The universal equivariance properties of exotic aromatic B-series

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May 18, 2023

Abstract

Exotic aromatic B-series were originally introduced for the calculation of order conditions for the high order numerical integration of ergodic stochastic differential equations in $\mathbb{R}^d$ and on manifolds. We prove in this paper that exotic aromatic B-series satisfy a universal geometric property, namely that they are characterised by locality and orthogonal-equivariance. This characterisation confirms that exotic aromatic B-series are a fundamental geometric object that naturally generalises aromatic B-series and B-series, as they share similar equivariance properties. In addition, we classify with stronger equivariance properties the main subsets of the exotic aromatic B-series, in particular the exotic B-series. Along the analysis, we present a generalised definition of exotic aromatic trees, dual vector fields, and we explore the impact of degeneracies on the classification.

Keywords: Butcher series, exotic aromatic B-series, equivariance, geometric numerical integration, stochastic differential equations.

AMS subject classification (2020): 15A72, 37C81, 41A58, 60H35, 65C30.

1 Introduction

Consider the ordinary differential equation

$$y'(t) = f(y(t)), \quad y(0) = y_0, \tag{1.1}$$

where $f\colon \mathbb{R}^d \to \mathbb{R}^d$ is a Lipschitz vector field and $y_0 \in \mathbb{R}^d$, and a one-step integrator for solving (1.1) of the form

$$y_{n+1} = \Phi(y_n, h), \tag{1.2}$$

where h is the timestep of the method. Following the backward error analysis idea [15], in order to study the properties of the integrator (preservation of invariants or measures, order, behaviour in long-time,...), it proves convenient to rewrite the scheme as the exact solution of a modified ODE

$$\tilde{y}'(t) = \tilde{f}(\tilde{y}(t)).$$

For large classes of integrators, such as Runge-Kutta methods, the modified vector field $\tilde{f}$ can be expressed as a formal Taylor series in f and its partial derivatives, called a B-series [10]. The paper [32] presents universal geometric conditions on $\tilde{f}$ to show that it can be written as a B-series. More precisely, any smooth local map that is invariant under affine change of coordinates can formally be written as a B-series.

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Originally introduced in [7, 16], Butcher series proved to be a powerful tool for the construction of numerical integrators for solving ODEs with a high order of accuracy and preserving geometric properties (see the textbooks [15, 8, 9] and the review [31]). The papers [11, 17] introduced simultaneously an extension of B-series called aromatic B-series for the study of volume preserving integrators (see also the recent works [3, 4, 25, 22, 6]). In this context, one is interested in finding methods (1.2) satisfying $\operatorname{div}(\tilde{f}) = 0$. The aromatic B-series proves to be a crucial tool as the standard operations on vector fields, the divergence operator, and Taylor expansions rewrite conveniently in aromatic B-series. One then wonders whether B-series and aromatic B-series are merely tools for manipulating tedious Taylor expansions or natural far-reaching algebraic objects. This question is answered in [30, 32] where universal geometric characterisations of B-series and aromatic B-series are given (see also [29, 31]).

In the context of stochastic differential equations (SDEs), it is known that there is no backward error analysis in the strong sense in general [33]. However, there exists a similar idea for ergodic SDEs. Consider overdamped Langevin dynamics with Stratonovich noise of the form

$$dY(t) = \Pi_{\mathcal{M}}(Y(t))f(Y(t))dt + \Pi_{\mathcal{M}}(Y(t)) \circ dW(t), \quad Y(0) = Y_0, \tag{1.3}$$

where $f\colon \mathbb{R}^d \to \mathbb{R}^d$ is a Lipschitz vector field, $Y_0 \in \mathbb{R}^d$, $\Pi_{\mathcal{M}}(x)$ is the orthogonal projection on the tangent bundle of $\mathcal{M}$ at the point $x \in \mathcal{M}$ (note that $\Pi_{\mathcal{M}}(x) = I_d$ if $\mathcal{M} = \mathbb{R}^d$), and W is a standard d-dimensional Brownian motion in $\mathbb{R}^d$ on a probability space equipped with a filtration and fulfilling the usual assumptions. Under a growth assumption on f, the solution of (1.3) is ergodic, that is, it follows a deterministic distribution, called the invariant measure, in long time [14, 12, 2]. In [23, 24, 21], an extension of the aromatic B-series, called exotic aromatic B-series, is introduced to write conveniently Taylor expansions (called Talay-Tubaro expansions [34] in this context) of the solutions of (1.3) and to build high-order approximations of the invariant measure of (1.3), with applications in molecular dynamics [27]. The main idea is to introduce two new types of edges to represent the Laplacian and the scalar product. Ergodic integrators for solving (1.3) have an invariant measure that can be written as the invariant measure of an exact problem of the form (1.3) with a modified vector field $\tilde{f}$ that typically has the form

$$h\tilde{f} = hf^i\partial_i + h^2[c_1 f^i_{jj} + c_2 f^i_j f^j + c_3 f^j f^j f^i]\partial_i + h^3[c_4 f^i_{jjkk} + c_5 f^j_k f^i_{jk} + c_6 f^k f^k f^j f^j f^i]\partial_i + \dots \tag{1.4}$$

where ∂_i is the vector basis of $\mathbb{R}^d$, the c_n are real constants, and each term is summed on all involved indices. Note that the expansion (1.4) is a linear combination of monomials in the components f^i and their partial derivatives, where we use pairs of indices. Note also that the power of h associated to a monomial is not given by the number of occurrences of f, in opposition to the deterministic context. For the integrators presented in [23, 24] for solving (1.3), the modified vector field can be expressed as an exotic B-series [6] in $\mathbb{R}^d$ (see examples in [23, Sec. 5.1]) and as a partitioned exotic aromatic B-series on manifolds at least for the first orders [24, 6]. Moreover, the Talay-Tubaro expansions presented in [23, 24] are exotic aromatic S-series [5].

For the high-order approximation of (1.3), the number of terms in the Taylor expansions explodes quickly, which makes the exotic aromatic B-series a crucial tool for the study of integrators for solving SDEs (see, for instance, the order two expansion in [24, App. D]). A natural question is the following: are exotic aromatic B-series just a technical tool used for carrying out tedious calculations? Or are they fundamental objects satisfying similar geometric properties as B-series and aromatic B-series? In this paper, we show that the exotic aromatic B-series satisfy a universal equivariance property, which justifies that the exotic aromatic B-series formalism is a natural extension of B-series and aromatic B-series. We extend this result to characterise subsets of the exotic aromatic B-series, such as the exotic B-series. This work also allows us to give a more general definition of exotic aromatic B-series, free of the degeneracies introduced in the numerical context.

The article is organized as follows. We present in Section 2 the definition of the geometric properties used in the characterisation, the general definition of the exotic aromatic B-series, and the main results of the paper. The characterisation of exotic aromatic B-series is proven in Section 3, while we derive the strong classification of exotic aromatic B-series in Section 4. We give outlooks on future works in Section 5.

2 Preliminaries and main results

This section is devoted to the definition of locality, equivariance and decoupling. We then give a new general definition of exotic aromatic trees and their associated elementary differential. The main results of the paper are presented in Subsection 2.3.

2.1 Locality, equivariance, and partitions

We define the geometric properties used in the characterisation of exotic aromatic B-series. A natural property of modified vector fields is locality.

Definition 2.1. *Let $d \geqslant 0$, a map $\varphi_d \colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d)$ is local if*

$$\operatorname{supp}(\varphi_d(f)) \subset \operatorname{supp}(f), \quad \operatorname{supp}(f) = \overline{\{x \in \mathbb{R}^d, f(x) \neq 0\}}.$$

In [32], the aromatic B-series are characterised by locality and a property of equivariance. Let $\mathfrak{X}(\mathbb{R}^d)$ be the set of smooth vector fields on $\mathbb{R}^d$ and G be a finite dimensional Lie subgroup of the set of diffeomorphisms $\operatorname{Diff}(\mathbb{R}^d)$ on $\mathbb{R}^d$. The group G has the form $H \ltimes \mathbb{R}^d$, where H is a subgroup of $\mathrm{GL}_d(\mathbb{R})$ called the isotropy group. An element $g = (A, b) \in G$ acts on a vector field $f \in \mathfrak{X}(\mathbb{R}^d)$ by

$$(g \cdot f)(x) = Af(A^{-1}(x - b)).$$

The G-equivariance is the compatibility with the action of G on vector fields.

Definition 2.2. *A map $\varphi_d \colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d)$ is G-equivariant if*

$$\varphi_d(g \cdot f) = g \cdot \varphi_d(f), \quad g \in G, \quad f \in \mathfrak{X}(\mathbb{R}^d).$$

In this work, we consider $G = H \ltimes \mathbb{R}^d$, where H is a matrix group called the isotropy group. If $H = \mathrm{GL}_d(\mathbb{R})$, the G-equivariance is written for simplicity GL-equivariance, while we write orthogonal-equivariance if $H = \mathrm{O}_d(\mathbb{R})$. The first main result of this paper is the characterization of exotic aromatic B-series with orthogonal-equivariance and locality.

The second goal of this work is to characterize the subsets of exotic aromatic B-series, in particular the exotic B-series. In this context, the dimension $d \geqslant 0$ of the problem plays an important role, so that we rely on sequences of maps $\varphi = (\varphi_d \colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d))_d$ indexed by the dimension d. Such a sequence is local (respectively G-equivariant) if φ_d is local (respectively G-equivariant) for all d. To observe the interactions between the dimensions, the notion of equivariance is extended to affine transformations [30], and we refer to such a property as strong equivariance in the following.

Definition 2.3. *Let the set of affine transformations*

$$\mathrm{Aff}(\mathbb{R}^{d_1},\mathbb{R}^{d_2}) = \{a\colon \mathbb{R}^{d_1} \to \mathbb{R}^{d_2},\ a(x) = Ax + b,\ (A,b) \in \mathbb{R}^{d_2\times d_1} \times \mathbb{R}^{d_2}\},$$

and $\mathcal{H}(\mathbb{R}^{d_1},\mathbb{R}^{d_2})$ be a subset defined for all dimensions d_1 and d_2. A sequence of smooth maps $\varphi = (\varphi_d\colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d))_d$ is equivariant with respect to $\mathcal{H}$ if for all d_1, d_2, for all $a(x) = Ax + b \in \mathcal{H}(\mathbb{R}^{d_1},\mathbb{R}^{d_2})$ and $x \in \mathbb{R}^{d_1}$, φ satisfies

$$f_2(a(x)) = Af_1(x) \ \Rightarrow\ \varphi_{d_2}(f_2)(a(x)) = A\varphi_{d_1}(f_1)(x), \quad f_1 \in \mathfrak{X}(\mathbb{R}^{d_1}), \quad f_2 \in \mathfrak{X}(\mathbb{R}^{d_2}).$$

A sequence of smooth maps $\varphi = (\varphi_d)_d$ is affine-equivariant if it is equivariant with respect to all affine transformations in Aff*.*

The different subsets of $\mathrm{Aff}(\mathbb{R}^{d_1},\mathbb{R}^{d_2})$ that we consider are associated to the classical homogeneous spaces corresponding to the Lie-group $H = \mathrm{O}_d(\mathbb{R})$:

$$\mathcal{S}(\mathbb{R}^{d_1},\mathbb{R}^{d_2}) = \{a(x) = Ax + b \in \mathrm{Aff}(\mathbb{R}^{d_1},\mathbb{R}^{d_2}),\ A^TA = I_{d_1}\}, \tag{2.1}$$
$$\mathcal{G}(\mathbb{R}^{d_1},\mathbb{R}^{d_2}) = \{a(x) = Ax + b \in \mathrm{Aff}(\mathbb{R}^{d_1},\mathbb{R}^{d_2}),\ AA^T = I_{d_2}\}. \tag{2.2}$$

The transformations in (2.1) are the left-orthogonal transformations and correspond to the Stiefel manifold, while the right-orthogonal transformations in (2.2) correspond to the Grassmann manifold. The associated equivariance properties are called Stiefel-equivariance and Grassmann-equivariance. A sequence φ is said to be semi-orthogonal-equivariant if it is both Stiefel-equivariant and Grassmann-equivariant.

The elementary differentials associated to standard B-series keep decoupled systems decoupled. Some exotic aromatic B-series also satisfy this property, which motivates the following definition. Similarly to [30], for $f_1 \in \mathfrak{X}(\mathbb{R}^{d_1})$ and $f_2 \in \mathfrak{X}(\mathbb{R}^{d_2})$, we use the notation

$$h = f_1 \oplus f_2 \in \mathfrak{X}(\mathbb{R}^{d_1+d_2}), \quad h(x,y) = (f_1(x), f_2(y)).$$

Definition 2.4. *A sequence $\varphi = (\varphi_d\colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d))_d$ is decoupling if for all $f_1 \in \mathfrak{X}(\mathbb{R}^{d_1})$ and $f_2 \in \mathfrak{X}(\mathbb{R}^{d_2})$, φ satisfies*

$$\varphi_{d_1+d_2}(f_1 \oplus f_2) = \varphi_{d_1}(f_1) \oplus \varphi_{d_2}(f_2),$$

that is, for all $x \in \mathbb{R}^{d_1}$, $y \in \mathbb{R}^{d_2}$,

$$\varphi_{d_1+d_2}((f_1(x), f_2(y))) = (\varphi_{d_1}(f_1)(x), \varphi_{d_2}(f_2)(y)).$$

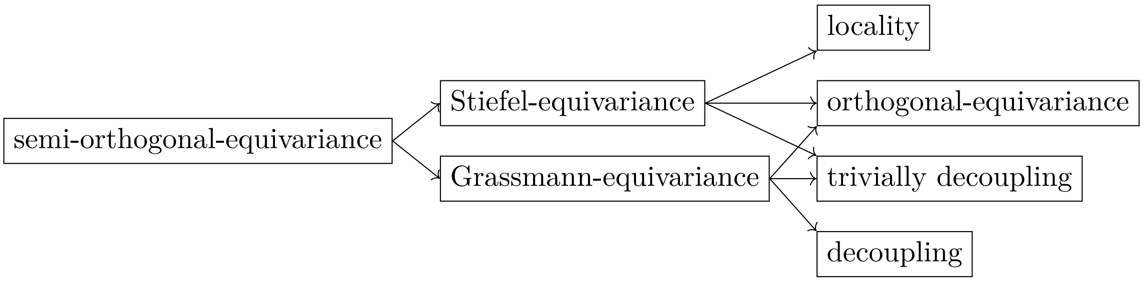
A sequence φ is trivially decoupling if for all $f \in \mathfrak{X}(\mathbb{R}^{d_1})$, φ satisfies

$$\varphi_{d_1+d_2}(f \oplus 0) = \varphi_{d_1}(f) \oplus 0.$$

The Stiefel-equivariance and Grassmann-equivariance properties are stronger than the orthogonal-equivariance in the following sense. The proof is omitted as it is nearly identical to [30, Lem. 4.2 and 6.1].

Proposition 2.5 ([30])**.** *If φ is Stiefel-equivariant, then φ is local, orthogonal-equivariant, and trivially decoupling. If $\varphi = (\varphi_d\colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d))_d$ is Grassmann-equivariant, then φ is orthogonal-equivariant, trivially decoupling, and decoupling.*

We summarise the links between the different geometric properties in the following graph for clarity.



2.2 Exotic aromatic trees

Introduced originally in [23, 24] for the calculation of the order conditions for the approximation of ergodic stochastic differential equations, the exotic aromatic trees are an extension of aromatic trees that involve two new kind of edges: lianas and stolons. The definition we give in the present paper is a generalization of the one originally presented in [23, 24] (see also [5, 6]). It reduces to the same definition under a regularity assumption discussed in Section 4.3. We choose an approach based on permutations as in [32] (see also [3, 22]).

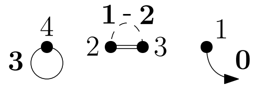
Definition 2.6. *We consider graphs of the form* $(V, \mathbf{A_0}, \sigma, \tau)$ *with* V *a finite set of vertices and* $\mathbf{A_0}$ *a finite set of arrows. The vertices are indexed from 1 to* $|V|$*, and the arrows from* $\mathbf{0}$ *to* $|\mathbf{A}|$*, where* $\mathbf{A} = \mathbf{A_0}\backslash\{\mathbf{0}\}$*. The map* $\tau\colon \mathbf{A} \to V$ *is the target map. The source map is a permutation* $\sigma\colon V \cup \mathbf{A_0} \to V \cup \mathbf{A_0}$ *that has no fixed points and satisfies* $\sigma \circ \sigma = id$*. Two such graphs are equivalent if there exists a bijection between their sets of nodes and arrows that are compatible with the source and target maps. An exotic aromatic tree is an equivalence class of such graphs. We denote* Γ *the set of exotic aromatic trees.*

Definition 2.6 differs from standard definitions of directed graphs as the source map usually sends arrows to nodes. The extension presented here allows arrows to be sources of arrows and vertices to be sources of vertices. If $\sigma(\mathbf{a_1}) = \mathbf{a_2}$, we say that the unordered tuple $(\mathbf{a_1}, \mathbf{a_2})$ is a liana and we represent it with a dashed edge between the two nodes $\tau(\mathbf{a_1})$ and $\tau(\mathbf{a_2})$, that can be identical. If $\sigma(v_1) = v_2$, we call the unordered tuple (v_1, v_2) a stolon and we draw it with a double edge between v_1 and v_2. The set of lianas is denoted L and the set of stolons is S. An exotic aromatic tree without lianas and stolons is called an aromatic tree, an extension of standard trees allowing for loops. A loop is a list of nodes $(v_1, \dots, v_K)$ such that there is a standard edge linking v_1 to v_2, …, v_K to v_1 (also called K-loop in [17]). Note that an exotic aromatic tree is an aromatic tree if and only if $\sigma(V) = \mathbf{A_0}$. In this case, Definition 2.6 reduces to an equivalent definition of the one in [32]. We refer to Table 1 for examples.

Example. *Let the exotic aromatic tree* $\gamma = (V, \mathbf{A_0}, \sigma, \tau)$ *with the nodes* $V = \{1, 2, 3, 4\}$*, the arrows* $\mathbf{A_0} = \{\mathbf{0}, \mathbf{1}, \mathbf{2}, \mathbf{3}\}$*, and the following source and target maps*

$$\sigma = (\mathbf{0}, 1)(\mathbf{1}, \mathbf{2})(2, 3)(\mathbf{3}, 4), \quad \tau = (2, 3, 4),$$

where we use the notation $\tau = (\tau(\mathbf{1}), \dots, \tau(|\mathbf{A}|))$*. The tree* γ *has one loop* (4)*, one liana* $(\mathbf{1}, \mathbf{2})$*, and one stolon* $(2, 3)$*. The associated graph is the following, where we detail the vertices and arrows for clarity.*

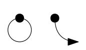
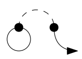
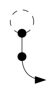


An exotic aromatic tree has a unique root r defined the following way. If $\sigma(\mathbf{0}) \in V$, $r = \sigma(\mathbf{0})$ is the root and $\mathbf{0}$ is called a ghost arrow. If $\sigma(\mathbf{0}) \in \mathbf{A}$, the liana $r = (\mathbf{0}, \sigma(\mathbf{0})) \in L$ is the root and is called a ghost liana. We draw the ghost arrow (respectively ghost liana) on the graphical representations of exotic aromatic trees as an edge (respectively dashed edge) with one end left unattached. In the aromatic context, the ghost arrow is usually omitted on the graphical representation, hence the name.

We say that two elements $x, y \in V \cup \mathbf{A_0}$ are neighbours if $\sigma(x) = y$ or $\tau(x) = y$ or $\tau(y) = x$. This defines a notion of connectedness on exotic aromatic trees. The connected components without the root are called aromas and a finite unordered collection of aromas is a multi-aroma. The connected component with the root is a connected exotic aromatic tree. We denote Γ_c the set of connected exotic aromatic trees and Γ^0 the set of multi-aromas, also represented as equivalence classes of graphs $(V, \mathbf{A}, \sigma, \tau)$ without the arrow $\mathbf{0}$. The aromas are gathered in Γ_c^0. An exotic aromatic tree decomposes into a number of aromas and one connected exotic aromatic tree. This notion of connectedness is a strong motivation to understand the exotic aromatic trees as graphs and not as trees as done beforehand in the literature. If there are no lianas and no stolons, we find the standard definition of aromas and rooted trees in the context of aromatic trees.

We define an exotic tree as an exotic aromatic tree that reduces to a standard Butcher tree when removing all the lianas. Note that there is a difference between the notions of exotic trees and connected exotic aromatic trees. A connected exotic aromatic tree does not reduce to a tree in general when removing the lianas.

Example. *Let the following exotic aromatic trees*

$\gamma_1 =$ , $\gamma_2 =$ , $\gamma_3 =$ .

The exotic aromatic tree γ_1 is a disconnected aromatic tree with one aroma. The graph γ_2 is connected, but is not an exotic tree as removing the lianas of γ_2 yields γ_1, which is not a tree. On the other hand, γ_3 is an exotic tree.

We denote the set of nodes that are the target of j arrows by V_j. For a given aromatic tree γ, we define its composition $\kappa\colon \mathbb{N} \to \mathbb{N}$ by $\kappa(j) = |V_j|$, and its derived composition by $\boldsymbol{\kappa}'(j) = j\kappa(j)$. A straightforward observation yields that the cardinals of V and $\mathbf{A}$ satisfy $|V| = |\kappa|$ and $|\mathbf{A}| = |\boldsymbol{\kappa}'|$, where $|\kappa| = \kappa(0) + \kappa(1) + \dots$ We write Γ_κ the set of exotic aromatic trees with composition κ and Γ_m the set of exotic aromatic trees such that $|\kappa| = m$. Note that Γ_κ is finite while Γ_m is infinite for all m. Contrary to the case of Butcher trees and aromatic trees, the order of an exotic aromatic tree is not given by the number of its nodes $|\kappa|$.

Lemma 2.7. *Define the order*[1] $|\gamma|$ *of an exotic aromatic tree* $\gamma \in \Gamma_\kappa$ *by* $|\gamma| = |V| + |L| - |S|$. *Then the following identity holds*

$$|\kappa| + |\boldsymbol{\kappa}'| + 1 = 2|\gamma|. \tag{2.3}$$

We mention that in the aromatic context, the order of an aromatic tree coincides with the number of nodes and (2.3) becomes

$$|\gamma| = |\kappa| = |\boldsymbol{\kappa}'| + 1. \tag{2.4}$$

[1]A similar definition of the order of an exotic aromatic tree is given in the works [23, 24]. Note that the order of an exotic aromatic tree is not the number of nodes in general.

If an exotic aromatic tree satisfies (2.4), it does not imply that γ is aromatic. In fact, there exists an infinite number of exotic aromatic trees satisfying (2.4) that do not reduce to aromatic trees: the exotic aromatic trees with the same number of stolons and lianas. In the context of branched rough paths, a similar identity to (2.4) on multi-indices is used in [28, eq. (6.3)], and the composition κ is called the fertility in this context.

Proof of Lemma 2.7. The arrows are either part of a liana or are standard arrows whose source are nodes. We denote $\mathbf{A}_\mathbf{0}^\diamond$ the latter set. Similarly, the nodes of $\gamma \in \Gamma_\kappa$ can be decomposed in two sets: the nodes that are the source of an arrow in $\mathbf{A}_\mathbf{0}^\diamond$, gathered in $V^\diamond$, and the ones that are the source of no arrows (the stolons). We observe that

$$|V| = |V^\diamond| + 2|S|, \quad |\mathbf{A}_\mathbf{0}| = |\mathbf{A}_\mathbf{0}^\diamond| + 2|L|.$$

Each node in $V^\diamond$ is the source of a unique arrow in $\mathbf{A}_\mathbf{0}^\diamond$, so that $|V^\diamond| = |\mathbf{A}_\mathbf{0}^\diamond|$. Thus, we deduce

$$|\kappa| + |\boldsymbol{\kappa}'| + 1 = |V| + |\mathbf{A}_\mathbf{0}| = 2(|V| + |L| - |S|) = 2|\gamma|,$$

which gives the desired identity (2.3). □

In Table 1, we present the list of the exotic aromatic trees of order one and two (see also Appendix A for the order three). On the contrary of the aromatic case, there exists an infinite number of exotic aromatic trees for a given number of nodes $|\kappa| > 0$. Indeed, adding any number of lianas to an exotic aromatic tree does not modify the value of $|\kappa|$, but gives a different tree.

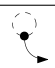
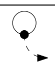
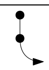
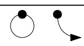
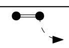
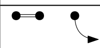
$\|\gamma\|$	$\|\kappa\|$	κ	$\boldsymbol{\kappa}'$	τ	σ	γ	$\mathcal{F}(\gamma)(f)$
1	1	(1)	(0)		$(\mathbf{0},1)$		$f^i\partial_i$
2	1	$(0,0,1)$	$(0,0,2)$	$(1,1)$	$(\mathbf{0},1)(\mathbf{1},\mathbf{2})$		$f^i_{jj}\partial_i$
					$(\mathbf{0},\mathbf{1})(\mathbf{2},1)$		$f^j_{ij}\partial_i$
2	2	$(1,1)$	$(0,1)$	(1)	$(\mathbf{0},1)(\mathbf{1},2)$		$f^i_j f^j\partial_i$
					$(\mathbf{0},2)(\mathbf{1},1)$		$f^j_j f^i\partial_i$
					$(\mathbf{0},\mathbf{1})(1,2)$		$f^j f^j_i\partial_i$
2	3	(3)	(0)		$(\mathbf{0},1)(2,3)$		$f^i f^j f^j\partial_i$

Table 1: List of the exotic aromatic trees of order one and two, with their associated composition, derived composition, target map, source map, and elementary differential (see Definition 2.8). We use the notation $\tau = (\tau(\mathbf{1}),\dots,\tau(|\boldsymbol{\kappa}'|))$.

2.3 Characterisation of exotic aromatic B-series

Butcher trees are used to represent elementary differentials, in order to represent conveniently Taylor expansions in numerical analysis [15]. We associate an elementary differential to each exotic aromatic tree. We use the standard notation ∂_i for the vector basis of $\mathbb{R}^d$.

Definition 2.8. *Given a smooth vector field $f \in \mathfrak{X}(\mathbb{R}^d)$ and $\gamma = (V, \mathbf{A_0}, \sigma, \tau) \in \Gamma$ an exotic aromatic tree, the elementary differential $\mathcal{F}_d(\gamma)$ associated to γ is the following vector field*

$$\mathcal{F}_d(\gamma)(f) = \sum_{\substack{i_1,\dots,i_{|\kappa|}\\ i_{\mathbf{0}},\dots,i_{|\boldsymbol{\kappa}'|}}} \prod_{v\in V} f^{i_v}_{i_{\tau^{-1}(\{v\})}} \delta_{i_\sigma} \partial_{i_{\mathbf{0}}},$$

where $i_{\tau^{-1}(\{v\})} = i_{l_1} \dots i_{l_m}$ for $\tau^{-1}(\{v\}) = \{l_1, \dots, l_m\}$ and $\delta_{i_\sigma} = \prod_{j=1}^{|\gamma|} \delta_{i_{p_j}, i_{q_j}}$ for the source map $\sigma = \prod_{j=1}^{|\gamma|}(p_j, q_j)$ with $\delta_{i,j} = 1$ if $i = j$ and 0 else. The elementary differential map of an exotic aromatic tree γ is the following sequence of maps indexed by the dimension of the problem

$$\mathcal{F}(\gamma) = (\mathcal{F}_d(\gamma) \colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d))_d.$$

The maps $\mathcal{F}_d$ are extended by linearity to $\operatorname{Span}(\Gamma)$*.*

Note that for a fixed dimension d, the elementary differential map $\mathcal{F}_d$ is not injective in general. There can be multiple ways to write a given elementary differential with exotic aromatic trees if the dimension d is too low. For instance, in dimension $d = 1$, all the trees with composition κ represent the same elementary differential

$$\mathcal{F}_1(\gamma)(f) = \prod_{j=0}^{\infty} (f^{(j)})^{\kappa(j)}.$$

This is a strong motivation for considering sequences of maps $\mathcal{F}(\gamma) = (\mathcal{F}_d(\gamma))_d$ indexed by the dimension of the problem.

Remark 2.9. *The elementary differential extends to multi-aromas $\gamma = (V, \mathbf{A}, \sigma, \tau) \in \Gamma^0$ by*

$$\mathcal{F}_d(\gamma)(f) = \sum_{\substack{i_1,\dots,i_{|\kappa|}\\ i_{\mathbf{1}},\dots,i_{|\boldsymbol{\kappa}'|}}} \prod_{v\in V} f^{i_v}_{i_{\tau^{-1}(\{v\})}} \delta_{i_\sigma}.$$

Example. *Consider the following exotic aromatic tree γ and its associated elementary differential*

$\gamma =$  $,\quad \mathcal{F}(\gamma) = \sum_{i_v, i_{\mathbf{a}}} f^{i_1} f^{i_2} f^{i_3}_{i_{\mathbf{1}} i_{\mathbf{2}}} \delta_{i_{\mathbf{0}}, i_1} \delta_{i_{\mathbf{1}}, i_{\mathbf{2}}} \delta_{i_2, i_3} \partial_{i_{\mathbf{0}}} = \sum_{i,j,k} f^i f^k f^k_{jj} \partial_i = (f, \Delta f) f.$

Further examples are presented in Table 1. Note that in the elementary differentials, every index appears twice. For aromatic trees, every index appears both at the top and at the bottom, while this is not the case in general for exotic aromatic trees.

An exotic aromatic B-series is a formal series indexed over exotic aromatic trees. As we consider Taylor expansions and thus use the grading by the number of nodes, we consider series with a finite number of trees with m nodes for all m. This assumption is not required in the numerical applications [23, 24] as the expansions are graded naturally by the order of the trees and not by the number of nodes.

Definition 2.10. *Given a coefficient map $b \colon \Gamma \to \mathbb{R}$ that has finite support on Γ_m for $m > 0$, the associated exotic aromatic B-series in dimension d is the following formal series*

$$B_d(b) = \sum_{m>0} \sum_{\gamma \in \Gamma_m} b(\gamma) \mathcal{F}_d(\gamma).$$

An exotic aromatic B-series is a sequence $B(b) = (B_d(b))_d$ indexed by the dimension.

The first main result of this paper is the characterization of exotic aromatic B-series with orthogonal-equivariance and locality.

Theorem 2.11. *Let $\varphi = (\varphi_d\colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d))_d$ be a sequence of smooth maps. Then, the Taylor expansion of φ_d around the trivial vector field 0 in dimension d is an exotic aromatic B-series $\varphi_d = B_d(b_d)$ if and only if φ_d is local and orthogonal-equivariant. If, in addition, φ is trivially decoupling, then there exists a coefficient map $b\colon \Gamma \to \mathbb{R}$ such that $\varphi = B(b)$.*

Theorem 2.11 provides a simple geometric criterion for checking whether a modified vector field corresponds to an exotic aromatic B-series. In addition, it confirms that the exotic aromatic B-series are a natural extension of the aromatic B-series as they both satisfy similar universal geometric properties [32].

We are then interested in characterising the different subsets of exotic aromatic B-series and in particular the exotic B-series, as they play an important role in stochastic numerical analysis [23]. We propose the following characterisation.

Theorem 2.12. *Let $\varphi = (\varphi_d\colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d))_d$ be a local sequence of smooth maps. Then, the Taylor expansion of φ around the trivial vector field 0 is:*

- *a connected exotic aromatic B-series if and only if φ is orthogonal-equivariant and decoupling,*
- *a B-series with stolons if and only if φ is Stiefel-equivariant,*
- *an exotic B-series if and only if φ is Grassmann-equivariant,*
- *a B-series if and only if φ is semi-orthogonal-equivariant.*

In particular, affine equivariance and semi-orthogonal-equivariance are equivalent notions as they both characterise B-series.

Remark 2.13. *The decoupling property exactly corresponds to the connectedness of the graphs involved in the expansion. This link was first observed in [30] in the context of aromatic B-series, where a decoupling aromatic B-series is showed to be a connected aromatic B-series, i.e., a standard B-series. Observe also that the elementary differential of an exotic aromatic tree can be factored through its connected components: let $\mu_1, \dots, \mu_m \in \Gamma_c^0$, $\tau \in \Gamma_c$ and the exotic aromatic tree $\gamma = \mu_1 \dots \mu_m \tau$, then*

$$F_d(\gamma)(f)(x) = F_d(\mu_1)(f)(x) \dots F_d(\mu_m)(f)(x) F_d(\tau)(f)(x). \tag{2.5}$$

The classification of exotic aromatic B-series is summarised in Table 2. To the best of our knowledge, the equivalence of affine-equivariance and semi-orthogonal-equivariance is a new non-trivial result. We derive in Subsection 4.3 a simplified characterisation related to the numerical analysis literature under a regularity assumption on the vector fields.

3 Geometric characterisation of exotic aromatic B-series

This section is devoted to the proof of Theorem 2.11. Following [32], we first restrict our study to symmetric multilinear local equivariant maps defined on the infinite jet bundle at one point in Section 3.1. We then decompose our space into invariant tensor spaces using the invariant tensor theorem. In Section 3.2, we draw a one-to-one correspondence between tensors in the invariant spaces and exotic aromatic trees. Section 3.3 contains the proof of Theorem 2.11 and a clarifying example.

geometric property	associated Butcher series
orthogonal-equivariance	exotic aromatic B-series
GL-equivariance	aromatic B-series
Stiefel-equivariance	B-series with stolons
Grassmann-equivariance	exotic B-series
affine/semi-orthogonal-equivariance	B-series

Table 2: Classification of B-series with respect to their equivariance properties (see Theorems 2.11 and 2.12).

3.1 Invariant tensor spaces and transfer of geometric properties

Let $\varphi_d \colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d)$ be a smooth local G-equivariant map with $G = H \ltimes \mathbb{R}^d$. The Taylor expansion of φ_d around the vector field 0 is

$$\sum_{m\geqslant 1} \frac{1}{m!} D^m\varphi_d(0)(f,\dots,f), \tag{3.1}$$

where $\varphi_d(0) = 0$ by locality [30, Lem. 6.1]. Following the transfer argument [32, Thm. 3.9], the m-th Taylor term $D^m\varphi_d(0)$ inherits the locality and orthogonal-equivariance properties. Moreover, the Peetre theorem [18, § 19.9] and the equivariance [32, Thm. 5.6] allow us to assume without loss of generality that the m-th Taylor term is in the space of multilinear symmetric local H-equivariant maps:

$$D^m\varphi_d(0) \in \mathcal{L}_H(S^m(M \otimes SM^*), M),$$

where $M = T_0\mathbb{R}^d \equiv \mathbb{R}^d$, the action of H on $S^m(M \otimes SM^*)$ is the natural action induced on tensor spaces, and for a vector space V, $SV := \bigoplus_{j=0}^{\infty} S^j V$ is the symmetric algebra. This result works for any isotropy group H.

Given a composition $\kappa \colon \mathbb{N} \to \mathbb{N}$, we define the tensor space $\mathcal{T}_\kappa$ and its symmetric counterpart $\mathcal{S}_\kappa$ by

$$\mathcal{T}_\kappa = M \otimes \bigotimes_{j=0}^{\infty} T^{\kappa(j)}(M^* \otimes T^j M), \quad \mathcal{S}_\kappa = M \otimes \bigotimes_{j=0}^{\infty} S^{\kappa(j)}(M^* \otimes S^j M),$$

and their H-invariant subspaces $\mathcal{T}_\kappa^H$ and $\mathcal{S}_\kappa^H$. Then, [32, Thm. 5.6] gives the isomorphism

$$\mathcal{L}_H(S^m(M \otimes SM^*), M) \equiv \bigoplus_{|\kappa|=m} \mathcal{S}_\kappa^H.$$

In the affine case $H = \mathrm{GL}_d(\mathbb{R})$, it is shown in [32, Thm. 6.3] with the description of H-invariant tensors [18, § 24.3] that $\mathcal{L}_H(S^m(M \otimes SM^*), M)$ is a finite dimensional space. In the orthogonal case $H = \mathrm{O}_d(\mathbb{R})$, this property does not hold in general, and we get the following instead.

Theorem 3.1. *Let $H = \mathrm{O}_d(\mathbb{R})$ and m a positive integer, the following isomorphism holds*

$$\mathcal{L}_H(S^m(M \otimes SM^*), M) \equiv \bigoplus_{\substack{|\kappa|=m \\ |\kappa|+|\kappa'|+1\in 2\mathbb{Z}}} \mathcal{S}_\kappa^H.$$

Proof. Following the description of $\mathrm{O}_d(\mathbb{R})$-invariant tensors [18, § 33.2], we deduce that $\mathcal{T}_\kappa^H$ is trivial when $|\kappa| + |\boldsymbol{\kappa}'| + 1$ is odd. As $\mathcal{S}_\kappa^H$ is naturally injected into $\mathcal{T}_\kappa^H$, we obtain the desired result. □

We write $\Delta^m \varphi_d\colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d)$ the term of order $m \geqslant 1$ in the expansion of φ_d around the vector field 0, that is,

$$\Delta^m \varphi_d(f) = D^m \varphi_d(0)(f, \dots, f).$$

Thanks to Theorem 3.1, $\Delta^m \varphi_d$ has the following form,

$$\Delta^m \varphi_d(f) = \sum_{\substack{|\kappa|=m \\ |\kappa|+|\boldsymbol{\kappa}'|+1 \in 2\mathbb{Z}}} \psi_{\kappa,d}(f^\kappa), \quad f^\kappa = (\underbrace{f, \dots, f}_{\kappa(0)}, \underbrace{f', \dots, f'}_{\kappa(1)}, \dots), \tag{3.2}$$

where only a finite number of the $\psi_{\kappa,d} \in \mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})}$ are non-zero.

Lemma 3.2. *Let φ be a local orthogonal-equivariant sequence of smooth maps. The strong equivariance, decoupling, or trivially decoupling properties of φ are transferred to the Taylor terms $\Delta^m \varphi$ in* (3.2)*.*

Proof. The proof for the transfer of equivariance properties is the same as in [30, Prop. 6.2]. Let us prove the transfer of the decoupling property. The transfer of the trivially decoupling property uses the same arguments. The Taylor terms of φ satisfy [20, § 5.11]

$$\Delta^m \varphi_d(f) = \partial_{t_1 \dots t_m} \varphi_d((t_1 + \dots + t_m) f)\Big|_{t_1 = \dots = t_m = 0}.$$

Thus, we find

$$\begin{aligned} \Delta^m \varphi_d(f_1 \oplus f_2) &= \partial_{t_1 \dots t_m} \varphi_d((t_1 + \dots + t_m) f_1 \oplus (t_1 + \dots + t_m) f_2)\Big|_{t_1 = \dots = t_m = 0} \\ &= \partial_{t_1 \dots t_m} \Big[\varphi_d((t_1 + \dots + t_m) f_1) \oplus \varphi_d((t_1 + \dots + t_m) f_2)\Big]\Big|_{t_1 = \dots = t_m = 0} \\ &= \Delta^m \varphi_d(f_1) \oplus \Delta^m \varphi_d(f_2). \end{aligned}$$

Hence the result. □

Thus, we restrict our study for the rest of the paper to the $\Delta^m \varphi = (\Delta^m \varphi_d)_d$ that can be expressed as finite sums of tensors in $\mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})}$. We show in Subsection 3.2 that the expansion (3.2) corresponds to the order m term of an exotic aromatic B-series.

3.2 Correspondence between exotic aromatic trees and invariant tensors

Let us now draw a correspondence between exotic aromatic trees and tensors in $\mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})}$.

Theorem 3.3. *For a given κ, there exists a surjective linear map $\widetilde{\mathcal{F}}_d\colon \mathrm{Span}(\Gamma_\kappa) \to \mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})}$. The map $\widetilde{\mathcal{F}}_d$ is a bijection if and only if $2d \geqslant |\kappa| + |\boldsymbol{\kappa}'| + 1$. Moreover, the elementary differential map $\mathcal{F}_d$ is injective on $\mathrm{Span}(\Gamma_\kappa)$ if $2d \geqslant |\kappa| + |\boldsymbol{\kappa}'| + 1$.*

Proof. **Decomposition of $\mathcal{T}_\kappa$.** Following Theorem 3.1, we assume without loss of generality that $|\kappa| + |\boldsymbol{\kappa}'| + 1 = 2d_0$ is even. We rewrite $\mathcal{T}_\kappa$ as

$$\mathcal{T}_\kappa = M \otimes \bigotimes_{j=0}^{\infty} \bigotimes_{i=1}^{\kappa(j)} T_i^j, \quad T_i^j = M^* \otimes T^j M.$$

We number the $2d_0$ components of $\mathcal{T}_\kappa$ in the following way. The copies of M^* in $\mathcal{T}_\kappa$ are numbered in an arbitrary manner from 1 to $|\kappa|$ and the copies of M from $\mathbf{0}$ to $|\boldsymbol{\kappa}'|$ so that

$$\mathcal{T}_\kappa = M_{\mathbf{0}} \otimes \bigotimes_{j=0}^{\infty} \bigotimes_{i=1}^{\kappa(j)} T_i^j.$$

If the numbering is given by

$$T_i^j = M_n^* \otimes M_{\mathbf{n_1}} \otimes \cdots \otimes M_{\mathbf{n_j}},$$

then we write

$$\tau(\mathbf{n_k}) = n, \quad k = 1, \dots, j.$$

This defines the target map $\tau\colon \mathbf{A} \to V$, the arrows $\mathbf{A} = \{\mathbf{1}, \dots, |\boldsymbol{\kappa}'|\}$, $\mathbf{A_0} = \{\mathbf{0}\} \cup \mathbf{A}$, and the vertices $V = \{1, \dots, |\kappa|\}$.

Definition of ω. We denote Σ_κ the set of permutations σ of the set $V \cup \mathbf{A_0}$ that have no fixed point and that satisfy $\sigma \circ \sigma = \mathrm{id}$. Given $\sigma \in \Sigma_\kappa$ and the target map τ, there exists a unique exotic aromatic tree $(V, \mathbf{A_0}, \sigma, \tau) \in \Gamma_\kappa$ according to Definition 2.6. This yields a map $\omega\colon \Sigma_\kappa \to \Gamma_\kappa$. We extend this map by linearity to obtain $\omega\colon \mathrm{Span}(\Sigma_\kappa) \to \mathrm{Span}(\Gamma_\kappa)$.

Definition of π. The projection map $\pi\colon \mathcal{T}_\kappa \to \mathcal{S}_\kappa$ is compatible with the action of $\mathrm{O}_d(\mathbb{R})$. Thus, it induces a surjective linear map (still denoted π for simplicity) from $\mathcal{T}_\kappa^{\mathrm{O}_d(\mathbb{R})}$ to $\mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})}$.

Definition of δ. Using the isomorphism $\mathcal{T}_\kappa \equiv \mathcal{L}(\bigotimes_{n\in V\cup\mathbf{A_0}} M_n, \mathbb{R})$, we define $\delta(\sigma)$ for a permutation $\sigma \in \Sigma_\kappa$ by

$$\delta(\sigma)(v) = \prod_{\substack{i,j\in V\cup\mathbf{A_0} \\ j=\sigma(i), i<j}} (v_i, v_j), \quad v = \bigotimes_{n\in V\cup\mathbf{A_0}} v_n \in \bigotimes_{n\in V\cup\mathbf{A_0}} M_n,$$

where $(.,.)$ is the standard scalar product in $\mathbb{R}^d$ and where we fixed an arbitrary total order on $V \cup \mathbf{A_0}$. We extend δ by linearity on $\mathrm{Span}(\Sigma_\kappa)$. The surjectivity of δ is a consequence of the $\mathrm{O}_d(\mathbb{R})$-invariant tensor theorem [18, § 33.2] (see also [35, Sec. II.9] and [19, Sec. 10.2]). Moreover, δ is a bijection if and only if $2d \geqslant |\kappa| + |\boldsymbol{\kappa}'| + 1 = |V| + |\mathbf{A_0}|$ (see [35, Sec. II.17]).

Intermediate diagram. We defined the linear maps π, ω and δ. We obtain the following diagram.

$$\begin{array}{ccc} \mathcal{T}_\kappa^{\mathrm{O}_d(\mathbb{R})} & \xrightarrow{\ \pi\ } & \mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})} \\ \delta\uparrow & & \\ \mathrm{Span}(\Sigma_\kappa) & \xrightarrow{\ \omega\ } & \mathrm{Span}(\Gamma_\kappa) \end{array}$$

Action of G_κ. The target function $\tau\colon \mathbf{A} \to V$ is an element of $V^{\mathbf{A}}$. We denote $\Sigma_{\mathbf{A}}$ the set of permutations of the arrows in $\mathbf{A}$, respectively Σ_V the set of permutations of the nodes in V, and $\Sigma_{\mathbf{A}} \times \Sigma_V$ the permutations of $V \cup \mathbf{A_0}$ that leave $\mathbf{0}$ fixed, permute the elements in V, and the elements of $\mathbf{A}$ without mixing them. The action of an element of $g \in \Sigma_{\mathbf{A}} \times \Sigma_V$ on $\xi \in V^{\mathbf{A}}$ is

$$g \cdot \xi = g \circ \xi \circ g^{-1}.$$

We denote G_κ the stabilizer of the target function τ, that is,

$$G_\kappa = \{g \in \Sigma_{\mathbf{A}} \times \Sigma_V, \quad g \cdot \tau = \tau\}.$$

The permutations in G_κ represent the permutations of arrows and nodes that are compatible with the target map τ.

Definition of K_Σ. An element $g \in \Sigma_{\mathbf{A}} \times \Sigma_V$ acts naturally on $\sigma \in \Sigma_\kappa$ by $g \cdot \sigma = g \circ \sigma \circ g^{-1}$. We observe that $\omega(\sigma_1) = \omega(\sigma_2)$ if and only if there exists $g \in G_\kappa$ such that $\sigma_1 = g \cdot \sigma_2$. We define K_Σ as the vector subspace of $\operatorname{Span}(\Sigma_\kappa)$ spanned by the $g_1 \cdot \sigma - g_2 \cdot \sigma$ for $g_1, g_2 \in G_\kappa$ and $\sigma \in \Sigma_\kappa$. By definition, K_Σ is the kernel of ω, so that the following sequence is exact.

$$0 \longrightarrow K_\Sigma \hookrightarrow \operatorname{Span}(\Sigma_\kappa) \xrightarrow{\omega} \operatorname{Span}(\Gamma_\kappa) \longrightarrow 0$$

Definition of $K_\otimes$. Using the identification $\mathcal{T}_\kappa \equiv \mathcal{L}(\bigotimes_{n \in V \cup \mathbf{A_0}} M_n, \mathbb{R})$, the action of an element of $\Sigma_{\mathbf{A}} \times \Sigma_V$ on $\mathcal{T}_\kappa$ is

$$(g \cdot \varphi)(v) = \varphi(\bigotimes_{n \in V \cup \mathbf{A_0}} v_{g(n)}), \quad \varphi \in \mathcal{L}(\bigotimes_{n \in V \cup \mathbf{A_0}} M_n, \mathbb{R}), \quad v = \bigotimes_{n \in V \cup \mathbf{A_0}} v_n.$$

We observe that by definition of τ, $\pi(\varphi_1) = \pi(\varphi_2)$ if and only if $\varphi_1 = g \cdot \varphi_2$ with $g \in G_\kappa$. We define $K_\otimes$ as the vector space spanned by the $g_1 \cdot \varphi - g_2 \cdot \varphi$ for $g_1, g_2 \in G_\kappa$, $\varphi \in \mathcal{T}_\kappa$. By definition, $K_\otimes$ is the kernel of π, and is also the kernel of the restriction $\pi \colon \mathcal{T}_\kappa^{\mathrm{O}_d(\mathbb{R})} \to \mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})}$. We have the following exact sequence.

$$0 \longrightarrow K_\otimes \hookrightarrow \mathcal{T}_\kappa^{\mathrm{O}_d(\mathbb{R})} \xrightarrow{\pi} \mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})} \longrightarrow 0$$

Definition of $\widetilde{\mathcal{F}}_d$. The action of G_κ commutes with δ, that is, $\delta(g \cdot \sigma) = g \cdot \delta(\sigma)$. Thus, δ induces a linear map from K_Σ to $K_\otimes$. By the fundamental theorem on homomorphisms, there exists a surjective map $\widetilde{\delta}$ from $\operatorname{Span}(\Sigma_\kappa)/K_\Sigma$ to $\mathcal{T}_\kappa^{\mathrm{O}_d(\mathbb{R})}/K_\otimes$. We obtain the following diagram, where $\widetilde{\mathcal{F}}_d = \pi \circ \widetilde{\delta} \circ \omega^{-1}$ is surjective.

$$\begin{array}{ccc} \mathcal{T}_\kappa^{\mathrm{O}_d(\mathbb{R})}/K_\otimes & \xrightarrow{\pi} & \mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})} \\ \uparrow{\scriptstyle \widetilde{\delta}} & & \uparrow{\scriptstyle \widetilde{\mathcal{F}}_d} \\ \operatorname{Span}(\Sigma_\kappa)/K_\Sigma & \xrightarrow{\omega} & \operatorname{Span}(\Gamma_\kappa) \end{array}$$

The map $\widetilde{\mathcal{F}}_d$ is bijective if and only if $\widetilde{\delta}$ is bijective, that is, if and only if $2d \geqslant |\kappa| + |\boldsymbol{\kappa}'| + 1$. The elementary differential map $\mathcal{F}_d$ in Definition 2.8 is related to the map $\widetilde{\mathcal{F}}_d$ on $\operatorname{Span}(\Gamma_\kappa)$ by

$$\mathcal{F}_d(\gamma)(f)(x) = \widetilde{\mathcal{F}}_d(\gamma)(f^\kappa), \quad f^\kappa(x) = (\underbrace{f(x), \dots, f(x)}_{\kappa(0)}, \underbrace{f'(x), \dots, f'(x)}_{\kappa(1)}, \dots), \quad f \in \mathfrak{X}(\mathbb{R}^d).$$

Thus, if $\widetilde{\mathcal{F}}_d$ is bijective on $\operatorname{Span}(\Gamma_\kappa)$, then $\mathcal{F}_d$ is injective on $\operatorname{Span}(\Gamma_\kappa)$. □

Remark 3.4. *There exists a finite number of exotic aromatic trees of composition κ, so that $\mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})}$ is finite-dimensional. However, on the contrary of the* GL*-equivariance setting, there is an infinite number of exotic aromatic trees with a given number of nodes $|\kappa|$, so that $\mathcal{L}_{\mathrm{O}_d(\mathbb{R})}(S^m(M \otimes SM^*), M)$ is infinite-dimensional.*

3.3 Characterisation of exotic aromatic B-series

As first mentioned in [21, Sec. 3.2.4], the exotic aromatic B-series satisfy geometric properties.

Proposition 3.5. *The exotic aromatic B-series are local, orthogonal-equivariant, and trivially decoupling.*

Proof. The locality and trivially decoupling properties are straightforward from Definition 2.8. Let $g = (A, b) \in O_d(\mathbb{R}) \ltimes \mathbb{R}^d$ and $\gamma \in \Gamma$, then

$$\begin{aligned}\mathcal{F}_d(\gamma)(g \cdot f)(x) &= \sum_{\substack{i_v, i_{\mathbf{a}} \\ v\in V, \mathbf{a}\in \mathbf{A_0}}} \prod_{v\in V} \sum_{\substack{k_v, k_{\mathbf{a_0}} \\ v\in V, \mathbf{a_0}\in \mathbf{A}}} a_{i_v,k_v} a_{i_{\tau^{-1}(\{v\})}, k_{\tau^{-1}(\{v\})}} f^{k_v}_{k_{\tau^{-1}(\{v\})}}(A^{-1}x - b)\delta_{i_\sigma}\partial_{i_{\mathbf{0}}} \\ &= \sum_{\substack{i_{\mathbf{0}}, k_v, k_{\mathbf{a}} \\ v\in V, \mathbf{a}\in \mathbf{A}}} a_{i_{\mathbf{0}}, k_{\sigma(\mathbf{0})}} \prod_{v\in V} f^{k_v}_{k_{\tau^{-1}(\{v\})}}(A^{-1}x - b)\delta_{k_\sigma}\partial_{i_{\mathbf{0}}} \\ &= (g \cdot \mathcal{F}_d(\gamma)(f))(x),\end{aligned}$$

where $a_{i_J,k_J} = \prod_{j\in J} a_{i_j,k_j}$ and we used that $A^T A = I_d$. By linearity, exotic aromatic B-series are orthogonal-equivariant. ☐

The trivially decoupling property characterises the sequences of elementary differentials associated to exotic aromatic trees independently of the dimension d.

Proposition 3.6. *Let $\varphi = (\mathcal{F}_d(\gamma_d))_d$ be trivially decoupling, with $\gamma_d \in \operatorname{Span}(\Gamma_\kappa)$, then there exists a unique $\gamma \in \operatorname{Span}(\Gamma_\kappa)$ such that $\varphi = \mathcal{F}(\gamma)$.*

Proof. Let $d_1 \leqslant d_2$, then we have $\mathcal{F}_{d_2}(\gamma_{d_2})(f_1 \oplus 0) = \mathcal{F}_{d_1}(\gamma_{d_1})(f_1) \oplus 0$ for $f_1 \in \mathfrak{X}(\mathbb{R}^{d_1})$ as φ is trivially decoupling. On the other hand, a close inspection of Definition 2.8 yields that $\mathcal{F}_{d_2}(\gamma_{d_2})(f_1 \oplus 0) = \mathcal{F}_{d_1}(\gamma_{d_2})(f_1) \oplus 0$, and we deduce

$$\mathcal{F}_{d_1}(\gamma_{d_1}) = \mathcal{F}_{d_1}(\gamma_{d_2}), \quad d_1 \leqslant d_2. \tag{3.3}$$

Let $d_0 = (|\kappa| + |\boldsymbol{\kappa}'| + 1)/2$. For $d \geqslant d_0$, equation (3.3) gives $\mathcal{F}_d(\gamma_d) = \mathcal{F}_d(\gamma_{d_0})$. For $d \leqslant d_0$, equation (3.3) gives $\mathcal{F}_{d_0}(\gamma_{d_0}) = \mathcal{F}_{d_0}(\gamma_d)$. As $\mathcal{F}_{d_0}$ is injective on $\operatorname{Span}(\Gamma_\kappa)$, $\gamma_d = \gamma_{d_0}$. Thus, we obtain $\varphi = \mathcal{F}(\gamma_{d_0})$. The uniqueness of γ_{d_0} is a consequence of the injectivity of $\mathcal{F}_{d_0}$ on $\operatorname{Span}(\Gamma_\kappa)$ (see Theorem 3.3). ☐

Let us now prove the characterisation of exotic aromatic B-series.

Proof of Theorem 2.11. Let $\varphi_d \colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d)$ be a local, and orthogonal-equivariant map. Thanks to Theorem 3.1, the term of order m in the Taylor expansion (3.1) of φ_d around the 0 vector field has the form (3.2). Theorem 3.3 gives the existence of $\gamma_{\kappa,d} \in \operatorname{Span}(\Gamma_\kappa)$ such that $\psi_{\kappa,d} = \widetilde{\mathcal{F}}_d(\gamma_{\kappa,d})$. The Taylor expansion of φ_d around the 0 vector field thus is the exotic aromatic B-series:

$$\sum_{m\geqslant 1} \frac{1}{m!} \sum_{\substack{|\kappa|=m \\ |\kappa|+|\boldsymbol{\kappa}'|+1\in 2\mathbb{Z}}} \mathcal{F}_d(\gamma_{\kappa,d})(f)(x).$$

If, in addition, φ is trivially decoupling, Proposition 3.6 gives the existence of the coefficient map $b \colon \Gamma \to \mathbb{R}$ such that $\varphi = B(b)$. ☐

Example. *Let us illustrate the tensor spaces and the different maps from the proof of Theorem 3.3 for* $\kappa = (2,0,1)$ *(in the spirit of the examples in [29, 32]). The tensor space has the form*

$$\mathcal{T}_\kappa = M_{\mathbf{0}} \otimes M_1^* \otimes M_2^* \otimes (M_3^* \otimes M_{\mathbf{1}} \otimes M_{\mathbf{2}}).$$

The associated set of nodes and arrows are $V = \{1,2,3\}$ *and* $\mathbf{A_0} = \{\mathbf{0},\mathbf{1},\mathbf{2}\}$*. The target map* $\tau\colon \mathbf{A} \to V$ *is given by* $\tau(\mathbf{1}) = \tau(\mathbf{2}) = 3$*. The stabilizer of* τ *is*

$$G_\kappa = \{\mathrm{id}, (1,2), (\mathbf{1},\mathbf{2}), (1,2)(\mathbf{1},\mathbf{2})\}.$$

We present the output of ω*,* $\widetilde{\delta}$ *and* $\widetilde{\mathcal{F}}$ *for the different* $\sigma \in \Sigma_\kappa$ *in Table 3, where we gather together the* G_κ*-orbits. We write* $\widetilde{\delta}(\sigma)$ *as an element of*

$$\mathcal{T}_\kappa / K_\otimes \equiv \mathcal{L}(T^2M \otimes \mathcal{L}(T^2M, M), M)/K_\otimes,$$

that is, for v*,* $w \in M$ *and a bilinear map* $\zeta \in \mathcal{L}(T^2M, M)$*, we have* $\widetilde{\delta}(\sigma)(v,w,\zeta) \in M$*. For* $\widetilde{\mathcal{F}}$*, we use the identification*

$$\mathcal{S}_\kappa \equiv \mathcal{L}(S^2M \otimes \mathcal{L}(S^2M, M), M).$$

Replacing $v = w = f(x)$ *and* $\zeta = f''(x)$ *yields the elementary differential* $\mathcal{F}(\gamma)(f)(x)$ *of Definition 2.8. Note that the first two lines of Table 3 are aromatic trees, and also appear in [32, Table 2]. It can be seen directly on the associated permutations* σ*, as each arrow is paired with a node and vice versa.*

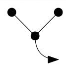
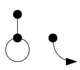
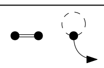
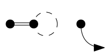
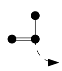
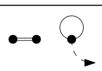
$\sigma \in \Sigma_\kappa$	$\gamma = \omega(\sigma)$	$\widetilde{\delta}(\sigma)(v,w,\zeta)$	$\widetilde{\mathcal{F}}(\gamma)(v,w,\zeta)$
$(\mathbf{0},3)(\mathbf{1},1)(\mathbf{2},2)$		$\zeta^i(v,w)\partial_i$	
$(\mathbf{0},3)(\mathbf{1},2)(\mathbf{2},1)$		$\zeta^i(w,v)\partial_i$	$\zeta^i(v,w)\partial_i$
$(\mathbf{0},1)(\mathbf{1},2)(\mathbf{2},3)$		$\zeta^j(w,\partial_j)v^i\partial_i$	
$(\mathbf{0},1)(\mathbf{1},3)(\mathbf{2},2)$		$\zeta^j(\partial_j,w)v^i\partial_i$	
$(\mathbf{0},2)(\mathbf{1},1)(\mathbf{2},3)$		$\zeta^j(v,\partial_j)w^i\partial_i$	
$(\mathbf{0},2)(\mathbf{1},3)(\mathbf{2},1)$		$\zeta^j(\partial_j,v)w^i\partial_i$	$\frac{1}{2}(\zeta^j(w,\partial_j)v^i + \zeta^j(v,\partial_j)w^i)\partial_i$
$(\mathbf{0},3)(\mathbf{1},\mathbf{2})(1,2)$		$(v,w)\zeta^i(\partial_j,\partial_j)\partial_i$	$(v,w)\zeta^i(\partial_j,\partial_j)\partial_i$
$(\mathbf{0},1)(\mathbf{1},\mathbf{2})(2,3)$		$(w,\zeta(\partial_j,\partial_j))v^i\partial_i$	
$(\mathbf{0},2)(\mathbf{1},\mathbf{2})(1,3)$		$(v,\zeta(\partial_j,\partial_j))w^i\partial_i$	$\frac{1}{2}((w,\zeta(\partial_j,\partial_j))v^i + (v,\zeta(\partial_j,\partial_j))w^i)\partial_i$
$(\mathbf{0},\mathbf{1})(\mathbf{2},1)(2,3)$		$(w,\zeta(\partial_i,v))\partial_i$	
$(\mathbf{0},\mathbf{1})(\mathbf{2},2)(1,3)$		$(v,\zeta(\partial_i,w))\partial_i$	
$(\mathbf{0},\mathbf{2})(\mathbf{1},1)(2,3)$		$(w,\zeta(v,\partial_i))\partial_i$	
$(\mathbf{0},\mathbf{2})(\mathbf{1},2)(1,3)$		$(v,\zeta(w,\partial_i))\partial_i$	$\frac{1}{2}((w,\zeta(\partial_i,v)) + (v,\zeta(\partial_i,w)))\partial_i$
$(\mathbf{0},\mathbf{1})(\mathbf{2},3)(1,2)$		$(v,w)\zeta^j(\partial_i,\partial_j)\partial_i$	
$(\mathbf{0},\mathbf{2})(\mathbf{1},3)(1,2)$		$(v,w)\zeta^j(\partial_j,\partial_i)\partial_i$	$(v,w)\zeta^j(\partial_j,\partial_i)\partial_i$

Table 3: Outputs of the functions ω, δ and $\widetilde{\mathcal{F}}$ appearing in the proof of Theorem 3.3 for the composition $\kappa = (2,0,1)$ and target map $\tau(\mathbf{1}) = \tau(\mathbf{2}) = 3$. The bilinear map ζ is assumed symmetric in the last column. The sums on all involved indices are omitted for simplicity.

4 Classification of exotic aromatic B-series

This section is devoted to the proof of the stronger classification of Theorem 2.12. The proof, presented in Subsection 4.2, relies heavily on the use of new dual vector fields, that we introduce in Subsection 4.1. We present the impact of degeneracies on the classification in Subsection 4.3.

4.1 Dual vector fields

The exotic aromatic trees given in Definition 2.6 produce independent elementary differentials. The standard method for proving this property is to consider dual vector fields, as presented in [15, 17, 30, 23]. In the proof of Theorem 2.12, we use the following new dual vector fields.

Proposition 4.1. *Given an exotic aromatic tree or multi-aroma $\gamma \in \Gamma^0 \cup \Gamma$, index the coordinates of $\mathbb{R}^{|\gamma|}$ by the uplets in $(V \cup \mathbf{A_0})/\sigma$ (respectively in $(V \cup \mathbf{A})/\sigma$ if $\gamma \in \Gamma^0$), where v and $\sigma(v)$ are identified. This corresponds to the nodes $(v, \mathbf{a}) \in V^\diamond$ that are not part of stolons, the stolons $s = (v_1, v_2) \in S$, and the lianas $l = (\mathbf{a_1}, \mathbf{a_2}) \in L$. Let θ^γ be the following parameter indexed by the standard nodes, the nodes in stolons, and the arrows in lianas,*

$$\theta^\gamma = (\theta^{V^\diamond}, \theta^S, \theta^L) = (\theta_1^{V^\diamond}, \dots, \theta_{|V^\diamond|}^{V^\diamond}, \theta_1^S, \dots, \theta_{2|S|}^S, \theta_{\mathbf{1}}^L, \dots, \theta_{\mathbf{2}|\mathbf{L}|}^L).$$

Define the associated vector field $f_\gamma^{(\theta^\gamma)} \in \mathfrak{X}(\mathbb{R}^{|\gamma|})$ by

$$\begin{aligned} f_\gamma^{(\theta^\gamma),v}(x) &= \theta_v^{V^\diamond} \prod_{\tau(\mathbf{a})=v} \theta_{\mathbf{a}}^L x_{\mathbf{a}}, \\ f_\gamma^{(\theta^\gamma),s}(x) &= \theta_{v_1}^S \prod_{\tau(\mathbf{a})=v_1} \theta_{\mathbf{a}}^L x_{\mathbf{a}} + \theta_{v_2}^S \prod_{\tau(\mathbf{a})=v_2} \theta_{\mathbf{a}}^L x_{\mathbf{a}}, \quad s = (v_1, v_2) \in S, \\ f_\gamma^{(\theta^\gamma),l}(x) &= 0, \end{aligned}$$

where an empty product equals 1 and $\theta_{\mathbf{a}}^L = 1$ if $\mathbf{a} \notin L$. By convention, if γ has a root, the coordinate of the root is the first one. Let γ, $\hat{\gamma} \in \Gamma^0 \cup \Gamma$, then

$$(\mathcal{F}_{|\hat{\gamma}|}(\gamma)(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})}))^1_{\theta^\gamma}\Big|_{\theta=0}(0) = 0 \text{ if } \hat{\gamma} \neq \mu\gamma, \quad \mu \in \Gamma_0.$$

In particular, the elementary differential map $\mathcal{F}$ is injective on $\operatorname{Span}(\Gamma)$*. Moreover, for connected graphs γ, $\hat{\gamma} \in \Gamma_c^0 \cup \Gamma_c$, we find*

$$(\mathcal{F}_{|\hat{\gamma}|}(\gamma)(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})}))^1_{\theta^\gamma}\Big|_{\theta=0}(0) = \sigma(\gamma) \neq 0 \text{ if and only if } \gamma = \hat{\gamma}.$$

In the latter case, the constant $\sigma(\gamma)$ is the symmetry coefficient of γ, that is, the number of bijections of the vertices and arrows of γ that preserve the graph structure.

Remark 4.2. *Given an exotic aromatic tree $\gamma = \mu_m \dots \mu_1 \tau$, we enforce an order on the aromas, so that $\mu_1\mu_2$ is now different from $\mu_2\mu_1$ if $\mu_1 \neq \mu_2$. Consider the additional parameter $\theta^\gamma = (\theta^\tau, \theta^{\mu_1}, \dots, \theta^{\mu_m})$, where the numbering of the nodes, lianas and stolons starts with τ, and continues in order with the μ_i. With this order on the aromas and the numbering of θ, the first statement of Proposition 4.1 is then replaced by*

$$(\mathcal{F}_{|\hat{\gamma}|}(\gamma)(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})}))^1_{\theta^\gamma}\Big|_{\theta=0}(0) \neq 0 \text{ if and only if } \hat{\gamma} = \mu\gamma, \quad \mu \in \Gamma_0.$$

Proof. Let $\gamma = (V, \mathbf{A}, \sigma, \tau)$, $\hat{\gamma} = (\hat{V}, \hat{\mathbf{A}}, \hat{\sigma}, \hat{\tau}) \in \Gamma^0 \cup \Gamma$. Definition 2.8 rewrites as

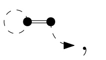
$$\begin{aligned}\mathcal{F}_{|\hat{\gamma}|}(\gamma)(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})})(x) &= \sum_{i\colon (V\cup\mathbf{A})/\sigma \to (\hat{V}\cup\hat{\mathbf{A}})/\hat{\sigma}} \prod_{v\in V} (f_{\hat{\gamma}})^{i_v}_{i_{\tau^{-1}(\{v\})}} \partial_{i_r} \\ &= \sum_{i\colon (V\cup\mathbf{A})/\sigma \to (\hat{V}\cup\hat{\mathbf{A}})/\hat{\sigma}} \prod_{v\in V} \Big(\theta^{V^\diamond}_{i_v} \theta^L_{\hat{\tau}^{-1}(i_v)} x_{\hat{\tau}^{-1}(i_v)} \mathbb{1}_{i_v\in \hat{V}_0} \\ &\quad + (\theta^S_{\hat{v}_1} \theta^L_{\hat{\tau}^{-1}(\hat{v}_1)} x_{\hat{\tau}^{-1}(\hat{v}_1)} + \theta^S_{\hat{v}_2} \theta^L_{\hat{\tau}^{-1}(\hat{v}_2)} x_{\hat{\tau}^{-1}(\hat{v}_2)}) \mathbb{1}_{i_v=(\hat{v}_1,\hat{v}_2)\in\hat{S}} \Big)_{i_{\tau^{-1}(\{v\})}} \partial_{i_r}.\end{aligned}$$

where we fix $\partial_{i_r} = \partial_1$ if $\gamma \in \Gamma^0$. By definition of the map i, if $\sigma(x) = y$, $\hat{\sigma}(i_x) = i_y$. Moreover, it is necessary that $\hat{\tau}^{-1}(i_v) = i_{\tau^{-1}(\{v\})}$ for $v \in V^\diamond$ (and analogously for $v \in S$) so that $(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})})^{i_v}_{i_{\tau^{-1}(\{v\})}}(0) \neq 0$. Thus, the map i is compatible with the source and target maps. In particular, i sends predecessors of v to predecessors of i_v.

On the other hand, the θ parameter enforces the injectivity of i and it forces i to send stolons to stolons, lianas to lianas, nodes in $V^\diamond$ to nodes in $\hat{V}^\diamond$. Thus i sends γ to a subgraph of $\hat{\gamma}$. If $\hat{\gamma} \neq \mu\gamma$, then at least an edge is missing and $\mathcal{F}_{|\hat{\gamma}|}(\gamma)(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})})(x)$ is a non-constant polynomial in x, so that it vanishes at $x = 0$.

If γ, $\hat{\gamma} \in \Gamma_c^0 \cup \Gamma_c$, the only maps i such that $(\mathcal{F}_{|\hat{\gamma}|}(\gamma)(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})}))^1_{\theta^\gamma}\Big|_{\theta=0}(0) \neq 0$ are the graph isomorphisms between γ and $\hat{\gamma}$. The number of such maps i is $\sigma(\gamma)$. □

Example. *Consider the following exotic aromatic tree with its associated vector field and elementary differential*

$\gamma =$ 

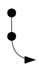
$$f_\gamma^{(\theta^\gamma)} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ \theta_1^S \theta_{\mathbf{2}}^L \theta_{\mathbf{3}}^L x_3^2 + \theta_2^S \theta_{\mathbf{1}}^L x_1 \\ 0 \end{pmatrix}, \quad (\mathcal{F}_3(\gamma)(f_\gamma^{(\theta^\gamma)}))^1_{\theta^\gamma}\Big|_{\theta=0}(0) = 2,$$

where the coordinates represent in descending order the root, the stolon, and the liana. Consider now the aroma

$\gamma =$ 

$$f_\gamma^{(\theta^\gamma)} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \theta_1^S \theta_{\mathbf{1}}^L x_2 + \theta_2^S \theta_{\mathbf{2}}^L x_2 \\ 0 \end{pmatrix}, \quad \theta^\gamma = (\theta_1^S, \theta_2^S, \theta_{\mathbf{1}}^L, \theta_{\mathbf{2}}^L),$$

and the tree

$\hat{\gamma} =$ 

$$f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \theta_1^{V^\diamond} x_2 \\ \theta_2^{V^\diamond} \end{pmatrix}, \quad \theta^{\hat{\gamma}} = (\theta_1^{V^\diamond}, \theta_2^{V^\diamond}).$$

A calculation yields

$$(\mathcal{F}_2(\gamma)(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})}))^1(x) = (\theta_1^{V^\diamond})^2, \quad (\mathcal{F}_2(\gamma)(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})}))^1_{\theta^\gamma}\Big|_{\theta=0}(0) = 0.$$

Note that fixing $\theta = \mathbb{1}$ yields $(\mathcal{F}_2(\gamma)(f_{\hat{\gamma}}^{(\mathbb{1})}))^1(0) = 1$, so that the dual vector field without the θ parameter fails to identify the difference between γ and $\hat{\gamma}$. The main use of the θ parameter in the proof of Proposition 4.1 is to enforce the map i to be injective and to preserve the nature of each pair $(v, \sigma(v))$. The dual vector field without the θ parameter is not sufficient, even in the aromatic context:

$\gamma =$ , $\hat{\gamma} =$ , $\mathcal{F}_{|\hat{\gamma}|}(\gamma)(f_{\hat{\gamma}}^{(\mathbb{1})})(0) = 1.$

This reveals a typographical error in [23, Rk. 4.8] where the remark only applies to exotic trees, and a minor error in [30, Sec. 4.2]. The further proofs of this paper can be adapted straightforwardly to fix the proofs in [30].

4.2 Strong characterisations

This section is devoted to the proof of Theorem 2.12. Following Subsection 3.1, as the regularity assumptions of Theorem 2.12 imply the locality, orthogonal-equivariance, and trivially decoupling properties, we work directly with $\varphi = \mathcal{F}(\gamma)$ and $\gamma \in \mathrm{Span}(\Gamma)$.

Proposition 4.3. *Connected exotic aromatic B-series are decoupling. B-series with stolons are Stiefel-equivariant and exotic B-series are Grassmann-equivariant.*

Proof. The decoupling property is straightforward from Definition 2.8. Let γ be an exotic aromatic tree without lianas and loops, $f \in \mathfrak{X}(\mathbb{R}^{d_1})$, $\hat{f} \in \mathfrak{X}(\mathbb{R}^{d_2})$, $a(x) = Ax + b \in \mathcal{S}(\mathbb{R}^{d_1}, \mathbb{R}^{d_2})$ with $d_1 \leqslant d_2$. Differentiating the identity $\hat{f}(a(x)) = Af(x)$ gives $a_{K,J}\hat{f}^i_K(a(x)) = a_{i,k}f^k_J(x)$. We call leaves the vertices in V that are not the target of any arrow. We say a node v has depth p if the shortest path of v to a leaf passes through p different nodes (not including the start and end points). The nodes of depth at most p are gathered in the set $V^{(p)}$. As γ does not have lianas or loops, $V^{(|\gamma|)} = V$. An induction on the depth yields

$$\begin{aligned}\mathcal{F}_{d_2}(\gamma)(\hat{f})(a(x)) &= \sum_{i,k} \prod_{v\in V^{(0)}} a_{i_v,k_v} f^{k_v}(x) \prod_{v\notin V^{(0)}} \hat{f}^{i_v}_{i_{\tau^{-1}(\{v\})}}(a(x))\delta_{i_\sigma}\partial_{i_{\mathbf{0}}} \\ &= \sum_{i,k} \prod_{v\in V^{(1)}} a^{(1)}_{i_v,k_v} a^{(1)}_{k_{\tau^{-1}(\{v\})}, i_{\tau^{-1}(\{v\})}} f^{k_v}_{k_{\tau^{-1}(\{v\})}}(x) \prod_{v\notin V^{(1)}} \hat{f}^{i_v}_{i_{\tau^{-1}(\{v\})}}(a(x))\delta^{(1)}_{i_\sigma}\delta^{(1)}_{k_\sigma}\partial_{i_{\mathbf{0}}} \\ &= \cdots = \sum_{i,k} \prod_{v\in V^{(|\gamma|)}} a^{(|\gamma|)}_{i_v,k_v} a^{(|\gamma|)}_{k_{\tau^{-1}(\{v\})}, i_{\tau^{-1}(\{v\})}} f^{k_v}_{k_{\tau^{-1}(\{v\})}}(x)\delta^{(|\gamma|)}_{i_\sigma}\delta^{(|\gamma|)}_{k_\sigma}\partial_{i_{\mathbf{0}}} \\ &= \sum_{i,k} \prod_{v\in V} a_{i_{\mathbf{0}},k_{\sigma(\mathbf{0})}} f^{k_v}_{k_{\tau^{-1}(\{v\})}}(x)\delta_{k_\sigma}\partial_{i_{\mathbf{0}}} = A\mathcal{F}_{d_1}(\gamma)(f)(x),\end{aligned}$$

where $a^{(p)}_{i_v,k_v} = a_{i_v,k_v}$ if $\sigma(v) \in \tau^{-1}(w)$ with $w \notin V^{(p)}$ and $a^{(p)}_{i_v,k_v} = 1$ else, $\delta^{(p)}_{i_\sigma}$, $\delta^{(p)}_{k_\sigma}$ contain the indices involved in the expression at step p, and the sums are on all involved indices.

On the other hand, let the exotic tree γ, the vector fields $f \in \mathfrak{X}(\mathbb{R}^{d_1})$, $\hat{f} \in \mathfrak{X}(\mathbb{R}^{d_2})$, and the affine transformation $a(x) = Ax + b \in \mathcal{G}(\mathbb{R}^{d_1}, \mathbb{R}^{d_2})$ with $d_1 \geqslant d_2$. We find

$$\begin{aligned}\mathcal{F}_{d_2}(\gamma)(g)(a(x)) &= \sum_{i,k} \prod_{v\in V} \hat{f}^{i_v}_{i_{\tau^{-1}(\{v\})}}(a(x))\delta_{i_\sigma}\partial_{i_{\mathbf{0}}} \\ &= \sum_{i,k} \prod_{v\in V} a_{i_{\tau^{-1}(\{v\})\cap L}, k_{\tau^{-1}(\{v\})\cap L}} \hat{f}^{i_v}_{i_{\tau^{-1}(\{v\})}}(a(x))\delta_{i_\sigma}\delta^{(L)}_{k_\sigma}\partial_{i_{\mathbf{0}}},\end{aligned}$$

where we used that $AA^T = I_{d_2}$ to add the coefficients associated to lianas and $\delta^{(L)}_{k_\sigma}$ identifies the coefficients k associated to lianas. The rest of the calculation is analogous to the Stiefel-equivariance case: we define the depth function on the tree without the lianas and we perform the calculation with an induction on the depth of the tree. □

Proposition 4.4. *Assume $\varphi = \mathcal{F}(\gamma)$ is decoupling, then $\gamma \in \mathrm{Span}(\Gamma_c)$.*

Proof. Let $\gamma \in \mathrm{Span}(\Gamma)$ and $\hat{\gamma} \in \Gamma$ be one of its exotic aromatic trees of maximal order among the ones that have at least one aroma, so that

$$\gamma = c\hat{\gamma} + R, \quad \hat{\gamma} = \mu_m \dots \mu_1\tau, \quad c \in \mathbb{R}, \quad R \in \mathrm{Span}(\Gamma). \tag{4.1}$$

Without loss of generality, we assume $c = 1$. Define $f^{(\theta^{\hat{\gamma}})}_{\hat{\gamma}}$ as in Proposition 4.1 and following the numbering of Remark 4.2,

$$f^{(\theta^{\hat{\gamma}})}_{\hat{\gamma}} = f^{(\theta^{\tau})}_{\tau} \oplus f^{(\theta^{\mu_1})}_{\mu_1} \oplus \cdots \oplus f^{(\theta^{\mu_m})}_{\mu_m} \in \mathfrak{X}(\mathbb{R}^d),$$

where the first entry of $f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})}$ corresponds to the root of τ. Using (2.5) and Proposition 4.1, we obtain

$$(\mathcal{F}_d(\gamma)(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})}))^1_{\theta^{\hat{\gamma}}}\Big|_{\theta=0}(0) = (\mathcal{F}_d(\hat{\gamma})(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})}))^1_{\theta^{\hat{\gamma}}}\Big|_{\theta=0}(0) \neq 0.$$

On the other hand, as $\mathcal{F}(\gamma)$ is decoupling, we find

$$(\mathcal{F}_d(\gamma)(f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})}))^1_{\theta^{\hat{\gamma}}}\Big|_{\theta=0}(0) = (\mathcal{F}_{|\tau|}(\gamma)(f_{\tau}^{(\theta^{\tau})}))^1_{\theta^{\hat{\gamma}}}\Big|_{\theta=0}(0) = 0,$$

as $\theta^{\hat{\gamma}}$ holds more parameters than θ^{τ}. We obtain a contradiction and $\gamma \in \mathrm{Span}(\Gamma_c)$. □

We now prove our second main result.

Proof of Theorem 2.12. Assume $\varphi = \mathcal{F}(\gamma)$ is decoupling, then Proposition 4.4 yields the connectedness of γ. Assume in addition that φ is local and Grassmann-equivariant and that at least one of the connected exotic aromatic trees τ in γ has a stolon or a loop. Consider $d_1 = |\tau|$, index the coordinates of $\mathbb{R}^{d_1}$ by $(V \cup \mathbf{A_0})/\sigma$ as in Proposition 4.1. We split the coordinates of $\mathbb{R}^{d_1}$ into $x = y \oplus z$, where $y \in \mathbb{R}^{d_2}$ contains the coordinates that are not stolons or nodes in a loop and z the others. Let $A \in \mathbb{R}^{d_2 \times d_1}$ be the projection matrix on $\mathbb{R}^{d_2}$, that is, $A(y \oplus z) = y$. Define $f_1 = f_{\tau}^{(\theta^{\tau})}$ and $f_2(Ax) = Af_1(x)$. The Grassmann-equivariance property and Proposition 4.1 yield

$$(\varphi_{d_2}(f_2))^1_{\theta^{\tau}}\Big|_{\theta=0}(0) = (\varphi_{|\tau|}(f_{\tau}^{(\theta^{\tau})}))^1_{\theta^{\tau}}\Big|_{\theta=0}(0) = (F_{|\tau|}(\tau)(f_{\tau}^{(\theta^{\tau})}))^1_{\theta^{\tau}}\Big|_{\theta=0}(0) = \sigma(\tau) \neq 0.$$

As $d_1 > d_2$, there is at least one $\theta_v^{V^\diamond}$ or θ_v^{S} that does not appear in f_2, but appears in θ^{τ}. Thus $(\varphi_{d_2}(f_2))^1_{\theta^{\tau}}\Big|_{\theta=0}(0) = 0$, which brings a contradiction.

Assume now that $\varphi = F(\gamma)$ is Stiefel-equivariant and that at least one of the exotic aromatic trees in γ has a liana or a loop. Consider the decomposition (4.1) of γ where $\hat{\gamma}$ is the term of maximal order among the ones that have a liana or a loop. For $d_2 = |\hat{\gamma}|$, we split the coordinates of $\mathbb{R}^{d_2}$ into $x = y \oplus z$ (or $x = z \oplus y$ if the root is a ghost liana, so that the root is still in first position), where $y \in \mathbb{R}^{d_1}$ contains the coordinates that are not lianas or nodes in a loop and z the others. Let $A \in \mathbb{R}^{d_2 \times d_1}$ be such that A^T is the projection matrix on $\mathbb{R}^{d_1}$, that is, $A^T(y \oplus z) = y$. Define $f_2 = f_{\hat{\gamma}}^{(\theta^{\hat{\gamma}})}$ and $f_1(y) = A^T f_2(y \oplus 0)$. Proposition 4.1 and the Stiefel-equivariance give

$$(\varphi_{d_1}(f_1))^1_{\theta^{\hat{\gamma}}}\Big|_{\theta=0}(0) = (\varphi_{d_2}(f_2))^1_{\theta^{\hat{\gamma}}}\Big|_{\theta=0}(0) \neq 0.$$

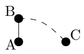
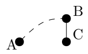
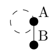
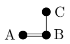
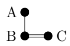
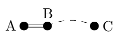
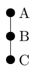
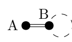
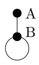
As $d_1 < d_2$, there is at least a node or a liana of $\hat{\gamma}$ that does not appear in f_1, but appears in $\theta^{\hat{\gamma}}$. We deduce $(\varphi_{d_1}(f_1))^1_{\theta^{\hat{\gamma}}}\Big|_{\theta=0}(0) = 0$, which brings a contradiction.

If φ is semi-orthogonal-equivariant, then γ is a linear combination of connected exotic aromatic trees without lianas, loops, and stolons, that is, a combination of standard Butcher trees. □

4.3 Impact of degeneracies on the classification

In a variety of contexts, the vector field f satisfies additional regularity properties. For instance, if f is a polynomial map of order p, then all exotic aromatic trees where at least a node is the target of more than p arrows have a trivial elementary differential. We mention in particular the work [4] on aromatic trees for quadratic differential equations that relies on such degeneracies. In the original numerical application of the exotic aromatic B-series in molecular dynamics [23, 24] (see also [27]), the vector fields f of interest are gradients, that is, $f = \nabla V$ for a smooth function $V\colon \mathbb{R}^d \to \mathbb{R}$. In [26, 13, 1], vector fields of the form $f = J\nabla V$ with J the symplectic matrix are used as perturbations to reduce the variance and accelerate the speed of convergence to equilibrium in the numerical integration of Langevin dynamics. In this section, we update the classification of Theorem 2.12 for gradient vector fields $f = \nabla V$, gathered in the set $\mathfrak{X}^\nabla(\mathbb{R}^d)$. As discussed in [23, Remark 4.8], the gradient property of f translates into degeneracies.

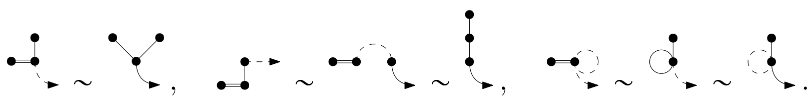
Proposition 4.5 ([23, 21])**.** *We say that two exotic aromatic trees γ_1 and γ_2 are equivalent on $\mathfrak{X}^\nabla(\mathbb{R}^d)$, written $\gamma_1 \sim \gamma_2$, if by performing the following operations, it is possible to transform γ_1 into γ_2:*

- *inversion edge-liana:*  $\sim$  *and*  $\sim$ ,
- *inversion edge-stolon:*  $\sim$ ,
- *simplification stolon-liana:*  $\sim$  *and*  $\sim$ .

The equivalence relation $\sim$ preserves the composition κ of the graph. Two equivalent exotic aromatic trees represent the same elementary differential $\mathcal{F}_d(\gamma_1) = \mathcal{F}_d(\gamma_2)$ on $\mathfrak{X}^\nabla(\mathbb{R}^d)$. Moreover, for any connected exotic aromatic tree, there exists a unique exotic tree in its equivalence class.

Proof. This is a direct consequence of the Schwarz theorem $f^i_{j_1\cdots j_q} = f^{j_p}_{j_1\cdots j_{p-1} i j_{p+1}\cdots j_q}$. ☐

Example. *The following connected exotic aromatic trees are equivalent to exotic trees:*



For further examples, the list of exotic aromatic trees of order 3 presented in Section A gathers the equivalent exotic aromatic trees in adjacent lines.

On $\mathfrak{X}^\nabla(\mathbb{R}^d)$, Theorem 2.11 and Theorem 2.12 simplify into the following simpler classification, which exactly characterises the exotic trees used in numerical analysis [23].

Theorem 4.6. *Let $\varphi = (\varphi_d\colon \mathfrak{X}^\nabla(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d))_d$ be a sequence of smooth maps. The Taylor expansion of φ around the trivial vector field 0 is an exotic B-series on $\mathfrak{X}^\nabla(\mathbb{R}^d)$ if and only if φ is local, orthogonal-equivariant, and decoupling.*

5 Conclusion and future works

In this work, we showed that smooth local orthogonal-equivariant maps and exotic aromatic B-series represent the same object. This universal property shows that exotic aromatic B-series are not just a tool for calculations in numerical analysis, but a natural algebraic object that is interesting in itself. The analysis relies on the invariant tensor theorem for orthogonal-equivariant tensors and the Peetre theorem, but also on a new generalised construction of exotic aromatic trees. In addition, we classified the intermediate subsets of exotic aromatic

B-series, and in particular the exotic B-series, with respect to strong equivariance properties. We also defined new dual vector fields and identified the effect of the degeneracies appearing in numerical analysis on the classification.

A variety of theoretical and applied questions arise from the present work. There exists different extensions of B-series such as partitioned B-series or Lie-Butcher series, and a variety of equivariance properties in $\mathbb{R}^d$ but also on manifolds. We mention in particular the equivariance with respect to symplectic tranformations. It would be interesting to link the different equivariance properties with the various B-series. This could allow us to create new extensions of B-series and to find corresponding applications in numerical analysis. For the B-series presented in this paper for instance, the B-series with stolons could be used in the study of projection methods for the approximation of ODEs on manifolds and modifications of the exotic aromatic formalism could be applied to the study of stochastic differential equations with multiplicative noise or to the creation of stochastic Lie-group methods of high weak order. This is matter for future work.

Acknowledgements. The work of Adrien Laurent was supported by the Research Council of Norway through project 302831 "Computational Dynamics and Stochastics on Manifolds" (CODYSMA).

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Appendices

A Exotic aromatic trees of order 3

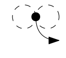
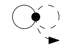
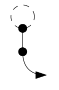
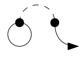
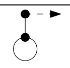
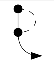
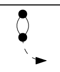
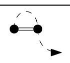
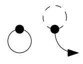
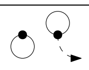
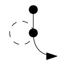
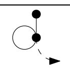
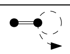
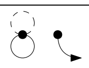
$\vert\kappa\vert$	κ	$\boldsymbol{\kappa}'$	τ	σ	γ	$\mathcal{F}(\gamma)(f)$
1	$(0,0,0,0,1)$	$(0,0,0,0,4)$	$(1,1,1,1)$	$(\mathbf{0},1)(\mathbf{1},\mathbf{2})(\mathbf{3},\mathbf{4})$		$f^i_{jjkk}\partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{2},1)(\mathbf{3},\mathbf{4})$		$f^j_{ijkk}\partial_i$
2	$(0,1,1)$	$(0,1,2)$	$(1,1,2)$	$(\mathbf{0},2)(\mathbf{1},\mathbf{2})(\mathbf{3},1)$		$f^i_j f^j_{kk}\partial_i$
				$(\mathbf{0},2)(\mathbf{1},1)(\mathbf{2},\mathbf{3})$		$f^i_j f^k_{jk}\partial_i$
				$(\mathbf{0},\mathbf{3})(1,2)(\mathbf{1},\mathbf{2})$		$f^j_i f^j_{kk}\partial_i$
				$(\mathbf{0},\mathbf{3})(\mathbf{1},1)(\mathbf{2},2)$		$f^j_i f^k_{jk}\partial_i$
				$(\mathbf{0},1)(\mathbf{1},2)(\mathbf{2},\mathbf{3})$		$f^i_{jk} f^j_k\partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{3},1)(\mathbf{2},2)$		$f^k_{ij} f^j_k\partial_i$
				$(\mathbf{0},\mathbf{1})(1,2)(\mathbf{2},\mathbf{3})$		$f^j_{ik} f^j_k\partial_i$
				$(\mathbf{0},1)(\mathbf{1},\mathbf{2})(\mathbf{3},2)$		$f^i_{jj} f^k_k\partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{2},1)(\mathbf{3},2)$		$f^j_{ij} f^k_k\partial_i$
2	$(1,0,0,1)$	$(0,0,0,3)$	$(1,1,1)$	$(\mathbf{0},1)(\mathbf{1},2)(\mathbf{2},\mathbf{3})$		$f^i_{jkk} f^j\partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{2},1)(\mathbf{3},2)$		$f^j_{ijk} f^k\partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{2},\mathbf{3})(1,2)$		$f^j_{ikk} f^j\partial_i$
				$(\mathbf{0},2)(\mathbf{1},1)(\mathbf{2},\mathbf{3})$		$f^i f^j_{jkk}\partial_i$

Table 3 (Part 1/2): List of the exotic aromatic trees of order three, with their associated composition, derived composition, target map, source map, and elementary differential (see Definition 2.8).

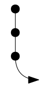
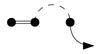
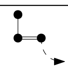
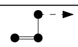
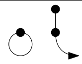
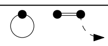
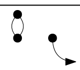
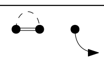
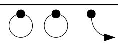
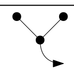
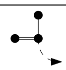
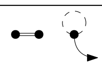
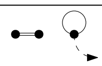
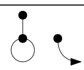
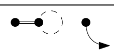
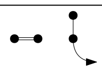
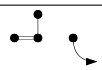
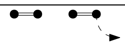
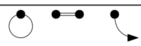
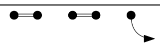
$\lvert\kappa\rvert$	κ	$\boldsymbol{\kappa}'$	τ	σ	γ	$\mathcal{F}(\gamma)(f)$
3	$(1,2)$	$(0,2)$	$(1,2)$	$(\mathbf{0},1)(\mathbf{1},2)(\mathbf{2},3)$		$f^i_j f^j_k f^k \partial_i$
				$(\mathbf{0},1)(\mathbf{1},\mathbf{2})(2,3)$		$f^i_j f^k_j f^k \partial_i$
				$(\mathbf{0},\mathbf{1})(1,2)(\mathbf{2},3)$		$f^j_i f^j_k f^k \partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{2},1)(2,3)$		$f^j_i f^k_j f^k \partial_i$
				$(\mathbf{0},1)(\mathbf{1},3)(\mathbf{2},2)$		$f^i_j f^j f^k_k \partial_i$
				$(\mathbf{0},\mathbf{2})(\mathbf{1},1)(2,3)$		$f^j_i f^j f^k_k \partial_i$
				$(\mathbf{0},3)(\mathbf{1},2)(\mathbf{2},1)$		$f^i f^j_k f^k_j \partial_i$
				$(\mathbf{0},3)(\mathbf{1},\mathbf{2})(1,2)$		$f^i f^j_k f^j_k \partial_i$
				$(\mathbf{0},3)(\mathbf{1},1)(\mathbf{2},2)$		$f^i f^j_j f^k_k \partial_i$
3	$(2,0,1)$	$(0,0,2)$	$(1,1)$	$(\mathbf{0},1)(\mathbf{1},2)(\mathbf{2},3)$		$f^i_{jj} f^j f^j \partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{2},2)(1,3)$		$f^j_{ik} f^j f^k \partial_i$
				$(\mathbf{0},1)(\mathbf{1},\mathbf{2})(2,3)$		$f^i_{jj} f^k f^k \partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{2},1)(2,3)$		$f^j_{ij} f^k f^k \partial_i$
				$(\mathbf{0},2)(\mathbf{1},1)(\mathbf{2},3)$		$f^i f^j_{jk} f^k \partial_i$
				$(\mathbf{0},3)(\mathbf{1},\mathbf{2})(1,2)$		$f^i f^j f^j_{kk} \partial_i$
4	$(3,1)$	$(0,1)$	(1)	$(\mathbf{0},1)(\mathbf{1},2)(3,4)$		$f^i_j f^j f^k f^k \partial_i$
				$(\mathbf{0},4)(1,2)(\mathbf{1},3)$		$f^i f^j f^j_k f^k \partial_i$
				$(\mathbf{0},\mathbf{1})(1,2)(3,4)$		$f^j_i f^j f^k f^k \partial_i$
				$(\mathbf{0},2)(\mathbf{1},1)(3,4)$		$f^i f^j f^j f^k_k \partial_i$
5	(5)	(0)		$(\mathbf{0},1)(2,3)(4,5)$		$f^i f^j f^j f^k f^k \partial_i$

Table 3 (Part 2/2): List of the exotic aromatic trees of order three, with their associated composition, derived composition, target map, source map, and elementary differential (see Definition 2.8).