

The Universal Pre-Lie–Rinehart Algebras of Aromatic Trees



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Abstract We organize colored aromatic trees into a pre-Lie–Rinehart algebra (i.e., a flat torsion-free Lie–Rinehart algebra) endowed with a natural trace map, and show the freeness of this object among pre-Lie–Rinehart algebras with trace. This yields the algebraic foundations of aromatic B-series.

Keywords Free pre-Lie algebra · Lie–Rinehart algebra · Aromatic tree · Trace map

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1 Introduction

In the analysis of structure preserving discretisation of differential equations, series developments indexed by trees are fundamental tools. The relationship between algebraic and geometric properties of such series has been extensively developed in recent years. The mother of all these series is B-series, introduced the seminal works of John Butcher in the 1960s [2, 3]. However, the fundamental idea of denoting analytical forms of differential calculus with trees was conceived already a century earlier by Cayley [4].

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A modern understanding of B-series stems from the algebra of flat and torsion-free connections naturally associated with locally Euclidean geometries. The vector fields on \mathbb{R}^d form a *pre-Lie* algebra L with product given by the connection \triangleright in (9). The *free pre-Lie algebra* is the vector space spanned by rooted trees with tree grafting as the product [5]. A B-series can be defined as an element B_a in the graded completion of the free pre-Lie algebra, yielding infinite series of trees with coefficients $a(t) \in \mathbb{R}$ for each tree t . By the universal property, a mapping $\bullet \mapsto f \in L$, sending the single node tree to a vector field, extends uniquely to a mapping $B_a \mapsto B_a(f)$, where $B_a(f)$ is an infinite series of vector fields

$$B_a(f) = a(\bullet)f + a(\downarrow)f \triangleright f + a(\uparrow)(f \triangleright f) \triangleright f + a(\vee)(f \triangleright (f \triangleright f) - (f \triangleright f) \triangleright f) + \dots$$

On the geometric side, it has recently been shown [11] that B-series are intimately connected with (strongly) affine equivariant families of mappings of vector fields on Euclidean spaces. An infinite family of smooth mappings $\Phi_n: \mathcal{X}\mathbb{R}^n \rightarrow \mathcal{X}\mathbb{R}^n$ for $n \in \mathbb{N}$ has a unique B-series expansion B_a if and only if the family respects all affine linear mappings $\varphi(x) = Ax + b: \mathbb{R}^m \rightarrow \mathbb{R}^n$. This means that $f \in \mathcal{X}\mathbb{R}^n$ being φ -related to $g \in \mathcal{X}\mathbb{R}^m$ implies $\Phi_n(f)$ being φ -related to $\Phi_m(g)$. Subject to convergence of the formal series we have $\Phi_n(f) = B_a(f)$.

Aromatic B-series is a generalization which was introduced for the study of volume preserving integration algorithms [6, 10], more recently studied in [1, 12]. The divergence of a tree is represented as a sum of “aromas”, graphs obtained by joining the tree root to any of the tree’s nodes. Aromas are connected directed graphs where each node has one outgoing edge. They consist of one cyclic sub-graph with trees attached to the nodes in the cycle. Aromatic B-series are indexed by *aromatic trees*, defined as a tree multiplied by a number of aromas.

The geometric significance of aromatic B-series is established in [12]. Consider a smooth local mapping of vector fields on a finite-dimensional vector space, $\Phi: \mathcal{X}\mathbb{R}^d \rightarrow \mathcal{X}\mathbb{R}^d$. “Local” means that the support is non-increasing, $\text{supp}(\Phi(f)) \subset \text{supp}(f)$. Such a mapping can be expanded in an aromatic B-series if and only if it is equivariant with respect to all affine (invertible) diffeomorphisms $\varphi(x) = Ax + b: \mathbb{R}^d \rightarrow \mathbb{R}^d$. An equivalent formulation of this result is in terms of the pre-Lie algebra $L = (\mathcal{X}\mathbb{R}^d, \triangleright)$ defined in the Canonical example of Sect. 2.4. The isomorphisms of L are exactly the pullback of vector fields by affine diffeomorphisms $\xi(f) = A^{-1}f \circ \varphi$, hence,

Theorem 1.1 *Let L be the canonical pre-Lie algebra of vector fields on a finite-dimensional euclidean space. A smooth local mapping $\Phi: L \rightarrow L$ can be expanded in an aromatic B-series if and only if $\Phi \circ \xi = \xi \circ \Phi$ for all pre-Lie isomorphisms $\xi: L \rightarrow L$.*

This result shows that aromatic B-series have a fundamental geometric significance. The question to be addressed in this paper is to understand their algebraic foundations. *In what sense can aromatic B-series be defined as a free object in some*

category? Trees represent vector fields and aromas represent scalar functions on a domain. The derivation of a scalar field by a vector field is modeled by grafting the tree on the aromas. A suitable geometric model for this is pre-Lie algebroids, defined as Lie algebroids with a flat and torsion-free connection [13]. Lie algebroids are vector bundles on a domain together with an “anchor map”, associating sections of the vector bundle with derivations of the ring of smooth scalar functions.

The algebraic structure of Lie algebroids is captured through the notion of *Lie–Rinehart algebras*; the aromatic trees form a module over the commutative ring of aromas, acting as derivations of the aromas through the anchor map given by grafting. However, it turns out that the operations of divergence of trees and the grafting anchor map are not sufficient to generate all aromas. Instead, a sufficient set of operations to generate everything is obtained by the graph versions of taking covariant exterior derivatives of vector fields and taking compositions and traces of the corresponding endomorphisms. These operations are well defined on any finite-dimensional pre-Lie algebroid. However, for the Lie–Rinehart algebra of aromas and trees the trace must be defined more carefully, since, e.g., the identity endomorphism on aromatic trees does not have a well-defined trace.

In this paper, we define the notion of *tracial pre-Lie–Rinehart algebras* and show that the aromatic B-series arise from the free object in this category.

2 Lie–Rinehart and Pre-Lie–Rinehart Algebras

Lie–Rinehart algebras were introduced by George S. Rinehart in 1963 [14]. They have been thoroughly studied by several authors since then, in particular by J. Hübschmann who emphasized their important applications in Poisson geometry [8]. After a brief reminder on these structures, we introduce pre-Lie–Rinehart algebras which are Lie–Rinehart algebras endowed with a flat and torsion-free connection. We also introduce the mild condition of traciality for Lie–Rinehart algebras. The main fact (Corollary 2.8) states the traciality of any finite-dimensional Lie algebroid over a smooth manifold.

2.1 Reminder on Lie–Rinehart Algebras

Let \mathbf{k} be a field, and let R be a unital commutative \mathbf{k} -algebra. Recall that a *Lie–Rinehart algebra* over R consists of an R -module L and an R -linear map

$$\rho : L \mapsto \text{Der}_{\mathbf{k}}(R, R)$$

(the *anchor map*), such that

- L is a \mathbf{k} -bilinear Lie algebra with bracket $\llbracket -, - \rrbracket$,

- The anchor map ρ is a homomorphism of Lie algebras,
- For $f \in R$ and $X, Y \in L$ the Leibniz rule holds:

$$\llbracket X, fY \rrbracket = (\rho(X)f)Y + f\llbracket X, Y \rrbracket. \tag{1}$$

Remark 2.1 In the original article [14], G.Rinehart does not state that the anchor map should be a Lie algebra homomorphism. However, all articles on Lie–Rinehart algebras from the last two decades seem to require this. In the much-cited article by J. Hübschmann [8] from 1990 it is not quite clear whether this is required, but again in later articles like [9] from 1998 and onwards, he explicitly requires the anchor map to be a Lie algebra homomorphism.

If one does not require the anchor map to be a Lie algebra homomorphism, then if $\text{Ann}(L)$ is the annihilator of L in R , it is easy to see that L will be a Lie–Rinehart algebra over $R/\text{Ann}(L)$, with the anchor map being a Lie algebra homomorphism. In particular, for Lie algebroids (see Sect. 2.2), then $\text{Ann}(L) = 0$, and the anchor map will automatically be a Lie algebra homomorphism.

A *homomorphism* $(\alpha, \gamma) : (L, R) \rightarrow (K, S)$ of Lie–Rinehart algebras consists of a Lie \mathbf{k} -algebra homomorphism α and \mathbf{k} -algebra homomorphism γ :

$$\alpha : L \rightarrow K, \quad \gamma : R \rightarrow S$$

such that for $f \in R$ and $X \in L$:

- $\alpha(fX) = \gamma(f)\alpha(X)$,
- $\gamma((\rho_L(X) \cdot f) = \rho_K(\alpha(X)) \cdot \gamma(f)$.

A *connection* on a R -module N is a R -linear map

$$\begin{aligned} \nabla : L &\longrightarrow \text{End}_{\mathbf{k}}(N) \\ X &\longmapsto \nabla_X \end{aligned}$$

such that

$$\nabla_X(fY) = (\rho(X).f)Y + f\nabla_X Y.$$

The curvature of the connection is given by

$$R(X, Y) := [\nabla_X, \nabla_Y] - \nabla_{\llbracket X, Y \rrbracket}.$$

If $N = L$, the torsion of the connection is given by

$$T(X, Y) := \nabla_X Y - \nabla_Y X - \llbracket X, Y \rrbracket.$$

The curvature vanishes if and only if N is a module over the Lie algebra L (via ∇). In that case, N is called a *module* over the Lie–Rinehart algebra (L, R) . This is equivalent to the map ∇ being a homomorphism of Lie algebras where $\text{End}_{\mathbf{k}}(N)$ is

endowed with the commutator as the Lie bracket. In particular, the \mathbf{k} -algebra R is a module over the Lie–Rinehart algebra (L, R) .

Let N be a R -module endowed with a connection ∇ with respect to the Lie–Rinehart algebra (L, R) . The R -module $\text{Hom}_R(N, N)$ can be equipped with the connection defined by (where $u \in \text{Hom}_R(N, N)$, $X \in L$ and $Y \in N$)

$$(\nabla_X u)(Y) := \nabla_X(u(Y)) - u(\nabla_X Y). \tag{2}$$

This connection verifies the Leibniz rule

$$\nabla_X(u \circ v) = \nabla_X u \circ v + u \circ \nabla_X v, \tag{3}$$

as can be immediately checked.

Proposition 2.2 *If the connection ∇ on N is flat, the corresponding connection ∇ on $\text{Hom}_R(N, N)$ given by (2) is also flat.*

Proof If ∇ is flat on N , it is well known that the corresponding L -module structure on N yields a L -module structure on $\text{Hom}_R(N, N)$ via (2), hence a flat connection. To be concrete, a direct computation using (2) yields

$$\begin{aligned} ([\nabla_X, \nabla_Y] - \nabla_{[[X, Y]])u}(Z) &= \nabla_X(\nabla_Y(u(Z)) - u(\nabla_Y Z)) - \nabla_Y(u(\nabla_X Z) + u(\nabla_Y \nabla_X Z)) \\ &\quad - \nabla_Y(\nabla_X(u(Z)) - u(\nabla_X Z)) + \nabla_X(u(\nabla_Y Z) - u(\nabla_X \nabla_Y Z)) \\ &\quad - \nabla_{[[X, Y]]}(u(Z)) + u(\nabla_{[[X, Y]]}Z) \\ &= ([\nabla_X, \nabla_Y] - \nabla_{[[X, Y]])u(Z) - u([\nabla_X, \nabla_Y] - \nabla_{[[X, Y]])Z). \end{aligned}$$

□

Definition 2.3 Let (L, R) be a Lie–Rinehart algebra. An R -module N is *tracial* if there exists a connection ∇ on N and a R -linear map $\tau : \text{Hom}_R(N, N) \rightarrow R$ such that

- $\tau(\alpha \circ \beta) = \tau(\beta \circ \alpha)$ (trace property),
- τ is compatible with the connection and the anchor, i.e., for any $X \in L$ and $\alpha \in \text{Hom}_R(N, N)$ we have

$$\tau(\nabla_X \alpha) = \rho(X) \cdot \tau(\alpha). \tag{4}$$

If N is a module over (L, R) , this means that τ is a homomorphism of (L, R) -modules.

2.2 Aside on Manifolds and Lie Algebroids

Recall that a *Lie algebroid* on a smooth manifold M is a Lie–Rinehart algebra over the \mathbb{C} -algebra of smooth \mathbb{C} -valued functions on M . It is given by the smooth sections of a vector bundle E , and the anchor map comes from a vector bundle morphism from E to the tangent bundle TM . The terminology “anchor map” and the notation ρ are often used for the bundle morphism in the literature on Lie algebroids.

Theorem 2.4 *Let M be a finite-dimensional smooth manifold, and let V be a Lie algebroid on M . Any finite-dimensional vector bundle W endowed with a V -connection is tracial, i.e., the $C^\infty(M)$ -module N of smooth sections of W is tracial with respect to the Lie–Rinehart algebra L of sections of V .*

Proof We can consider the fiberwise trace on the algebra $\text{Hom}_{C^\infty(M)}(N, N)$ of smooth sections of the endomorphism bundle $\text{End } W$: it is given fiber by fiber by the ordinary trace of an endomorphism of a finite-dimensional vector space. The trace property is obviously verified.

To prove the invariance property (4), choose two V -connections ∇^1 and ∇^2 on W . It is well known (and easily verified) that $c_X := \nabla_X^2 - \nabla_X^1$ belongs to $\text{Hom}_{C^\infty(M)}(N, N)$, hence is a section of the vector bundle $\text{End}(W)$. Now for any section φ of $\text{End}(W)$ we have for any $X \in L$ and $\alpha \in N$:

$$\begin{aligned} (\nabla_X^2 \varphi)(\alpha) &= \nabla_X^2(\varphi(\alpha)) - \varphi(\nabla_X^2(\alpha)) \\ &= (\nabla_X^1 + c_X)(\varphi(\alpha)) - \varphi(\nabla_X^1(\alpha) + c_X(\alpha)) \\ &= (\nabla_X^1 \varphi)(\alpha) + [c_X, \varphi](\alpha). \end{aligned}$$

The trace of a commutator vanishes, hence we get

$$\text{Tr}(\nabla_X^2 \varphi) = \text{Tr}(\nabla_X^1 \varphi). \quad (5)$$

In other words, the trace of $\nabla_X \varphi$ does not depend on the choice of the connection. We can locally (i.e., on any open chart of M trivializing the vector bundle W) choose the canonical flat connection with respect to a coordinate system, namely

$$\nabla_X^0 \alpha := (\rho(X)\alpha_1, \dots, \rho(X)\alpha_p)$$

for which (4) is obviously verified (here p is the dimension of the fiber bundle W). Hence, from (5), we get that (4) is verified for any choice of connection ∇ . \square

2.3 Tracial Lie–Rinehart Algebras

When the module N is the Lie–Rinehart algebra itself, it may be convenient to restrict the algebra on which the trace is defined:

Definition 2.5 Suppose that $N = L$, and let us introduce the \mathbf{k} -linear operator

$$d : L \longrightarrow \text{Hom}_R(L, L)$$

defined by

$$dX(Z) := \nabla_Z X. \tag{6}$$

Let the *algebra of elementary R -module endomorphisms* be the R -module subalgebra of $\text{Hom}_R(L, L)$ generated by $\{\nabla_{Y_1} \cdots \nabla_{Y_n} dX : X, Y_1, \dots, Y_n \in L\}$. It will be denoted by $El_R(L, L)$.

Remark 2.6 The Leibniz rule (3) implies that the (L, R) -module structure on $\text{Hom}_R(L, L)$ (via the connection ∇) restricts to $El_R(L, L)$, making this an (L, R) -submodule of $\text{Hom}_R(L, L)$.

Definition 2.7 A Lie–Rinehart algebra L over the unital commutative \mathbf{k} -algebra R is *tracial* if there exists a connection ∇ on L and a R -linear map $\tau : El_R(L) \rightarrow R$ such that

- $\tau(\alpha \circ \beta) = \tau(\beta \circ \alpha)$ (trace property),
- τ is a homomorphism of L -modules, i.e., for any $X \in L$ and $\alpha \in El_R(L)$ we have

$$\tau(\nabla_X \alpha) = \rho(X) \cdot \tau(\alpha). \tag{7}$$

In this case, the *divergence* on L is the composition $\text{Div} = \tau \circ d$ of

$$L \xrightarrow{d} El_R(L) \xrightarrow{\tau} R.$$

Corollary 2.8 Any finite-dimensional Lie algebroid is tracial for its natural canonical trace map.

Proof It is an immediate consequence of Theorem 2.4. □

We also have an analog for the differential of a function, the first term in the De Rham complex:

$$d : R \rightarrow \text{Hom}_R(L, R), \quad f \mapsto (X \mapsto \rho(X)(f)).$$

Given an element Y in L , we get a map in $\text{Hom}_R(L, L)$ denoted $df \cdot X$:

$$X \mapsto \rho(X)(f) \cdot Y. \tag{8}$$

2.4 Pre-Lie–Rinehart Algebras

Definition 2.9 A *pre-Lie–Rinehart algebra* is a Lie–Rinehart algebra L endowed with a flat torsion-free connection

$$\nabla : L \rightarrow \text{End}_{\mathbf{k}}(L, L).$$

We have then, with the notation $X \triangleright Y := \nabla_X Y$:

- $\llbracket X, Y \rrbracket = X \triangleright Y - Y \triangleright X$,
- $X \triangleright (Y \triangleright Z) - (X \triangleright Y) \triangleright Z = Y \triangleright (X \triangleright Z) - (Y \triangleright X) \triangleright Z$ (left pre-Lie relation).

A *module* over the pre-Lie–Rinehart algebra is the same as a module over the underlying Lie–Rinehart algebra. If N is a module and n and element, we write $X \triangleright n$ for $\nabla_X n$. In particular, for $f \in R$, the action of the anchor map $\rho(X) \cdot f$ is written $X \triangleright f$.

Canonical example [4]: Let $\mathbf{k} = \mathbb{R}$, let $R = C^\infty(\mathbb{R}^d)$ and let L be the space of smooth vector fields on \mathbb{R}^d . Let $X, Y \in L$, which are written in coordinates:

$$X = \sum_{i=1}^d f^i \partial_i, \quad Y = \sum_{j=1}^d g^j \partial_j.$$

Then

$$X \triangleright Y = \sum_{j=1}^d \left(\sum_{i=1}^d f^i (\partial_i g^j) \right) \partial_j. \tag{9}$$

For a vector field $X = \sum_{i=1}^d f^i \partial_i$, the endomorphism dX sends

$$\sum_{i=1}^d g^j \partial_j \mapsto \sum_{i,j=1}^d g^j \partial_j (f^i) \partial_i.$$

In particular $\partial_j \mapsto \sum_{i=1}^d \partial_j (f^i) \partial_i$, so the trace of dX is the divergence $\sum_{i=1}^d \partial_i (f^i)$.

Proposition 2.10 *In a pre-Lie–Rinehart algebra L , the algebra $E\ell_R(L)$ of elementary module homomorphisms is generated by $\{dX : X \in L\}$.*

Proof In view of Definition 2.5, we first show that for any $X, Y \in L$, the endomorphism $\nabla_Y(dX)$ is obtained by linear combinations of products of endomorphisms of the form dZ , $Z \in L$. It derives immediately from the left pre-Lie relation, via the following computation (recall (2)):

$$\begin{aligned} (\nabla_Y dX)(Z) &= \nabla_Y(dX(Z)) - dX(\nabla_Y Z) \\ &= \nabla_Y(Z \triangleright X) - (\nabla_Y Z) \triangleright X \\ &= Y \triangleright (Z \triangleright X) - (Y \triangleright Z) \triangleright X \\ &= Z \triangleright (Y \triangleright X) - (Z \triangleright Y) \triangleright X \\ &= (d(Y \triangleright X) - dX \circ dY)(Z). \end{aligned}$$

To then show further that $\nabla_{Y_1} \nabla_{Y_2} dX$ is a linear combination of products of endomorphisms, we use the Leibniz rule

$$\nabla_{Y_1}(dX \circ dY_2) = (\nabla_{Y_1} dX) \circ dY_2 + dX \circ \nabla_{Y_1} dY_2.$$

In this way we may continue. □

Proposition 2.11 *Let L be a pre-Lie–Rinehart algebra.*

a. *For any $X, Y \in L$:*

$$X \triangleright dY = d(X \triangleright Y) - dY \circ dX.$$

b. *For $f \in R$ (recall (8) for $df \cdot Y$):*

$$X \triangleright (df \cdot Y) = df \cdot (X \triangleright Y) + d(X \triangleright f) \cdot Y - (df \cdot Y) \circ dX.$$

Proof a. Using (2):

$$\begin{aligned} (X \triangleright dY)(Z) &= X \triangleright (Z \triangleright Y) - (X \triangleright Z) \triangleright Y \\ &= Z \triangleright (X \triangleright Y) - (Z \triangleright X) \triangleright Y \\ &= d(X \triangleright Y)(Z) - dY \circ dX(Z) \end{aligned}$$

b. Again using (2) this map sends Z to

$$\begin{aligned} (X \triangleright (df \cdot Y))(Z) &= X \triangleright ((Z \triangleright f)Y) - (df \cdot Y)(X \triangleright Z) \\ \text{(connection property)} &= (X \triangleright (Z \triangleright f))Y + (Z \triangleright f)(X \triangleright Y) - ((X \triangleright Z) \triangleright f)Y \\ &= (Z \triangleright (X \triangleright f))Y - ((Z \triangleright X) \triangleright f)Y + (Z \triangleright f)(X \triangleright Y). \end{aligned}$$

This is the map:

$$d(X \triangleright f) \cdot Y - (df \cdot Y) \circ dX + df \cdot (X \triangleright Y).$$

□

Definition 2.12 Let (L, R) and (K, S) be tracial pre-Lie–Rinehart algebras, and $(\alpha, \gamma) : (L, R) \rightarrow (K, S)$ a homomorphism of pre-Lie–Rinehart algebras. For each $X \in L$ there is a commutative diagram:

$$\begin{array}{ccc} L & \xrightarrow{dX} & L \\ \alpha \downarrow & & \downarrow \alpha \\ K & \xrightarrow{d\alpha(X)} & K. \end{array}$$

An elementary endomorphism $\phi : L \rightarrow L$ is an R -linear combination of compositions $dX_1 \circ \cdots \circ dX_r$. It induces an elementary endomorphism $\psi : K \rightarrow K$ which

is the corresponding R -linear combination of compositions of $d\alpha(X_i)$'s. *Note:* This ψ may not be unique since expressing ϕ as an R -linear combination of compositions may not be done uniquely. For instance it could be that dX is the zero map, while $d\alpha(X)$ is *not* the zero map.

The homomorphism (α, γ) is a *homomorphism of tracial pre-Lie algebras* if for each elementary endomorphism ϕ the trace of ϕ maps to the trace of ψ : $\gamma(\tau\phi) = \tau\psi$. (This is regardless of which ψ that corresponds to ϕ .)

3 Aromatic Trees

In this section we define rooted trees, aromas and aromatic trees, the latter being the relevant combinatorial objects for building up the free pre-Lie–Rinehart algebra.

3.1 Rooted Trees and Aromas

Let \mathcal{C} be a finite set, whose elements we shall think of as colors. We introduce some notation:

Definition 3.1 $T_{\mathcal{C}}$ is the vector space freely generated by rooted trees whose vertices are colored with elements of \mathcal{C} . We denote by $V_{\mathcal{C}}$ the vector space freely generated by pairs (v, t) where t is a \mathcal{C} -colored tree and v is a vertex of t .

There is an injective map

$$V_{\mathcal{C}} \rightarrow \text{End}_{\mathbf{k}}(T_{\mathcal{C}}), \quad (v, t) \mapsto (s \mapsto s \triangleright_v t)$$

where \triangleright_v is grafting the root of s on the vertex v .

The composition $\beta \circ \alpha$ of maps β, α in $\text{End}_{\mathbf{k}}(T_{\mathcal{C}})$ induces a multiplication (composition) \circ on $V_{\mathcal{C}}$ given by $(v, t) \circ (u, s) = (u, s \triangleright_v t)$. We may then identify $V_{\mathcal{C}}$ as a \mathbf{k} -subalgebra of $\text{End}_{\mathbf{k}}(T_{\mathcal{C}})$. Then

$$d : T_{\mathcal{C}} \rightarrow \text{End}_{\mathbf{k}}(T_{\mathcal{C}}), \quad t \mapsto \sum_{v \in t} (v, t). \tag{10}$$

Definition 3.2 A connected directed graph with vertices colored by \mathcal{C} and where each vertex has precisely one outgoing edge is called a \mathcal{C} -colored *aroma* or just an *aroma* since we will only consider this situation. It consists of a central cycle with trees attached to the vertices of this cycle. The arrows of each tree are oriented towards the cycle, which will be oriented counterclockwise by convention when an aroma is drawn in the two-dimensional plane. We let $A_{\mathcal{C}}$ be the vector space freely generated by \mathcal{C} -colored aromas. See Fig. 1 where the first four connected graphs are aromas.

Now consider the linear map

$$\tau : V_C \longrightarrow A_C \tag{11}$$

which maps the pair (v, t) to an aroma by joining the root of t to the vertex v .

Lemma 3.3 *The vector space A_C spanned by the aromas can be naturally identified with the quotient $V_C/[V_C, V_C]$, where $[V_C, V_C]$ is the vector space spanned by the commutators in V_C , so that the map τ becomes the natural projection from V_C onto $V_C/[V_C, V_C]$.*

Proof An aroma has a unique interior cycle. Let r_1, \dots, r_n be the vertices on this cycle. At r_{j-1} there is a tree t'_j with root r_{j-1} . Let t_j be this tree with r_{j-1} grafted onto r_j , so r_j is the root of t_j . We may write the aroma as

$$a = \tau((r_1, t_1) \circ \dots \circ (r_n, t_n)). \tag{12}$$

and this is invariant under any cyclic permutation of the elements (r_i, t_i) . On the other hand, any tree t with marked point v admits the decomposition:

$$(v, t) = (v_1, t_1) \circ \dots \circ (v_j, t_j) \tag{13}$$

where v_1 (resp. v_j) is the root of t (resp. the marked vertex v) and (v_1, v_2, \dots, v_j) is the path from the root to v in t . Each vertex v_i of this path is the root of the tree t_i . Now if $(v', t') = (v_{j+1}, t_{j+1}) \circ \dots \circ (v_{j+k}, t_{j+k})$ is another tree with marked vertex, we have

$$\begin{aligned} (v, t) \circ (v', t') &= (v_1, t_1) \circ \dots \circ (v_{j+k}, t_{j+k}) \text{ and} \\ (v', t') \circ (v, t) &= (v_{j+1}, t_{j+1}) \circ \dots \circ (v_{j+k}, t_{j+k}) \circ (v_1, t_1) \circ \dots \circ (v_j, t_j). \end{aligned}$$

The trace property $\tau((v, t) \circ (v', t')) = \tau((v', t') \circ (v, t))$ is then obvious by cyclic invariance of the decomposition of an aroma. Now any aroma is the image by τ of at most n trees with marked points, where n is the length of the cycle. It is clear that two such trees admit the same decomposition as above modulo cyclic permutation, which implies that they differ by a commutator. Now, we have to prove that any element $T \in V_C$ with $\tau(T) = 0$ is a linear combination of commutators. Decomposing T in the basis of trees with one marked points:

$$\begin{aligned} T &= \sum_{(v,t)} \alpha_{(v,t)}(v, t) \\ &= \sum_a \sum_{(v,t), \tau(v,t)=a} \alpha_{(v,t)}(v, t), \end{aligned}$$

from $\tau(T) = 0$ we get $\sum_{(v,t), \tau(v,t)=a} \alpha_{(v,t)} = 0$ for any aroma a . Hence, the sum $\sum_{(v,t), \tau(v,t)=a} \alpha_{(v,t)}(v, t)$ is a sum of commutators for any aroma a , which proves that T is also a sum of commutators. \square

The canonical embedding of \mathcal{C} into $T_{\mathcal{C}}$ is given by $c \mapsto \bullet_c$. It is well-known [5, 7] that $T_{\mathcal{C}}$ with grafting as the operation \triangleright is the free pre-Lie algebra on the set \mathcal{C} . Then $(T_{\mathcal{C}}, k)$ becomes a pre-Lie–Rinehart algebra, with anchor map zero.

Lemma 3.4 *The algebra $El_k(T_{\mathcal{C}})$ of elementary module morphisms of Definition 2.5, for the pre-Lie–Rinehart algebra $(T_{\mathcal{C}}, k)$, coincides with the algebra $V_{\mathcal{C}}$ of trees with one marked point.*

Proof Since $dt = \sum_{v \in t} (v, t)$ by (10) we need only to show that each marked tree (v, t) is in $El_k(T_{\mathcal{C}})$. Let t_v be the subtree of t which has v as root. If v is not the root of t , it is attached to a node w . Take t_v away from t and let t' be the resulting tree. Then $(v, t) = (w, t') \circ (v, t_v)$. We now show by induction on the number of nodes of (i) $|t|$ and (ii) $|t_v|$, that (v, t) is in $El_k(T_{\mathcal{C}})$.

- (i) If the marked tree is (\bullet_c, \bullet_c) , then it is $d(\bullet_c)$ and is in $El_k(T_{\mathcal{C}})$.
- (ii) If v is a root, then

$$d(t) = (v, t) + \sum_{w \neq v} (w, t).$$

The left term is in $El_k(T_{\mathcal{C}})$, and the right term also by induction.

- (iii) If v is not a root then both (w, t') and (v, t_v) are in $El_k(T_{\mathcal{C}})$ by induction, and so also (v, t) . \square

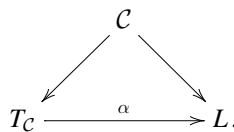
As a result $V_{\mathcal{C}}$ is a $T_{\mathcal{C}}$ -module by grafting:

$$s \triangleright (v, t) = (v, s \triangleright t),$$

where the latter is a sum of pairs (v, t_i) coming from that $s \triangleright t$ is a sum of trees t_i . The aromas $A_{\mathcal{C}}$ also form a $T_{\mathcal{C}}$ -module by grafting the trees on all vertices in an aroma. Lastly, the map $\tau : V_{\mathcal{C}} \rightarrow A_{\mathcal{C}}$ is a $T_{\mathcal{C}}$ -module map.

3.2 The Free Pre-Lie Algebra

Let L be a pre-Lie algebra over the field \mathbf{k} . The pre-Lie algebra $T_{\mathcal{C}}$ has the universal property that given any map $\mathcal{C} \rightarrow L$ there is a unique morphism of pre-Lie algebras $T_{\mathcal{C}} \rightarrow L$ such that the diagram below commutes:



Theorem 3.5 *Let L be a tracial pre-Lie–Rinehart algebra over the \mathbf{k} -algebra R , with trace map $\text{End}_R(L, L) \xrightarrow{\tau} R$.*

- a. *Given a set map $\psi : \mathcal{C} \rightarrow L$, the unique pre-Lie algebra homomorphism $T_{\mathcal{C}} \xrightarrow{\alpha} L$ such that $\alpha(\bullet_c) = \psi(c)$ for any $c \in \mathcal{C}$ induces a unique morphism of associative algebras $V_{\mathcal{C}} \xrightarrow{\beta} \text{El}_R(L)$ such that the following diagram commutes:*

$$\begin{array}{ccc} T_{\mathcal{C}} & \xrightarrow{d} & V_{\mathcal{C}} \\ \alpha \downarrow & & \beta \downarrow \\ L & \xrightarrow{d} & \text{El}_R(L). \end{array} \tag{14}$$

- b. *Moreover, there is a unique linear map γ extending the diagram (14) to a commutative diagram*

$$\begin{array}{ccccc} T_{\mathcal{C}} & \xrightarrow{d} & V_{\mathcal{C}} & \xrightarrow{\tau} & A_{\mathcal{C}} \\ \alpha \downarrow & & \beta \downarrow & & \gamma \downarrow \\ L & \xrightarrow{d} & \text{El}_R(L) & \xrightarrow{\tau} & R. \end{array}$$

- c. *These maps fulfill the following for an aroma a , tree t , and $\phi \in V_{\mathcal{C}} \subseteq \text{End}_{\mathbf{k}}(T_{\mathcal{C}})$:*

- i. $\beta(\phi)(\alpha(t)) = \alpha(\phi(t))$,
- ii. $\beta(t \triangleright \phi) = \alpha(t) \triangleright \beta(\phi)$,
- iii. $\gamma(t \triangleright a) = \alpha(t) \triangleright \gamma(a)$.

Proof Part a. Any tree (v, t) with one marked point different from the root can be written as

$$(v, t) = (v'', t'') \circ (v, t'), \tag{15}$$

where the associative product on $V_{\mathcal{C}}$ has been described in Sect. 3.1. Here, t' is any upper sub tree containing the marked vertex v , and t'' is the remaining tree, on which the marked vertex v'' comes from the vertex immediately below the root of t' . We then proceed by induction on the number of vertices: if t is reduced to the vertex v colored by $c \in \mathcal{C}$, we obviously have

$$\beta(v, t)(x) = d\alpha(\bullet_c)(x) = x \triangleright \alpha(\bullet_c) \tag{16}$$

for any $x \in L$. Suppose that the map β has been defined for any tree up to n vertices. Now if t has $n + 1$ vertices and one marked vertex v different from the root, we must have:

$$\beta(v, t) = \beta((v'', t'') \circ (v, t')) = \beta(v'', t'') \circ \beta(v, t'). \tag{17}$$

It is easily seen that this does not depend on the choice of the decomposition. Indeed, if v is not the root of t' , then $(v, t') = (v', s')(v, s)$ where s is the subtree with root v ,

and s' is the remaining tree inside t' . The vertex v' comes from the vertex immediately below v in t' . We have then

$$\beta(v, t) = \beta(v'', t'') \circ \beta(v', s') \circ \beta(v, s) = \beta(v', \tilde{t}) \circ \beta(v, s)$$

where \tilde{t} is obtained by grafting s' on t'' at vertex v'' . Hence any decomposition boils down to the unique one with minimal upper tree, for which the marked vertex is the root. Now if t has $n + 1$ vertices and if the marked vertex is the root, we must define $\beta(v, t)$ as follows:

$$\beta(v, t) = d\alpha(t) - \sum_{v' \neq v} \beta(v', t). \quad (18)$$

Part b. The map β is an algebra morphism, hence induces a map

$$\bar{\beta} : V_C/[V_C, V_C] \rightarrow \text{Hom}_R(L, L)/[\text{Hom}_R(L, L), \text{Hom}_R(L, L)].$$

The map τ of the bottom line of the diagram being a trace, it induces a map $\bar{\tau} : \text{Hom}_R(L, L)/[\text{Hom}_R(L, L), \text{Hom}_R(L, L)] \rightarrow L$. In view of Lemma 3.3, the map $\gamma := \bar{\tau} \circ \bar{\beta}$ then makes Diagram (14) commute.

Part c. We prove first ii. Let t, s be trees and first consider $\phi = ds$. Recall by Proposition 2.11a:

$$\begin{aligned} t \triangleright ds &= d(t \triangleright s) - ds \circ dt \\ \beta(t \triangleright ds) &= \beta d(t \triangleright s) - \beta d(s) \circ \beta d(t) \\ &= d\alpha(t \triangleright s) - d\alpha(s) \circ d\alpha(t) \\ &= d(\alpha(t) \triangleright \alpha(s)) - d\alpha(s) \circ d\alpha(t) \end{aligned}$$

Again by Proposition 2.11a this equals:

$$\alpha(t) \triangleright d\alpha(s) = \alpha(t) \triangleright \beta(ds).$$

Now if part ii holds for ϕ_1 and ϕ_2 it is an immediate computation to verify that

$$\beta(t \triangleright (\phi_1 \circ \phi_2)) = \alpha(t) \triangleright \beta(\phi_1 \circ \phi_2),$$

thus showing part ii.

Part i is shown in a similar way. First consider $\phi = du$. Then

$$\begin{aligned} \beta(du)(\alpha(t)) &= d\alpha(u)(\alpha(t)) \\ &= \alpha(t) \triangleright \alpha(u) \\ &= \alpha(t \triangleright u) \\ &= \alpha(du(t)). \end{aligned}$$

Lastly one may show that if i holds for ϕ_1 and ϕ_2 , it holds for their composition.

For Part iii, the aroma a is an image $\tau\phi$ for a marked tree ϕ . Hence,

$$\begin{aligned}
 \gamma(t \triangleright a) &= \gamma(t \triangleright \tau\phi) \\
 \text{(trace is an } L\text{-homomorphism)} &= \gamma\tau(t \triangleright \phi) \\
 &= \tau\beta(t \triangleright \phi) \\
 \text{(use Part ii.)} &= \tau(\alpha(t) \triangleright \beta(\phi)) \\
 \text{(trace is an } L\text{-homomorphism)} &= \alpha(t) \triangleright \tau\beta(\phi) \\
 &= \alpha(t) \triangleright \gamma\tau(\phi) \\
 &= \alpha(t) \triangleright \gamma(a).
 \end{aligned}$$

□

3.3 The Pre-Lie–Rinehart Algebra of Aromatic Trees

Definition 3.6 Let R_C be the vector space freely generated by C -colored directed graphs (not necessarily connected) where each vertex has precisely one outgoing edge. Such a directed graph is a multiset of aromas, and we call it a multi-aroma.

The vector space R_C has a commutative unital \mathbf{k} -algebra structure coming from the monoid structure on multisets of aromas. Note that R_C is the symmetric algebra $\text{Sym}_{\mathbf{k}}(A_C)$ on the vector space of C -colored aromas.

Remark 3.7 Denote $[n] = \{1, 2, \dots, n\}$. In the case of one color, a multi-aroma on n vertices is simply a map $f : [n] \rightarrow [n]$. More precisely the multi-aromas identify as orbits of such maps by the action of the symmetric group S_n .

Definition 3.8 Denote $R_C \otimes_{\mathbf{k}} T_C$ by L_C . As a vector space it has as basis all expressions $r \otimes_{\mathbf{k}} t$ where r is a multi-aroma and t is a tree. For short we write this as rt and call it an *aromatic tree*, [12]. See Fig. 1.

On L_C we have the product

$$\begin{aligned}
 L_C \times L_C &\longrightarrow L_C \\
 (qs, rt) &\longmapsto \nabla_{qs}rt = qs \triangleright rt
 \end{aligned}$$

given by grafting the root of the tree s on any vertex of the aromatic tree rt and summing up. Similarly, we can graft an aromatic tree on an aroma. From this, we get induced maps:

$$\begin{array}{lll}
 \nabla : L_C \rightarrow \text{Hom}_{\mathbf{k}}(L_C, L_C) & \rho : L_C \rightarrow \text{Der}_{\mathbf{k}}(R_C, R_C) & d : L_C \rightarrow \text{Hom}_{R_C}(L_C, L_C) \\
 rt \mapsto (qs \mapsto rt \triangleright qs) & rt \mapsto (q \mapsto rt \triangleright q) & rt \mapsto (qs \mapsto qs \triangleright rt)
 \end{array}$$

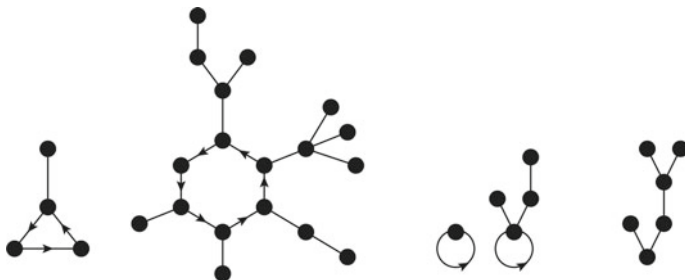


Fig. 1 An example of aromatic tree made of four aromas and a rooted tree

Proposition 3.9 L_C is a pre-Lie-Rinehart algebra over the commutative algebra R_C spanned by multi-aromas, with anchor map ρ and connection ∇ defined above.

Proof Checking the Leibniz rule for the anchor map and the left pre-Lie relation for \triangleright is an easy exercise left to the reader. □

3.4 The Algebra of Marked Aromatic Trees

Definition 3.10 Let \hat{E}_C be the free R_C -module spanned by all pairs (v, rt) where rt is an aromatic tree and v is a vertex of rt . It identifies naturally as an R_C -submodule of $\text{End}_{R_C}(L_C)$ by

$$(v, rt) \mapsto (u \mapsto u \triangleright_v rt).$$

In fact by composition \circ it is an R_C -submodule subalgebra.

Extending the map τ of (11) we get an R_C -linear map

$$\tau : \hat{E}_C \rightarrow R_C.$$

It maps an element (v, rt) to the multi-aroma we get by joining the root of t to the vertex v .

Lemma 3.11

- a. \hat{E}_C is an L_C -submodule of $\text{End}_{R_C}(L_C)$,
- b. τ is an L_C -module map,
- c. τ is a trace map, i.e., it vanishes on commutators.

Proof a. For an aromatic tree rt and a marked aromatic tree $\alpha = (v, qs)$, one obtains $rt \triangleright \alpha$ by grafting the root of t on any vertex of qs and by summing up all possibilities, keeping of course the marked vertex v in each term.

b. Consider the operations:

- First graft t on each vertex of qs and then attach the root of s to v . This gives $\tau(rt \triangleright (v, qs))$.
- First attach the root of s on v and then graft the root of t to any vertex of the resulting aroma. This gives $rt \triangleright \tau(v, qs)$.

We see these operations give the same result, and so

$$\tau(rt \triangleright (v, qs)) = rt \triangleright \tau(v, qs).$$

c. Look at $\tau((w, rt) \circ (v, qs))$. We get this by

1. Composition \circ : Graft the root of s on w .
2. Map τ : Graft the root of t on v .

But the order of these two operations can be switched without changing the result. Hence τ is a trace map. \square

3.5 The Algebra of Elementary Endomorphisms

Let B_C be the vector space freely generated by pairs (v, a) where a is an aroma in A_C and v a vertex of a . There is an injection

$$B_C \rightarrow \text{Hom}_{\mathbf{k}}(T_C, A_C), \quad (v, a) \mapsto (s \mapsto s \triangleright_v a),$$

where the tree s is grafted on the vertex v in a . The T_C -module structure on A_C gives by adjunction an injective linear map

$$d : A_C \rightarrow \text{Hom}_{\mathbf{k}}(T_C, A_C), \quad a \mapsto (t \mapsto t \triangleright a).$$

Its image lies in the image of B_C . Thus A_C may be considered a subspace of B_C , identifying $da = \sum_{v \in a} (v, a)$. Let D_C be the \mathbf{k} -vector space generated by expressions $da \cdot t$, where a is an aroma and t a tree. It identifies as $dA_C \otimes_{\mathbf{k}} T_C$.

We have compositions:

$$\begin{aligned} V_C \circ V_C \rightarrow V_C & : & (v, s) \circ (w, t) &= (w, t \triangleright_w s) \\ D_C \circ V_C & : & (da \cdot t) \circ (v, s) &= \sum_{u \in a} (v, s \triangleright_u a) \cdot t \\ V_C \circ D_C \rightarrow D_C & : & (v, s) \circ (da \cdot t) &\mapsto da \cdot (t \triangleright_v s) \\ D_C \circ D_C \rightarrow R_C \otimes_{\mathbf{k}} D_C & : & (da \cdot t) \circ (db \cdot s) &\mapsto (s \triangleright a) \cdot db \cdot t \end{aligned} \tag{19}$$

Proposition 3.12 *The R_C -submodule E_C of \hat{E}_C generated by D_C , V_C and their composition $D_C \circ V_C$, is the algebra of elementary endomorphisms $El_{R_C}(L_C)$.*

It decomposes as a free R_C -module:

$$E_C = (R_C \otimes_{\mathbf{k}} V_C) \bigoplus (R_C \otimes_{\mathbf{k}} D_C) \bigoplus (R_C \otimes_{\mathbf{k}} (D_C \circ V_C)). \quad (20)$$

Proof By the relations (19) above, we see that E_C is an R_C -module subalgebra of \hat{E}_C .

Inclusion $E\ell_{R_C}(L_C) \subseteq E_C$: Considering the map d :

$$d(rt) = dr \cdot t + r \cdot dt.$$

Looking at the right side of this, the first term is in D_C , and the second term in $R_C \otimes_{\mathbf{k}} V_C$.

Inclusion $E_C \subseteq E\ell_{R_C}(L_C)$: By Lemma 3.4, $V_C \subseteq E\ell_{R_C}(L_C)$. Since

$$d(at) - adt = da \cdot t,$$

also $D_C \subseteq E\ell_{R_C}(L_C)$.

Free decomposition: An element of $R_C \otimes_{\mathbf{k}} V_C$ has its marks on trees, and so cannot be an R -linear combination of the two other parts. Any element of $R_C \otimes_{\mathbf{k}} D_C$ must have a term with a mark on the interior cycle of an aroma and so cannot be a sum of terms in $D_C \circ V_C$. \square

By Lemma 3.11 and Proposition 3.12 above we have

Corollary 3.13 *The pre-Lie–Rinehart algebra L_C of aromatic trees is tracial.*

4 The Universal Tracial Pre-Lie–Rinehart Algebra

We show that the pair (L_C, R_C) is a *universal tracial* pre-Lie–Rinehart algebra.

Remark 4.1 Originally we aimed to show that the pair (L_C, R_C) was a universal pre-Lie–Rinehart algebra. However from a given map of sets

$$\mathcal{C} \rightarrow L$$

we could not extend this to maps

$$L_C \rightarrow L, \quad R_C \rightarrow R.$$

The problem is that one cannot generate all of L_C or R_C by starting from \mathcal{C} and using the operations $\text{Div} = \tau \circ d$ and \triangleright applied on the algebra L_C , either between aromatic trees $s \triangleright t$ or on an aroma $s \triangleright a$. In particular, one cannot generate all of the multi-aromas R_C .

To remedy this we have introduced the subalgebra V_C of $\text{End}_k(T_C)$ generated by the image of $T_C \rightarrow \text{End}_k(T_C)$ together with its trace map τ . From this subalgebra, one can get all aromas by applying the trace map. Furthermore, V_C is “fattened up” to the subalgebra El_C of $\text{End}_{R_C}(L_C)$ over R_C . To get the universality property, we have therefore introduced the class of tracial pre-Lie–Rinehart algebras.

The map γ of Theorem 3.5 extends to $\hat{\gamma} : R_C \rightarrow R$ given by

$$\hat{\gamma}(a_1 \cdots a_p) := \gamma(a_1) \cdots \gamma(a_p).$$

The map α of Theorem 3.5 extends to $\hat{\alpha} : L_C \rightarrow L$ given by

$$\hat{\alpha}(a_1 \cdots a_i t) := \hat{\gamma}(a_1 \cdots a_p) \alpha(t) = \gamma(a_1) \cdots \gamma(a_i) \alpha(t)$$

for any $a_1, \dots, a_i \in A_C$ and $t \in T_C$.

Theorem 4.2 (Universality property) *Let (L, R) be a tracial pre-Lie–Rinehart algebra, and $C \rightarrow L$ a map of sets.*

a. *This extends to a unique homomorphism of tracial pre-Lie–Rinehart algebras:*

$$(\hat{\alpha}, \hat{\gamma}) : (L_C, R_C) \rightarrow (L, R).$$

b. *The map β of Theorem 3.5 extends to a homomorphism $\hat{\beta}$ of associative algebras giving a commutative diagram*

$$\begin{array}{ccccc} L_C & \xrightarrow{d} & El_C & \xrightarrow{\tau} & R_C \\ \hat{\alpha} \downarrow & & \hat{\beta} \downarrow & & \hat{\gamma} \downarrow \\ L & \xrightarrow{d} & El_R(L) & \xrightarrow{\tau} & R. \end{array} \tag{21}$$

c. *It fulfills the following for $u \in L_C$ and $\phi \in E_C$:*

- i. $\hat{\beta}(\phi)(\hat{\alpha}(u)) = \hat{\alpha}(\phi(u))$,
- ii. $\hat{\beta}(u \triangleright \phi) = \hat{\alpha}(u) \triangleright \hat{\beta}(\phi)$.

Proof Part a. We show

- ai. $\hat{\gamma}$ is a k -algebra homomorphism,
- aii. For an aromatic tree rt and a multi-aroma q : $\hat{\gamma}(rt \triangleright q) = \hat{\alpha}(rt) \triangleright \hat{\gamma}(q)$. Note: It is to establish this property that we require the trace map τ to be an L -module homomorphism.
- aiii. $\hat{\alpha}$ is a homomorphism of pre-Lie algebras,
- aiv. For a multi-aroma q and an aromatic tree rt : $\hat{\alpha}(q \cdot rt) = \hat{\gamma}(q) \cdot \hat{\alpha}(rt)$.
- av. Uniqueness of $\hat{\alpha}$ and $\hat{\gamma}$.

Property ai is by construction since R_C is a free commutative algebra. Property aiv is by definition of $\hat{\alpha}$.

Since the action of \triangleright of L_C on R_C is a derivation (the anchor map), it is enough for Property aii to show for an aroma a and tree t that:

$$\gamma(t \triangleright a) = \alpha(t) \triangleright \gamma(a)$$

and this is done in Theorem 3.5.

For Property aiii, we have for multi-aromas r, q and trees t, s that

$$\begin{aligned} \hat{\alpha}(rt \triangleright qs) &= \hat{\alpha}(r(t \triangleright q)s + rq(t \triangleright s)), \\ &= \hat{\gamma}(r(t \triangleright q))\alpha(s) + \hat{\gamma}(rq)\alpha(t \triangleright s) \\ &= \hat{\gamma}(r)(\alpha(t) \triangleright \hat{\gamma}(q))\alpha(s) + \hat{\gamma}(r)\hat{\gamma}(q)(\alpha(t) \triangleright \alpha(s)). \end{aligned}$$

This again equals:

$$\hat{\alpha}(rt) \triangleright \hat{\alpha}(qs) = \hat{\gamma}(r)\alpha(t) \triangleright \hat{\gamma}(q)\alpha(s).$$

The uniqueness, Property av, of $\hat{\alpha}$ is by L_C being the free pre-Lie algebra. As for $\hat{\gamma}$ it is determined by its restriction $A_C \rightarrow R$. By the requirement of Definition 2.12 and the uniqueness of γ for making a commutative diagram in Theorem 3.5 we see that the $\hat{\gamma}$ restricted to A_C must equal γ .

Part b. Definition of $\hat{\beta}$: E_C decomposes as a free R_C -module (20). We let $\hat{\beta}(r\phi) = \hat{\gamma}(r)\hat{\beta}\phi$ when ϕ is a basis element for these free modules. On V_C we let $\hat{\beta}$ be given by β . On D_C we define

$$\hat{\beta}(da \cdot t) = d\alpha(t) \cdot \alpha(t).$$

Lastly consider the map

$$D_C \otimes_{\mathbf{k}} V_C \rightarrow D_C \circ V_C,$$

where by the latter we mean the vector space spanned by all compositions. This map is a bijection. To see this, consider (19). Note that an element ω in $D_C \circ V_C$ has no marked point on the interior cycle of the aroma. Let then v be a marked point in a term of the element ω which has minimal distance from v to the interior cycle. Following the path from v to the interior cycle, the vertex attached to the interior cycle (but not *on* the cycle), must be the root of a tree s with $v \in s$, which is grafted onto an aroma a . Thus, we have reconstructed a , (v, s) and t and can subtract the image of a multiple of $(da \cdot t) \circ (v, s)$ from ω . In this way, we may continue and get ω as the image of a unique element in $D_C \otimes_{\mathbf{k}} V_C$.

We may then define $\hat{\beta}$ on $D_C \otimes_{\mathbf{k}} V_C$ by

$$\hat{\beta}((da \cdot t) \circ (v, s)) = (d\gamma(a) \cdot \alpha(t)) \circ \beta(v, s).$$

Now we show the homomorphism property of $\hat{\beta}$. It respects composition of V_C since β does. It respects compositions $D_C \circ V_C$ by the above definition. It respects composition $D_C \circ D_C$ by

$$\begin{aligned}
 \hat{\beta}((da \cdot t) \circ (db \cdot s)) &= \hat{\beta}((s \triangleright a)db \cdot t) \\
 &= \gamma(s \triangleright a)\hat{\beta}(db \cdot t) \\
 &= \gamma(s \triangleright a)d\gamma(b) \cdot \alpha(t) \\
 &= (\alpha(s) \triangleright \gamma(a))d\gamma(b) \cdot \alpha(t) \\
 &= (d\gamma(a) \cdot \alpha(t)) \circ (d\gamma(b) \cdot \alpha(s)) \\
 &= \hat{\beta}(da \cdot t) \circ \hat{\beta}(db \cdot s).
 \end{aligned}$$

Applying $\hat{\beta}$ to the composition $V_C \circ D_C$

$$\begin{aligned}
 \hat{\beta}((v, s) \circ (da \cdot t)) &= \hat{\beta}(da \cdot (t \triangleright_v s)) \\
 &= d\gamma(a) \cdot \alpha(t \triangleright_v s) \\
 \text{(use Part i. of Theorem 3.5)} &= d\gamma(a) \cdot \beta((v, s))(\alpha(t)).
 \end{aligned}$$

This map sends $u \in L_C$ to $(u \triangleright \gamma(a)) \cdot \beta((v, s))(\alpha(t))$, and so does the map

$$\hat{\beta}((v, s)) \circ d\gamma(a) \cdot \alpha(t) = \hat{\beta}((v, s)) \circ \hat{\beta}(da \cdot t).$$

So these maps are equal and $\hat{\beta}$ respects composition on $D_C \circ V_C$.

Part c. i. For ϕ in V_C , this follows easily from Part i in Theorem 3.5. For ϕ in D_C , it is an easy computation. Since $\hat{\beta}$ respects compositions, we then derive it for general ϕ .

ii. When ϕ is in V_C this is by Part ii in Theorem 3.5. When ϕ is in D_C we have the following computation using Proposition 2.11b :

$$\begin{aligned}
 \hat{\beta}(t \triangleright (da \cdot s)) &= \hat{\beta}(da \cdot (t \triangleright s) + d(t \triangleright a) \cdot s - (da \cdot s) \circ dt) \\
 &= d\gamma(a) \cdot \alpha(t \triangleright s) + d(\gamma(t \triangleright a)) \cdot \alpha(s) - d\gamma(a) \cdot \alpha(s) \circ \beta d(t) \\
 &= d\gamma(a) \cdot (\alpha(t) \triangleright \alpha(s)) + d(\alpha(t) \triangleright \gamma(a)) \cdot \alpha(s) - (d\gamma(a) \cdot \alpha(s)) \circ d\alpha(t) \\
 \text{(use Proposition 2.11b)} &= \alpha(t) \triangleright (d\gamma(a) \cdot \alpha(s)) \\
 &= \alpha(t) \triangleright \hat{\beta}(da \cdot s).
 \end{aligned}$$

Now ii follows by the easily checked fact that it holds for compositions if it holds for each factor. \square

5 Remarks on Equivariance

We finally return to some remarks on Theorem 1.1 in the light of the universal diagram (21). Consider the canonical example (L, \triangleright) of vector fields on \mathbb{R}^d , where $R = C^\infty(\mathbb{R}^d)$. Let $\mathcal{C} = \{\bullet\}$ and choose a mapping $\bullet \mapsto f \in L$ inducing the universal arrows $\hat{\alpha}, \hat{\beta}, \hat{\gamma}$ in (21). Any affine diffeomorphism $\xi(x) = Ax + b$ on \mathbb{R}^d induces isomorphisms on L , $\text{End}_R(L, L)$ and R by pullback of tensors:

$$\begin{aligned} \xi \cdot f &:= A^{-1} f \circ \xi \\ (\xi \cdot G)(f) &:= \xi \cdot (G(\xi \cdot f)) \\ \xi \cdot r &:= r \circ \xi \end{aligned}$$

for $f \in L$, $G \in \text{End}_R(L, L)$ and $r \in R$.

Given three finite series $B_L \in L_{\mathcal{C}}$, $B_E \in E\ell_{\mathcal{C}}$, $B_R \in R_{\mathcal{C}}$ we obtain three mappings

$$\begin{aligned} \Phi_L(f) &:= \hat{\alpha}(B_L): L \rightarrow L \\ \Phi_E(f) &:= \hat{\beta}(B_E): L \rightarrow \text{End}_R(L, L) \\ \Phi_R(f) &:= \hat{\beta}(B_R): L \rightarrow R. \end{aligned}$$

It is straightforward to check that these are all equivariant with respect to the action of affine diffeomorphisms: $\Phi_L(\xi \cdot f) = \xi \cdot (\Phi_L(f))$, $\Phi_E(\xi(f)) = \xi \cdot (\Phi_E(f))$ and $\Phi_R(\xi(f)) = \xi \cdot (\Phi_R(f))$. Theorem 1.1 states that any smooth local affine equivariant mapping $\Phi: L \rightarrow L$ has an aromatic B -series $\overline{B_L} \in \overline{L_{\mathcal{C}}}$, where the overline denotes the graded completion, i.e., the space of formal infinite series. The proof technique [12], seems to work also for smooth local mappings between different tensor bundles. Hence, we claim:

Claim 5.1 *A smooth, local mapping $\Phi_E: L \rightarrow \text{End}_R(L, L)$ has an aromatic series $\overline{B_E} \in \overline{E\ell_{\mathcal{C}}}$ if and only it is affinely equivariant. A smooth, local mapping $\Phi_R: L \rightarrow R$ has an aromatic series $\overline{B_R} \in \overline{R_{\mathcal{C}}}$ if and only it is affinely equivariant. Subject to convergence, the mappings are represented by their aromatic B -series.*

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References

1. Geir Bogfjellmo, Algebraic structure of aromatic B-series. *Journal of Computational Dynamics* 6(2), 199 (2019)
2. J.C. Butcher, Coefficients for the study of Runge-Kutta integration processes. *J. Aust. Math. Soc.* 3(2), 185–201 (1963)

3. J.C. Butcher, An algebraic theory of integration methods. *Math. Comput.* **26**(117), 79–106 (1972)
4. A. Cayley, On the theory of the analytical forms called trees. *Lon. Edinburgh Dublin Philosoph. Mag. J. Sci.* **13**(85), 172–176 (1857)
5. F. Chapoton, M. Livernet, Pre-Lie algebras and the rooted trees operad. *Int. Math. Res. Not.* **2001**(8), 395–408 (2001)
6. P. Chartier, A. Murua, Preserving first integrals and volume forms of additively split systems. *IMA J. Numer. Anal.* **27**(2), 381–405 (2007)
7. A. Dzhamalil'daev, C. Löffwall, Trees, free right-symmetric algebras, free Novikov algebras and identities. *Homol. Homot. Appl.* **4**(2), 165–190 (2002)
8. J. Huebschmann, Poisson cohomology and quantization. *J. f.d. Reine u. Angew. Math.* **408**, 57–113 (1990)
9. J. Huebschmann, Twilled Lie-Rinehart algebras and differential Batalin-Vilkovisky algebras (1998). [arXiv:math/9811069](https://arxiv.org/abs/math/9811069)
10. A. Iserles, G.R.W. Quispel, P.S.P. Tse, B-series methods cannot be volume-preserving. *BIT Num. Math.* **47**(2), 351–378 (2007)
11. R.I. McLachlan, K. Modin, H. Munthe-Kaas, O. Verdier, B-series methods are exactly the affine equivariant methods. *Numerische Mathematik* **133**(3), 599–622 (2016)
12. H. Munthe-Kaas, O. Verdier, Aromatic Butcher series. *Found. Comput. Math.* **16**(1), 183–215 (2016)
13. H.Z. Munthe-Kaas, A. Stern, O. Verdier, Invariant connections, Lie algebra actions, and foundations of numerical integration on manifolds. *SIAM J. Appl. Algebra Geom.* **4**(1), 49–68 (2020)
14. G.S. Rinehart, Differential forms on general commutative algebras. *Trans. Amer. Math. Soc.* **108**(2), 195–222 (1963)