$. Various aspects of this theory can also be found in [27, 29, 22, 21]. Here we develop the core theory from the axiomatic definition of a post-Lie algebra, and establish the functorial relationship between post-Lie algebras and the enveloping D-algebra. Moreover, we find that a magmatic view of planar trees and forests give rise to recursive formulas for various algebraic operations, which simplify computer implementations.

3.1 Free post-Lie algebras

In [7] Chapoton and Livernet gave an explicit description of the free pre-Lie algebra in terms of decorated rooted trees and grafting. In this section we will see that there is a similar description of the free post-Lie algebra. In fact, we will show that the free post-Lie algebra can be described as the free Lie algebra over planar rooted trees, extended with a connection given by left grafting of trees. Furthermore, we will relate post-Lie algebras to D-algebras, studied in connection with numerical Lie group integration [29, 22]. The universal enveloping algebra of a post-Lie algebra is a D-algebra, and the post-Lie algebra is recovered as the derivations in the D-algebra.

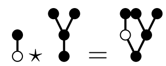
Trees. Let $\mathcal{C}$ be a set, henceforth called *colors*. We define $\mathrm{T}_\mathcal{C}$ the set of all planar (or ordered)[2] rooted trees with nodes colored by $\mathcal{C}$. Formally we define this as the free magma

$$\mathrm{T}_\mathcal{C} := \mathrm{Magma}(\mathcal{C}).$$

Recall that a *magma* is a set with a binary operation $\star$ without any algebraic relations imposed. The free magma over $\mathcal{C}$ consists of all possible ways to parenthesize binary operations on $\mathcal{C}$. We

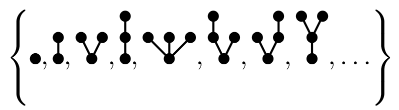
[2]Trees with different orderings of the branches are considered different, as when pictured in the plane.

identify Magma($\mathcal{C}$) with planar trees, where the nodes are decorated with colors from $\mathcal{C}$. On trees we interpret $\star$ as the *Butcher-product* [4]: $\tau_1 \star \tau_2 = \tau$ is a tree where the root of the tree τ_1 is attached on the left part of the root of the tree τ_2. For example:



$$= (\bullet \star \circ) \star ((\bullet \star (\bullet \star \bullet)) \star \bullet).$$

If $\mathcal{C} = \{\bullet\}$ has only one element, we write $\mathrm{T} := \mathrm{T}_{\{\bullet\}}$. The first few elements of T are:

$\mathrm{T} =$ 

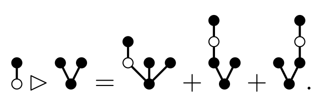
Note that any $\tau \in \mathrm{T}_{\mathcal{C}}$ has a unique maximal right factorization

$$\tau = \tau_1 \star (\tau_2 \star (\cdots (\tau_k \star c))), \quad \text{where } c \in \mathcal{C} \text{ and } \tau_1, \dots, \tau_k \in \mathrm{T}_{\mathcal{C}}.$$

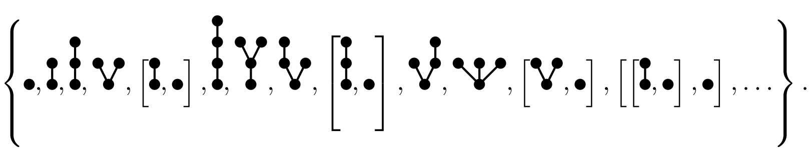
Here c is the root, k is the *fertility* of the root and $\tau_1, \dots, \tau_k$ are the branches of the root. Let k be a field of characteristic zero and write $\mathrm{k}\{\mathrm{T}_{\mathcal{C}}\}$ for the free k-vector space over the set $\mathrm{T}_{\mathcal{C}}$, i.e. all k-linear combinations of trees. We define *left grafting*[3] $\rhd\colon \mathrm{T}_{\mathcal{C}} \times \mathrm{T}_{\mathcal{C}} \to \mathrm{k}\{\mathrm{T}_{\mathcal{C}}\}$ by the recursion

$$\begin{aligned} \tau \rhd c :=& \; \tau \star c, \quad \text{for } c \in \mathcal{C} \\ \tau \rhd (\tau_1 \star (\tau_2 \star (\cdots (\tau_k \star c)))) :=& \; \tau \star (\tau_1 \star (\tau_2 \star (\cdots (\tau_k \star c)))) \\ &+ (\tau \rhd \tau_1) \star (\tau_2 \star (\cdots (\tau_k \star c))) \\ &+ \tau_1 \star ((\tau \rhd \tau_2) \star (\cdots (\tau_k \star c))) \\ &+ \cdots \\ &+ \tau_1 \star (\tau_2 \star (\cdots ((\tau \rhd \tau_k) \star c))). \end{aligned} \tag{33}$$

Thus $\tau_1 \rhd \tau_2$ is the sum of all the trees resulting from attaching the root of τ_1 from the left to all the nodes of the tree τ_2. Example:



Free Lie algebras of trees. Let $\mathfrak{g} = \mathrm{Lie}(\mathrm{T}_{\mathcal{C}})$ denote the free Lie algebra over the set $\mathrm{T}_{\mathcal{C}}$ [35]. For $\mathcal{C} = \{\bullet\}$, a Lyndon basis is given up to order four as [27]:

$\mathrm{Lie}(\mathrm{T}_{\mathcal{C}}) = \mathrm{k}$ 

Proposition 3.1. *Let the free Lie algebra $\mathfrak{g} = \mathrm{Lie}(\mathrm{T}_{\mathcal{C}})$ be equipped with a product $\rhd\colon \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, extended from the left grafting defined on $\mathrm{T}_{\mathcal{C}}$ in (33) as*

$$u \rhd [v, w] = [u \rhd v, w] + [v, u \rhd w] \tag{34}$$

$$[u, v] \rhd w = a(u, v, w) - a(v, u, w) \tag{35}$$

for all $u, v, w \in \mathfrak{g}$. Then $\{\mathrm{Lie}(\mathrm{T}_{\mathcal{C}}), [\cdot,\cdot], \rhd\}$ is post-Lie.

Proof. Since any $u, v, w \in \mathfrak{g}$ can be written as a sum of trees and commutators of trees, the connection is well-defined on $\mathfrak{g}$. By construction it satisfies the axioms of a post-Lie algebra. $\square$

[3] Various notations for similar grafting products are found in the literature, e.g. $u \rhd v = u[v] = u \curvearrowright v$.

Free post-Lie algebras. Proposition 3.1 shows that the free Lie algebra of ordered trees has naturally the structure of an post-Lie algebra $\mathrm{postLie}(\mathcal{C}) := \{\mathrm{Lie}(\mathrm{T}_{\mathcal{C}}), [\cdot,\cdot], \rhd\}$. We call this the *free post-Lie algebra* over the set $\mathcal{C}$ for the following reason:

Theorem 3.2. *For any post-Lie algebra $\{\mathcal{A}, [\cdot,\cdot], \rhd\}$ and any function $f\colon \mathcal{C} \to \mathcal{A}$, there exists a unique morphism of post-Lie algebras $\mathcal{F}\colon \mathrm{postLie}(\mathcal{C}) \to \mathcal{A}$ such that $\mathcal{F}(c) = f(c)$ for all $c \in \mathcal{C}$.*

Proof. We construct $\mathcal{F}$ in two stages. First we show, using $\rhd$, that f extends uniquely to a function $\mathcal{F}_{\mathrm{T}_{\mathcal{C}}}\colon \mathrm{T}_{\mathcal{C}} \to \mathcal{A}$. Then by universality of the free Lie algebra, there is a unique Lie algebra homomorphism $\mathcal{F}\colon \mathrm{Lie}(\mathrm{T}_{\mathcal{C}}) \to \mathcal{A}$. We show that this is also a homomorphism for the connection product $\rhd$.

To construct the extension to $\mathrm{T}_{\mathcal{C}}$ we first observe that the magmatic product $\tau \star \tau'$ on $\mathrm{T}_{\mathcal{C}}$ (the Butcher product of two trees) can be expressed in terms of left grafting $\rhd$. This is done by induction in the fertility of τ'. For fertility 0, i.e. $\tau' = c \in \mathcal{C}$, we have $\tau \star c = \tau \rhd c$. For fertility k we write $\tau' = \tau_1 \star (\tau_2 \star (\cdots (\tau_k \star c)))$ and find from (33)

$$\tau \star \tau' = \tau \rhd \tau' - (\tau \rhd \tau_1) \star (\tau_2 \star (\cdots (\tau_k \star c))) - \cdots - (\tau_1 \star (\tau_2 \star (\cdots (\tau \rhd \tau_k \star c))).$$

In the right hand side of the equation, the fertility of any term on the right hand side of a $\star$-product is smaller than k, which completes the induction. The fact that $\mathrm{T}_{\mathcal{C}}$ is freely generated from $\mathcal{C}$ by the product $\star$ ensures that $\mathcal{F}_{\mathrm{T}_{\mathcal{C}}}$ is uniquely defined by

$$\begin{aligned} \mathcal{F}_{\mathrm{T}_{\mathcal{C}}}(c) &= f(c) \quad \text{for all } c \in \mathcal{C} \\ \mathcal{F}_{\mathrm{T}_{\mathcal{C}}}(\tau \rhd \tau') &= \mathcal{F}_{\mathrm{T}_{\mathcal{C}}}(\tau) \rhd \mathcal{F}_{\mathrm{T}_{\mathcal{C}}}(\tau'), \end{aligned}$$

and hence that also $\mathcal{F}\colon \mathrm{Lie}(\mathrm{T}_{\mathcal{C}}) \to \mathcal{A}$ is uniquely defined as a Lie algebra homomorphism.

Finally, by induction on the length of iterated commutators, we see that $\mathcal{F}(u \rhd v) = \mathcal{F}(u) \rhd \mathcal{F}(v)$ for all $u, v \in \mathrm{Lie}(\mathrm{T}_{\mathcal{C}})$: If $u, v \in \mathrm{T}_{\mathcal{C}}$ this holds by construction. Assuming that $\mathcal{F}(u \rhd v) = \mathcal{F}(u) \rhd \mathcal{F}(v)$ whenever u and v are iterated commutators of length at most k, we find by using (34)–(35) that $\mathcal{F}([u, \tau_1] \rhd [v, \tau_2]) = \mathcal{F}([u, \tau_1]) \rhd \mathcal{F}([v, \tau_2])$ for all $\tau_1, \tau_2 \in \mathrm{T}_{\mathcal{C}}$. □

Proposition 3.3. *Let $\mathrm{postLie}(\mathcal{C})$ be graded with the number n counting the number of nodes in the trees. Then*

$$\mathit{dim}(\mathrm{postLie}(\mathcal{C})_n) = \frac{1}{2n} \sum_{d|n} \mu(\frac{n}{d}) \binom{2d}{d} n^{|\mathcal{C}|},$$

where μ is the Möbius function. For $|\mathcal{C}| = 1$ the dimensions are $1, 1, 3, 8, 25, 75, 245, \ldots$. See also [37, A022553].

Proof. See [28] and [27]. □

Remark 3.4. The same dimensions also appear for the primitive Lie algebra of the Hopf algebra CQSym (Catalan Quasi-Symmetric functions) [31]. We believe that also this theory is founded on post-Lie algebras.

3.2 Universal enveloping algebras

D-algebras. In Section 4 we describe certain algebraic structures that occur naturally in the study of numerical integration methods on manifolds [29]. Central to this work are algebras of derivations, called *D*-algebras. We will see that post-Lie algebras relate to D-algebras similarly to the relationship between a Lie algebra and its universal enveloping algebra.

Definition 3.5 (D-algebra [29])**.** Let B be a unital associative algebra with product $u, v \mapsto uv$, unit $\mathbb{I}$ and equipped with a non-associative product $\cdot \rhd \cdot\colon B \otimes B \to B$ such that $\mathbb{I} \rhd v = v$ for all $v \in B$. Write $\mathrm{Der}(B)$ for the set of all $u \in B$ such that $u \rhd \cdot$ is a derivation:

$$\mathrm{Der}(B) = \{u \in B \mid u \rhd (vw) = (u \rhd v)w + v(u \rhd w) \ \text{ for all } v, w \in B\}.$$

B is called a *D-algebra* if the product $u, v \mapsto uv$ generates B from $\{\mathbb{I}, \mathrm{Der}(B)\}$ and furthermore for any $u \in \mathrm{Der}(B)$ and any $v, w \in B$ we have

$$\begin{aligned} v \rhd u &\in \mathrm{Der}(B) && (36)\\ (uv) \rhd w &= u \rhd (v \rhd w) - (u \rhd v) \rhd w. && (37)\end{aligned}$$

Proposition 3.6. *If B is a D-algebra then the derivations $\mathrm{Der}(B)$ form a post-Lie algebra, with torsion $[u, v] = uv - vu$ and connection $\rhd$.*

Proof. If $u, v \in \mathrm{Der}(B)$ we note that

$$(uv - vu) \rhd \cdot = u \rhd (v \rhd \cdot) - v \rhd (u \rhd \cdot) + (u \rhd v) \rhd \cdot - (v \rhd u) \rhd \cdot.$$

The first two terms on the right is a commutator of two derivations and is therefore a derivation. The last two terms are derivations separately. Hence, $[u, v] \in \mathrm{Der}(B)$ and $\{\mathrm{Der}(B), [\cdot, \cdot]\}$ is a Lie algebra. The other axioms of being post-Lie follows easily from the definition of a D-algebra. □

Universal enveloping algebras. Let $\{A, [\cdot, \cdot], \rhd\}$ be an post-Lie algebra, and let $U(A)$ be the universal enveloping algebra of the Lie algebra $\{A, [\cdot, \cdot]\}$. By the Poincaré–Birkhoff–Witt theorem we can embed A as a linear subspace of $U(A)$, such that $[u, v] = uv - vu$. The embedding is also denoted by A. The product $\rhd$ on A can be extended to $U(A)$ according to:

$$\begin{aligned} \mathbb{I} \rhd v &= v && (38)\\ u \rhd (vw) &= (u \rhd v)w + v(u \rhd w) && (39)\\ (uv) \rhd w &= u \rhd (v \rhd w) - (u \rhd v) \rhd w, && (40)\end{aligned}$$

for all $u \in A$ and $v, w \in U(A)$.

Proposition 3.7. *Equations (38)–(40) define a unique extension of $\rhd$ from A to $U(A)$. With the non-associative product $\rhd$, $U(A)$ is a D-algebra with derivations $\mathrm{Der}(U(A)) = A$.*

Proof. See [16, Theorem V.1] for a proof that a derivation on a Lie algebra A extends uniquely to a derivation on $U(A)$. This justifies the extension on the right (39). The extension on the left, given by (38) and (40), is compatible with the the embedding $[u, v] \mapsto uv - vu$ due to the flatness condition (10) for post-Lie algebras. From the PBW basis on $U(A)$ it follows that these equations extend $\rhd$ uniquely to all of $U(A)$ also on the left. It is clear that $A \subset \mathrm{Der}(U(A))$. To check that $A = \mathrm{Der}(U(A))$ we verify from (38)–(40) that $\mathbb{I}$ is not a derivation and that $u_1, u_2 \in \mathrm{Der}(U(A)) \Rightarrow u_1u_2 \notin \mathrm{Der}(U(A))$, thus $\mathrm{Der}(U(A))$ cannot be larger than A. □

Definition 3.8 (Universal enveloping algebras)**.** We call $U(A)$ equipped with this D-algebra structure $\rhd$ the universal enveloping algebra of the post-Lie algebra A.

Proposition 3.9. *For any D-algebra B and any post-Lie morphism $f : A \to \mathrm{Der}(B)$ there exists a unique D-algebra morphism $\mathcal{F} : U(A) \to B$ such that $\mathcal{F}(u) = f(u)$ for all $u \in A$.*

Proof. $\mathcal{F}$ is uniquely defined as a unital associative algebra morphism. It remains to verify that $\mathcal{F}(u \rhd v) = \mathcal{F}(u) \rhd \mathcal{F}(v)$. $U(A)$ has a grading by the length of the monomial basis of PBW. Using (38)–(40) it follows by induction in the grading that $\mathcal{F}(u \rhd v) = \mathcal{F}(u) \rhd \mathcal{F}(v)$. □

Remark 3.10. The preceding results establishes a pair of adjoint functors between the categories of D-algebras and post-Lie algebras:

$$U(\cdot) : \text{post-Lie} : \rightleftarrows \text{D-alg} : \mathrm{Der}(\cdot).$$

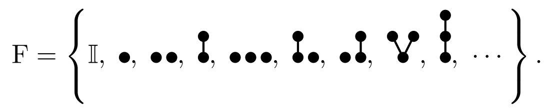
In other words, there is a natural isomorphism

$$\mathrm{Hom}_{\mathrm{postLie}}(\mathrm{Der}(A), B) \to \mathrm{Hom}_{\mathrm{D}}(A, U(B)).$$

Free D-algebras. A direct consequence of Theorem 3.2 and Proposition 3.9 is the following characterization of a free D-algebra:

Corollary 3.11 ([29, Proposition 1])**.** *The algebra* $\mathrm{D}_{\mathcal{C}} := U(\mathrm{postLie}(\mathcal{C}))$ *is the free D-algebra over the set* $\mathcal{C}$*, i.e. for any D-algebra* B *and any function* $f\colon \mathcal{C} \to \mathrm{Der}(B)$ *there exists a unique D-algebra morphism* $\mathcal{F}\colon \mathrm{D}_{\mathcal{C}} \to B$ *such that* $\mathcal{F}(c) = f(c)$ *for all* $c \in \mathcal{C}$*.*

The unital associative algebra of $\mathrm{D}_{\mathcal{C}}$ is $U(\mathrm{Lie}(\mathrm{T}_{\mathcal{C}}))$, which by the Cartier–Milner–Moore theorem is the free associative algebra over $\mathrm{T}_{\mathcal{C}}$. I.e. it is the noncommutative polynomials over rooted trees: $\mathrm{D}_{\mathcal{C}} = \mathrm{k}\langle \mathrm{T}_{\mathcal{C}}\rangle = \mathrm{k}\{\mathrm{F}_{\mathcal{C}}\}$, where $\mathrm{k}\{\mathrm{F}_{\mathcal{C}}\}$ denotes the free vector space over the set of *ordered forests*. $\mathrm{F}_{\mathcal{C}} := \mathrm{T}_{\mathcal{C}}^{*}$ consist of all words of finite length over the alphabet $\mathrm{T}_{\mathcal{C}}$, including the empty word $\mathbb{I}$. For $\mathcal{C} = \{\bullet\}$ these are



We can create a tree from a forest ω by applying the operator $\mathrm{B}_c^+ : \mathrm{F}_{\mathcal{C}} \to \mathrm{T}_{\mathcal{C}}$, attaching the trees in ω onto a common root labelled by $c \in \mathcal{C}$ and we can create a forest from a tree using the operator $\mathrm{B}^- : \mathrm{T}_{\mathcal{C}} \to \mathrm{F}_{\mathcal{C}}$ removing the root. The concatenation product $\omega_1, \omega_2 \mapsto \omega_1\omega_2$ is the associative operation of sticking shorter words together to create longer words.

Summarizing, the free D-algebra $\mathrm{D}_{\mathcal{C}}$ is the vector space of forests $\mathrm{k}\{F_{\mathcal{C}}\}$ with unit $\mathbb{I}$, concatenation product and the left grafting product $\triangleright$ defined on trees in (33) and extended to forests by (38)–(40). This free D-algebra carries a Hopf algebra structure, closely related to the Connes–Kreimer Hopf algebra, to be discussed in the sequel.

The composition product $\circ$ on D-algebras. A *dipterous* algebra [19] is a triple $\{B, \circ, \triangleright\}$, where B is a vector space and $\circ$ and $\triangleright$ are two binary operations on B satisfying:

$$x\circ(y\circ z) = (x\circ y)\circ z \tag{41}$$

$$x \triangleright (y \triangleright z) = (x\circ y) \triangleright z \tag{42}$$

for all $x, y, z \in B$. Let B be a D-algebra with concatenation $x, y \mapsto xy$ and connection product $x \triangleright y$. Define a product $\circ\colon B \times B \to B$ as

$$\begin{aligned} \mathbb{I}\circ y &= y \\ x\circ y &:= xy + x \triangleright y \\ (xy)\circ z &:= x\circ(y\circ z) - (x \triangleright y)\circ z \quad \text{for all } x \in \mathrm{Der}(B), y, z \in B. \end{aligned} \tag{43}$$

Proposition 3.12. *If* B *is a D-algebra then* $\{B, \circ, \triangleright\}$ *is a dipterous algebra.*

Proof. Proof by induction in the grading on B provided by the PBW basis. □

The product $x, y \mapsto x\circ y$ will be referred to as the *composition product*, while $x, y \mapsto xy$ is called either concatenation of *frozen composition*, due to the interpretation for differential operators on manifolds. Let $A = \Omega^0(\mathcal{M}, \mathfrak{g})$ be the post-Lie algebra defined in Proposition 2.10, and let $B = U(A) = \Omega^0(\mathcal{M}, U(\mathfrak{g}))$. For $f, g \in B$ the frozen composition is $(fg)(p) = f(p)g(p)$, where we 'freeze' the value of f and g in a point $p \in \mathcal{M}$ and obtain the product from $U(\mathfrak{g})$. The composition $f, g \mapsto f\circ g$, on the other hand, corresponds to the fundamental operation of composing two differential operators on $\mathcal{M}$. For $f, g \in \mathrm{Der}(B)$ we have $f\circ g = fg + f \triangleright g$, splitting the composition in a term fg where g is 'frozen' (constant) and a term $f \triangleright g$ where the variation of g along f is taken into account.

On the free D-algebra $D_{\mathcal{C}}$ the composition is computed on two forests $\omega_1, \omega_2 \in \mathrm{F}_{\mathcal{C}}$ as ([29] Definition 2):

$$\omega_1\circ\omega_2 = B^-(\omega_1 \triangleright B^+(\omega_2)). \tag{44}$$

We call this the planar Grossman–Larson product, since it is a planar forest analogue of the Grossman–Larson product [15] of unordered trees appearing in the Connes–Kreimer Hopf algebra.

3.3 Hopf algebras

Hopf algebraic structures related to the free D-algebra $\mathrm{D}_{\mathcal{C}} = U(\mathrm{postLie}(\mathcal{C}))$ has been studied in [29, 22, 21]. These Hopf algebras can both be seen as generalizations of the shuffle–concatenation Hopf algebras of free Lie algebras as well as of the Connes–Kreimer Hopf algebra, which is closely related to pre-Lie algebras [7].

Shuffle product. From the classical theory of free Lie algebras, it follows that the derivations $\mathrm{Der}(\mathrm{D}_{\mathcal{C}})$ can be characterized in terms of shuffle products. Define the shuffle product $⧢ : \mathrm{D}_{\mathcal{C}} \otimes \mathrm{D}_{\mathcal{C}} \to \mathrm{D}_{\mathcal{C}}$ on the free D-algebra $\mathrm{D}_{\mathcal{C}}$ by $\mathbb{I}⧢\omega = \omega = \omega⧢\mathbb{I}$ and

$$(\tau_1\omega_1)⧢(\tau_2\omega_2) = \tau_1(\omega_1⧢\tau_2\omega_2) + \tau_2(\tau_1\omega_1⧢\omega_2)$$

for $\tau_1, \tau_2 \in \mathrm{T}$, $\omega_1, \omega_2 \in \mathrm{F}$. Let $(\cdot, \cdot)$ be an inner product on $\mathrm{D}_{\mathcal{C}}$ defined such that the forests form an orthonormal basis, and let the coproduct $\Delta_{⧢}\colon \mathrm{D}_{\mathcal{C}} \to \mathrm{D}_{\mathcal{C}} \otimes \mathrm{D}_{\mathcal{C}}$ be the adjoint of $⧢$.

Proposition 3.13. *The free D-algebra $\mathrm{D}_{\mathcal{C}}$ has the structure of a cocommutative Hopf algebra $\mathcal{H}'_N = \{\mathrm{k}\{\mathrm{F}_{\mathcal{C}}\}, \epsilon, \circ, \eta, \Delta_{⧢}, S\}$ with product being the planar Grossman–Larson product $\circ$ defined in (44), the coproduct $\Delta_{⧢}$ is the adjoint of the shuffle and the unit η and counit ϵ are given as*

$$\begin{aligned} \eta(1) &= \mathbb{I} \\ \epsilon(\mathbb{I}) &= 1, \quad \epsilon(\omega) = 0 \quad \text{for all } \omega \in \mathrm{F}_{\mathcal{C}} \setminus \{\mathbb{I}\}. \end{aligned}$$

The primitive elements are $Prim(\mathcal{H}'_N) = \mathrm{Der}(\mathrm{D}_{\mathcal{C}})$. The antipode S is defined in [29].

Proof. The Hopf algebraic structure (for the dual of $\mathcal{H}'_N$) is proven in [29]. Characterization of the primitive elements follows from the free Lie algebra structure [35]. ☐

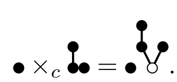
The Hopf algebra $\mathcal{H}_N$, a magmatic view In the study of numerical integration on manifolds it is important to characterize flows and parallel transport on manifolds with connections algebraically. It is convenient to base this on the dual Hopf algebra of $\mathcal{H}'_N$. Let $\mathcal{H}_N = \{\mathrm{k}\{\mathrm{F}_{\mathcal{C}}\}, \epsilon, ⧢, \eta, \Delta_\circ, S\}$ be the commutative Hopf algebra of planar forests, where the product is the shuffle product $⧢$ and the coproduct $\Delta_\circ$ the adjoint of the planar Grossman–Larson product. Various expressions for $\Delta_\circ$ and the antipode S are derived in [29]. Our definition of $\mathrm{F}_{\mathcal{C}}$ and $\mathcal{H}_N$ is rather involved, going via trees and enveloping algebras extending $\rhd$ from derivations, introducing the dipterous composition $\circ$ and dualizing to obtain $\Delta_\circ$. However, both $\mathrm{F}_{\mathcal{C}}$ and the Hopf algebra $\mathcal{H}_N$ can alternatively be defined in a compact, recursive manner. We will review this definition, which is the foundation for a computer implementation of $\mathcal{H}_N$ currently under construction.

Definition 3.14 (Magmatic definition of $\mathrm{F}_{\mathcal{C}}$)**.** Given a set $\mathcal{C}$ we let $\{\times_c\}_{c\in\mathcal{C}}$ be a collection of magmatic products, without any defining relations. Let $\mathbb{I}$ denote the unity and we define $\mathrm{F}_{\mathcal{C}}$ as the free magma generated from $\mathbb{I}$ by the magmatic products.

This definition is related to our previous definition of $\mathrm{F}_{\mathcal{C}}$ by interpreting $\omega_1 \times_c \omega_2$ in terms of forests as

$$\omega_1 \times_c \omega_2 = \omega_1 B_c^+(\omega_2) \tag{45}$$

for all $\omega_1, \omega_2 \in \mathrm{F}_{\mathcal{C}}$, $c \in \mathcal{C}$. Thus, e.g. for $c = \circ$ we have $\mathbb{I} \times_c \mathbb{I} = \circ$, and



Any $\omega \in \mathrm{F}_{\mathcal{C}} \setminus \{\mathbb{I}\}$ can be written uniquely as $\omega = \omega_L \times_c \omega_R$, where $c \in \mathcal{C}$ is the root of the rightmost tree in the forest. We call ω_L and ω_R the left and right parts of ω and c the right root.

Definition 3.15 (Shuffle product)**.** The shuffle product $⧢\colon \mathrm{k}\{\mathrm{F}_{\mathcal{C}}\} \otimes \mathrm{k}\{\mathrm{F}_{\mathcal{C}}\} \to \mathrm{k}\{\mathrm{F}_{\mathcal{C}}\}$ is defined by k-linearity and the recursion

$$\begin{aligned} &\mathbb{I}⧢\omega = \omega⧢\mathbb{I} = \omega, \quad \text{for all } \omega \in \mathrm{F}_{\mathcal{C}}, \\ &v⧢\omega = (v_L⧢\omega) \times_c v_R + (v⧢\omega_L) \times_d \omega_R, \quad \text{for } v = v_L \times_c v_R,\ \omega = \omega_L \times_d \omega_R. \end{aligned} \tag{46}$$

Definition 3.16 (Coproduct.)**.** The coproduct $\Delta_\circ\colon \mathrm{k}\{\mathrm{F}_\mathcal{C}\} \to \mathrm{k}\{\mathrm{F}_\mathcal{C}\}\otimes\mathrm{k}\{\mathrm{F}_\mathcal{C}\}$ is defined by k-linearity and the recursion

$$\begin{aligned}\Delta_\circ(\mathbb{I}) &= \mathbb{I}\otimes\mathbb{I}\\ \Delta_\circ(\omega) &= \omega\otimes\mathbb{I} + \Delta_\circ(\omega_L)\sqcup\!\!\sqcup\!\times_d\Delta_\circ(\omega_R), \quad \text{for } \omega = \omega_L \times_d \omega_R,\end{aligned} \tag{47}$$

where $\sqcup\!\!\sqcup\!\times_d$ is the shuffle product on the left and the magmatic product $\times_d$ on the right:

$$(u_1\otimes u_2)\sqcup\!\!\sqcup\!\times_d(v_1\otimes v_2) := (u_1\sqcup\!\!\sqcup v_1)\otimes(u_2 \times_d v_2).$$

Proposition 3.17 ([29])**.** *$\mathcal{H}_N = \{\mathrm{k}\{\mathrm{F}_\mathcal{C}\}, \epsilon, \sqcup\!\!\sqcup, \eta, \Delta_\circ, S\}$ is a commutative Hopf algebra.*

The Hopf algebra $\mathcal{H}_N$ is the setting for *Lie–Butcher series.*

4 Lie–Butcher series and moving frames

Lie–Butcher series are formal power series for flows and vector fields on manifolds, which combine Butcher series with Lie series. An extensive overview of this field can be found in [22]. We will briefly review the basic definitions and point to some relations between LB-series and moving frames, which have not been discussed elsewhere.

Definition 4.1 (Lie–Butcher series)**.** Let $\mathcal{H}_N^* = \mathrm{Hom}_\mathrm{k}(\mathcal{H}_N, \mathrm{k})$ denote the linear dual space of $\mathcal{H}_N$. An element $\alpha \in \mathcal{H}_N^*$ is called a Lie–Butcher series. We identify α with an infinite series

$$\alpha = \sum_{\omega\in\mathrm{F}_\mathcal{C}} \alpha(\omega)\omega,$$

via a dual pairing $(\cdot,\cdot)\colon \mathcal{H}_N^* \times \mathcal{H}_N \to \mathrm{k}$ defined such that

$$\alpha(\omega) = (\alpha, \omega) \quad \text{for all } \omega \in \mathrm{F}_\mathcal{C}.$$

Define *characters* $G(\mathcal{H}_N) \subset \mathcal{H}_N^*$ and *infinitesimal characters* $\mathfrak{g}(\mathcal{H}_N) \subset \mathcal{H}_N^*$ as

$$G(\mathcal{H}_N) = \{\alpha \in \mathcal{H}_N^*\colon \alpha(\mathbb{I}) = 1,\ \alpha(\omega_1\sqcup\!\!\sqcup\omega_2) = \alpha(\omega_1)\alpha(\omega_2) \text{ for } \omega_1, \omega_2 \in \mathrm{F}_\mathcal{C}\} \tag{48}$$

$$\mathfrak{g}(\mathcal{H}_N) = \{\alpha \in \mathcal{H}_N^*\colon \alpha(\mathbb{I}) = 0,\ \alpha(\omega_1\sqcup\!\!\sqcup\omega_2) = 0 \text{ for } \omega_1, \omega_2 \in \mathrm{F}_\mathcal{C}\setminus\{\mathbb{I}\}\}\,. \tag{49}$$

The convolution product on $\mathcal{H}_N^*$ is defined in the standard way:

$$\alpha\circ\beta(\omega) = \sum_{(\omega)} \alpha(\omega_{(1)})\beta(\omega_{(2)}), \tag{50}$$

using the Sweedler notation. The convolution is the extension of the planar Grossman–Larson product from finite series to infinite series by considering $\mathcal{H}_N^*$ as the projective limit $\mathcal{H}_N^* = \varprojlim \mathcal{N}_k$, where $\mathcal{N}_k = \mathrm{span}\{\omega \in \mathrm{F}\colon |\omega| \le k\}$. Note that the series are formal power series, and convergence in concrete cases, such as flows on manifolds, must be addressed by additional theory.

$G(\mathcal{H}_N)$ with the convolution product forms a group called the character group of $\mathcal{H}_N$, where the unit and the inverse is given by the unit and the antipode in the Hopf algebra $\mathcal{H}_N$, see [22]. In the special case where the post-Lie algebra is pre-Lie, this is the Butcher group, first introduced in [4] as a tool to study numerical integration. More generally, the elements in $\mathfrak{g}(\mathcal{H}_N)$ can represent vector fields and elements in $G(\mathcal{H}_N)$ diffeomorphisms on a manifold $\mathcal{M}$. The convolution represents the composition of diffeomorphisms. Parallel transport of $g \in \mathcal{H}_N^*$ along the $t = 1$ flow of $f \in \mathfrak{g}(\mathcal{H}_N)$ is represented by the exponential of the connection, which using (42) becomes

$$\exp(f\rhd)g := g + f \rhd g + \frac{1}{2} f \rhd (f \rhd g) + \cdots = (\mathbb{I} + f + \frac{1}{2} f\circ f + \cdots) \rhd g = \exp^\circ f \rhd g,$$

where $\exp^\circ$ is the exponential with respect to the composition product. The map $\exp^\circ\colon \mathfrak{g}(\mathcal{H}_N) \to G(\mathcal{H}_N)$ is 1–1, with the inverse given by the eulerian idempotent [22].

We will now be more concrete and discuss basic application of LB-series in numerical analysis of integration on a homogeneous space $\mathcal{M}$. Consider the post-Lie algebra on $\mathcal{M}$ introduced in Section 2.2.3, written compactly as $\mathfrak{g}^{\mathcal{M}} := \Omega^0_H(G,\mathfrak{g}) \simeq \Gamma(G\times_H \mathfrak{g})$, and define the enveloping algebra $U(\mathfrak{g})^{\mathcal{M}} := \Omega^0_H(G,U(\mathfrak{g})) \simeq \Gamma(G\times_H U(\mathfrak{g}))$. Let $\sigma\colon \mathcal{M}\to G$ be a Cartan gauge (left partial moving frame), with $\sigma_*\colon T\mathcal{M}\to G\times_H \mathfrak{g}$ and $\rho_*\colon G\times_H\mathfrak{g}\to T\mathcal{M}$ as defined in Section 2.2.3.

Suppose we want to integrate a differential equation on $\mathcal{M}$ given as

$$y'(t) = F(y(t)),\quad y(0) = y_0 \in \mathcal{M},$$

where $F\in \mathcal{X}\mathcal{M}$. We represent the vector field as $F = \rho_*(f)$, where

$$f = \omega_*(F) \in \mathfrak{g}^{\mathcal{M}}.$$

A numerical method with timestep $0 < h \in \mathbb{R}$ is a diffeomorphism $\Psi_{hf}\colon \mathcal{M}\to\mathcal{M}$, which is not identical to the exact flow Φ_{hf} (but preferably quite close). Many numerical methods are maps which can be represented as LB-series, and the analysis of the LB-series of the numerical solution is a fundamental tool to answer many questions about accuracy and geometric properties of the numerical algorithm. We will not go into details about this here, but merely discuss some different ways a LB-series can be interpreted as a flow Ψ_{hf} on $\mathcal{M}$. Consider $\mathcal{H}_N^*$, where $\mathcal{C}=\{\bullet\}$, and an identification $\bullet\mapsto f\in\mathfrak{g}^{\mathcal{M}}$. This extends uniquely to a map $\mathcal{F}_f\colon \mathcal{H}_N^*\to U(\mathfrak{g})^{\mathcal{M}}$. For a forest $\omega\in \mathrm{F}_{\mathcal{C}}$, $\mathcal{F}_f(\omega)$ is called an *elementary differential operator*. Note that for $t\in\mathbb{R}$ we have $\mathcal{F}_{tf}(\omega) = t^{|\omega|}\mathcal{F}_f(\omega)$. B-series and LB-series are traditionally considered as time-dependent series of differential operators on $\mathbb{R}^n$ and on $\mathcal{M}$ respectively, for $\alpha\in\mathcal{H}_N^*$ given as

$$\mathcal{F}_{tf}(\alpha) = \sum_{\omega\in \mathrm{F}_{\mathcal{C}}} t^{|\omega|}\alpha(\omega)\mathcal{F}_f(\omega).$$

There are (at least) three different ways LB-series are used to represent the numerical method.

Parallel transport. Find $\alpha\in G(\mathcal{H}_N)$ such that

$$\mathcal{F}_{hf}(\alpha)\rhd g = \Psi^*_{hf} g,\qquad \text{for all } g\in U(G)^{\mathcal{M}}, \tag{51}$$

where $\Psi^*_{hf}g$ denotes parallel transport of g along Ψ_{hf}.

Backward error. Find $\beta\in\mathfrak{g}(\mathcal{H}_N)$ such that Ψ_{hf} is exactly the $t=1$ flow of an autonomous vector field $\widetilde{F}_h = \rho_*\widetilde{f}_h$, where

$$\widetilde{f}_h = \mathcal{F}_{hf}(\beta)\in\mathfrak{g}^{\mathcal{M}}. \tag{52}$$

Development. Given a curve $t\mapsto \widetilde{y}(t)\colon I\subset\mathbb{R}\mapsto\mathcal{M}$ and a left (possibly partial) moving frame $\sigma\colon\mathcal{M}\to G$ with Darboux derivative $\omega_\sigma\in\Omega^1(\mathcal{M},\mathfrak{g})$. The curve $\delta\colon I\subset\mathbb{R}\to\mathfrak{g}$ given as $\delta(t) = \omega_\sigma\circ\widetilde{y}'(t)$ is called the *development* of $\widetilde{y}(t)$ with respect to the moving frame[4]. A computation yields:

Proposition 4.2. *Let $\widetilde{y}(t)\in\mathcal{M}$ be an integral curve of a differential equation*

$$\widetilde{y}'(t) = \widetilde{F}(\widetilde{y}(t)),\quad \widetilde{y}(0) = y_0. \tag{53}$$

The development of $\widetilde{y}$ with respect to σ is $\delta(t) = \widetilde{f}(\sigma(\widetilde{y}(t)))$, where $\widetilde{f} = \sigma_*\widetilde{F}\in\mathfrak{g}^{\mathcal{M}}\simeq\Omega^0_H(G,\mathfrak{g})$. Equivalently

$$\delta(t) = \Psi^*_{t\widetilde{f}}\widetilde{f}(\sigma(y_0)), \tag{54}$$

where $\Psi^*_{t\widetilde{f}}\widetilde{f}$ denotes parallel transport of $\widetilde{f}$ along the flow of itself.

[4]Example: The classical Frenet–Serret frame of a curve in $\mathbb{R}^3$ is the development with respect to the full moving frame obtained by prolongation of the Euclidean motion group acting on $\mathbb{R}^3$.

We can represent the curve in $\widetilde{y}(t)$ in (53) algebraically by finding $\gamma \in \mathfrak{g}(\mathcal{H}_N)$ such that

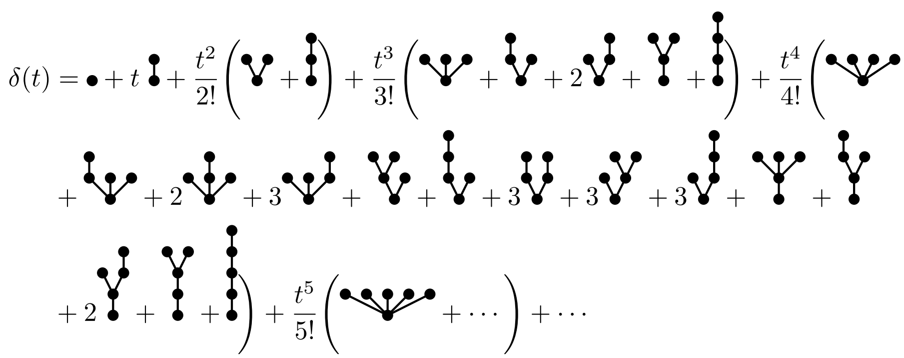
$$\delta(t) = \frac{\partial}{\partial t}\mathcal{F}_{tf}(\gamma)(y_0) \tag{55}$$

is the development of $\widetilde{y}(t)$.

Remark 4.3. The three ways of representing the numerical method, as $\alpha \in G(\mathcal{H}_N)$ representing parallel transport along the numerical flow Ψ_{hf}, as $\beta \in \mathfrak{g}(\mathcal{H}_N)$ representing the backward error vector field $\widetilde{F}$ and as $\gamma \in \mathfrak{g}(\mathcal{H}_N)$ representing the development of the integral curve of the numerical flow, are all discussed in [22]. However, the third representation γ is presented differently, and the close relationship between this representation and moving frames is therefore not obvious.

The algebraic relationship between α, β and γ is discussed in [22]. We find α from β by applying $\exp^\circ$ and β from α via the eulerian idempotent in $\mathcal{H}_N$. From α we find γ by applying the Dynkin idempotent in $\mathcal{H}_N$, and conversely α is found from γ by a formula involving certain non-commutative Bell polynomials.

Remark 4.4. Consider the *exact* flow Φ_{tf} of the differential equation $y' = F(y)$. In this case, obviously, $\beta = \bullet$. From this we can compute explicitly the development $\delta(t) \in \mathfrak{g}$ of the solution curve $y(t) \in \mathcal{M}$, see [22], yielding



For instance, given a curve $y(t) \in \mathbb{R}^3$ where the moving frame is obtained by prolongation of the euclidean motion group acting on $\mathbb{R}^3$, this expresses the Taylor expansion of the classical euclidean curvature and torsion of the space curve $y(t)$, in terms of elementary differentials of f.

Concluding remarks

The theory in this paper opens several interesting areas of further investigation. We are convinced that post-Lie algebraic structures will find applications in many areas also outside numerical analysis, such as stochastic differential equations, control theory and sub-Riemannian geometry. Within numerical analysis, the paper points to different ways of applying moving frame techniques in geometrically 'nice' ways of choosing isotropy in Lie group integration. This still has to be investigated numerically and computationally.

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