What is an exotic aromatic B-series, really?

Adrien Laurent – Project CODYSMA
Joint work with H. Z. Munthe-Kaas

UNIVERSITETET I BERGEN
Det matematisk-naturvitenskapelige fakultet

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Backward error analysis

Consider an ODE with a vector field $f \in \mathfrak{X}(\mathbb{R}^d)$ and an integrator

$$y'(t) = f(y(t)), \quad y_{n+1} = \Phi(y_n, h).$$

Backward error analysis: the integrator can be rewritten as the exact solution of a modified equation

$$\tilde{y}'(t) = \tilde{f}(\tilde{y}(t)), \quad \tilde{f} \in \mathfrak{X}(\mathbb{R}^d).$$

The numerical properties (order, invariants, long-time behaviour,...) of the integrator can be read directly on $\tilde{f}$.

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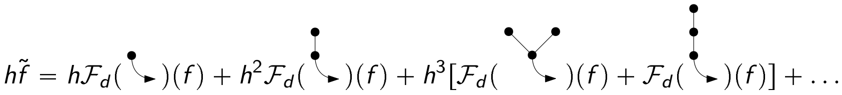
The modified vector field $\tilde{f}$ typically has the form[1]

$$h\tilde{f} = hf^i\partial_i + h^2 f^i_j f^j \partial_i + h^3[f^i_{jk} f^j f^k + f^i_j f^j_k f^k]\partial_i + \dots,$$

or equivalently with trees



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Stochastic backward error analysis

Consider overdamped Langevin dynamics in $\mathbb{R}^d$ or on manifolds:

$$dY(t) = \Pi_{\mathcal{M}}(Y(t))f(Y(t))dt + \Pi_{\mathcal{M}}(Y(t)) \circ dW(t).$$

Shardlow, 2006: there is no stochastic backward error analysis!

[2] Reference: L., Vilmart, 2020 ; L., Vilmart, 2022 ; Bronasco, 2023 ; Bronasco, L., in preparation.

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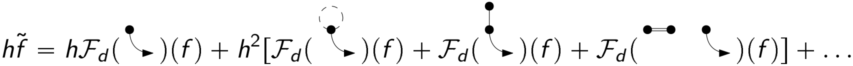
or equivalently with exotic aromatic trees[2]



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Application of exotic aromatic B-series

Forest γ	Differential $F(\gamma)(\phi)$	Exact $e(\gamma)$	Numerical approximation $a(\gamma)$
Terms of order 4 w.r.t. ϕ			
	$\sigma^4\Delta^2\phi$	$\frac{1}{8}$	$\frac{1}{8}$
	$\sigma^4 G^{-1}\Delta\phi''(g,g)$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$\sigma^4 G^{-2}\phi^{(4)}(g,g,g,g)$	$\frac{1}{8}$	$\frac{1}{8}$
Terms of order 3 w.r.t. ϕ			
	$\sigma^2\Delta\phi' f$	$\frac{1}{2}$	$\frac{1}{2}$
	$\sigma^2 G^{-1}\phi^{(3)}(g,g,f)$	$-\frac{1}{2}$	$-\frac{1}{2}$
	$\sigma^4 G^{-2}\phi^{(3)}(g,g,g'g)$	1	1
	$\sigma^4 G^{-1}\sum\phi^{(3)}(g,g'e_i,e_i)$	$-\frac{1}{2}$	$-\frac{1}{2}$
	$\sigma^2 G^{-2}(g,f)\phi^{(3)}(g,g,g)$	$\frac{1}{2}$	$\frac{1}{2}$
	$\sigma^4 G^{-2}\,\mathrm{div}(g)\phi^{(3)}(g,g,g)$	$\frac{1}{4}$	$\frac{1}{4}$
	$\sigma^4 G^{-2}(g,g'g)\phi^{(3)}(g,g,g)$	$-\frac{3}{4}$	$-\frac{3}{4}$
	$\sigma^2 G^{-1}(g,f)\Delta\phi'(g)$	$-\frac{1}{2}$	$-\frac{1}{2}$
	$\sigma^4 G^{-1}\,\mathrm{div}(g)\Delta\phi'(g)$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$\sigma^4 G^{-2}(g,g'g)\Delta\phi'(g)$	$\frac{1}{4}$	$\frac{1}{4}$
Terms of order 2 w.r.t. ϕ			
	$\phi''(f,f)$	$\frac{1}{2}$	$\frac{1}{2}$
	$\sigma^2\sum\phi''(f'e_i,e_i)$	$\frac{1}{2}$	$b^T d$
	$\sigma^2 G^{-1}\phi''(g,g'f)$	-1	-1
	$\sigma^2 G^{-1}\phi''(g,f'g)$	-1	$-b^T d-\widehat{b}^T d$
	$\sigma^4 G^{-2}\phi''(g,g'g'g)$	$\frac{3}{2}$	$-2\widehat{b}^T(d\bullet\widehat{A}d)-(\widehat{b}^T d)^2+2\widehat{b}^T d+1$

Question:

Are exotic aromatic B-series just a useful tool for the calculation of order conditions?

Figure: Coefficients in exotic aromatic forests of the Talay-Tubaro operators - Part 1/7

Contents

References of this talk:

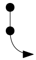
• A. Laurent and G. Vilmart. Exotic aromatic B-series for the study of long time integrators for a class of ergodic SDEs. arXiv:1707.02877. *Math. Comp.* (2020).
• A. Laurent and G. Vilmart. Order conditions for sampling the invariant measure of ergodic stochastic differential equations on manifolds, arXiv:2006.09743, *Found. Comput. Math.* (2022).
• A. Laurent and H. Z. Munthe-Kaas. The universal equivariance properties of exotic aromatic B-series, *In preparation*.

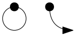
Contents

Prototypes of exotic aromatic trees

References on aromatic B-series: Iserles, Quispel, Tse, 2007 ; Chartier Murua, 2007 ; Markl, 2008 ; Bogfjellmo, 2019 ; Bogfjellmo, Celledoni, McLachlan, Owren, Quispel, 2022 ; L., McLachlan, Munthe-Kaas, Verdier, 2023

Examples of aromatic trees:

$\mathcal{F}_d($  $)(f) = f'f = f^i_j f^j \partial_i$

$\mathcal{F}_d($  $)(f) = \mathrm{div}(f)f = f^j_j f^i \partial_i$

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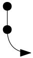
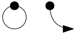
$\mathcal{F}_d($  $)(f) = f'f = f^i_j f^j \partial_i$

$\mathcal{F}_d($  $)(f) = \mathrm{div}(f)f = f^j_j f^i \partial_i$

Examples of exotic aromatic trees:

$\mathcal{F}_d($  $)(f) = \Delta f = f^i_{jj} \partial_i$

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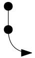
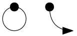
$\mathcal{F}_d($  $)(f) = f'f = f^i_j f^j \partial_i$

$\mathcal{F}_d($  $)(f) = \mathrm{div}(f) f = f^j_j f^i \partial_i$

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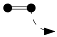
New exotic aromatic trees:

$\mathcal{F}_d($  $)(f) = \nabla \mathrm{div}(f) = f^j_{ij} \partial_i$

$\mathcal{F}_d($  $)(f) = (f, \nabla f) = f^j f^j_i \partial_i$

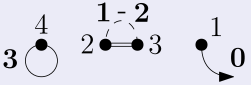
Exotic aromatic trees

Definition

Let the exotic aromatic tree $\gamma = (V, \mathbf{A_0}, \sigma, \tau)$ with the nodes $V = \{1, 2, 3, 4\}$, the arrows $\mathbf{A_0} = \{\mathbf{0}, \mathbf{1}, \mathbf{2}, \mathbf{3}\}$, the target map $\tau \colon \mathbf{A} \to V$ and source map σ given by

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

The associated graph and elementary differential are



$$\mathcal{F}_d(\gamma)(f) = f^{i_1} f^{i_2}_{i_\mathbf{1}} f^{i_3}_{i_\mathbf{2}} \delta_{i_\mathbf{0}, i_1} \delta_{i_\mathbf{1}, i_2} \delta_{i_2, i_3} \delta_{i_\mathbf{3}, i_4} \partial_{i_\mathbf{0}} = f^i f^j_k f^j_k f^l_l \partial_i$$

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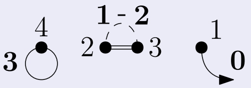

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- An aroma is a connected component without root.
- An exotic tree is an exotic aromatic tree that reduces to a tree when removing the lianas.
- the order of a tree is $|\gamma| = (|V| + |\mathbf{A_0}|)/2$.
- An exotic aromatic B-series is

$$B(b) = (B_d(b))_d, \qquad B_d(b) = \sum_{m>0} \sum_{|\kappa|=m} \sum_{\gamma \in \Gamma_\kappa} b(\gamma) \mathcal{F}_d(\gamma).$$

Examples of exotic aromatic trees

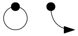
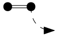
$\lvert\gamma\rvert$	$\lvert V\rvert$	τ	σ	γ	$\mathcal{F}(\gamma)(f)$
1	1		$(\mathbf{0},1)$		$f^i\partial_i$
2	1	$(1,1)$	$(\mathbf{0},1)(\mathbf{1},\mathbf{2})$		$f^i_{jj}\partial_i$
			$(\mathbf{0},\mathbf{1})(\mathbf{2},1)$		$f^j_{ij}\partial_i$
2	2	(1)	$(\mathbf{0},1)(\mathbf{1},2)$		$f^i_j f^j\partial_i$
			$(\mathbf{0},2)(\mathbf{1},1)$		$f^j_j f^i\partial_i$
			$(\mathbf{0},\mathbf{1})(1,2)$		$f^j f^j_i\partial_i$
2	3		$(\mathbf{0},1)(2,3)$		$f^i f^j f^j\partial_i$

Table: List of the exotic aromatic trees of order one and two.

Contents

Equivariance properties

Definition

A sequence of smooth maps $\varphi = (\varphi_d \colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d))_d$ is $\mathcal{A}$-equivariant if for $a(x) = Ax + b \colon \mathbb{R}^{d_1} \to \mathbb{R}^{d_2} \in \mathcal{A}$, φ satisfies for $f_1 \in \mathfrak{X}(\mathbb{R}^{d_1})$, $f_2 \in \mathfrak{X}(\mathbb{R}^{d_2})$,

$$f_2(a(x)) = Af_1(x) \;\Rightarrow\; \varphi_{d_2}(f_2)(a(x)) = A\varphi_{d_1}(f_1)(x).$$

- GL-equivariance: $A \in \mathrm{GL}_d(\mathbb{R})$,
- Affine-equivariance: $A \in \mathbb{R}^{d_2 \times d_1}$,
- Orthogonal-equivariance: $A \in \mathrm{O}_d(\mathbb{R})$,
- Stiefel-equivariance: $A^T A = I_{d_1}$,
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- Semi-orthogonal-equivariance= Stiefel + Grassmann equivariance.

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Theorem (McLachlan, Modin, Munthe-Kaas, Verdier, 2016)

B-series are exactly the affine equivariant maps. Aromatic B-series are exactly the local GL*-equivariant maps.*

The exotic aromatic classification

Theorem (L., Munthe-Kaas, 2023)

The exotic aromatic classification of sequences of smooth local maps $\varphi = (\varphi_d \colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d))_d$ is the following.

Geometric property	*Associated Butcher series*
orthogonal-equivariance	*exotic aromatic B-series*
Stiefel-equivariance	*B-series with stolons*
Grassmann-equivariance	*exotic B-series*
GL-*equivariance*	*aromatic B-series*
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Moreover, exotic aromatic B-series keep decoupled systems decoupled if and only if they are connected.

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affine/semi-orthogonal-equivariance	*B-series*

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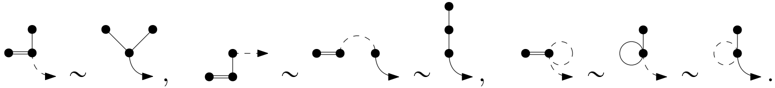
Remark: degeneracies impact the classification. For instance, if we consider $f = \nabla V$, connected exotic aromatic trees can be rewritten as exotic trees.



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Invariant tensors and combination of trees

Let $\varphi_d \colon \mathfrak{X}(\mathbb{R}^d) \to \mathfrak{X}(\mathbb{R}^d)$ be a smooth local orthogonal-equivariant map. The Taylor expansion of φ_d around 0 is, by Peetre's theorem,

$$\sum_{m \geqslant 1} \frac{1}{m!} \sum_{\substack{\kappa \colon \mathbb{N} \to \mathbb{N} \\ |\kappa| = m}} \psi_{\kappa,d}(f^\kappa), \quad f^\kappa = (\underbrace{f, \dots, f}_{\kappa(0)}, \underbrace{f', \dots, f'}_{\kappa(1)}, \dots),$$

where $\psi_{\kappa,d} \in \mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})}$, $\mathcal{S}_\kappa = M \otimes \bigotimes_{j=0}^\infty S^{\kappa(j)}(M^* \otimes S^j M)$, and $M = T_0\mathbb{R}^d \equiv \mathbb{R}^d$.

Theorem (Weyl, 1939)

The tensor space $\mathcal{S}_\kappa^{\mathrm{O}_d(\mathbb{R})}$ is trivial if $|\kappa| + |\boldsymbol{\kappa}'| + 1 \notin 2\mathbb{Z}$.

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Theorem (L., Munthe-Kaas, 2023)

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

Interaction between the dimensions

The proof of the classification uses dual vector fields $f_\gamma^{(\theta^\gamma)}$:

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

Example

Consider the following exotic aromatic tree with its dual vector field

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

and the elementary differential is $(\mathcal{F}_3(\gamma)(f_\gamma^{(\theta^\gamma)}))^1_{\theta^\gamma}\Big|_{\theta=0}(0) = 2.$

The classification of exotic aromatic B-series is obtained with proofs by contradiction using the dual vector fields.

Conclusion and outlook

Summary:

- We presented a generalised definition of exotic aromatic B-series and characterised them with a universal geometric property. This confirms that exotic aromatic B-series are an algebraic object interesting in itself, and not just a tool for calculations.
- We classified the different subsets of exotic aromatic B-series according to a variety of natural equivariance properties. We defined dual vector fields for exotic aromatic trees.
- The classification confirms that the exotic extension of aromatic B-series is natural as both exotic aromatic and aromatic B-series satisfy similar universal geometric properties.

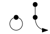
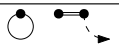
Outlooks and future works:

- Characterisation of other B-series (partitioned B-series, Lie-Butcher series, exponential B-series,...) with different equivariance properties (especially on manifolds).
- In the manifold case, it is not known yet whether the modified vector field can be written as an exotic aromatic B-series at any order. The $\mathbb{R}^d$ case is presented in Bronasco, L., in preparation.
- Numerical application of B-series with stolons with projection methods.

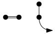
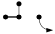
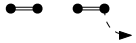
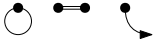
Exotic aromatic trees of order 3

$\|\kappa\|$	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	$(1,0,0,1)$	$(0,0,0,3)$	$(1,1,1)$	$(\mathbf{0},1)(\mathbf{1},2)(\mathbf{2},\mathbf{3})$		$f^i_{jkk} f^j\partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{2},1)(\mathbf{3},2)$		$f^j_{ijk} f^k\partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{2},\mathbf{3})(1,2)$		$f^j_{ikk} f^j\partial_i$
				$(\mathbf{0},2)(\mathbf{1},1)(\mathbf{2},\mathbf{3})$		$f^i f^j_{jkk}\partial_i$

Exotic aromatic trees of order 3

$\lvert\kappa\rvert$	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	$(2,0,1)$	$(0,0,2)$	$(1,1)$	$(\mathbf{0},1)(\mathbf{1},2)(\mathbf{2},3)$		$f^i_{jj} f^j f^j \partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{2},2)(1,3)$		$f^j_{ik} f^j f^k \partial_i$
				$(\mathbf{0},1)(\mathbf{1},\mathbf{2})(2,3)$		$f^i_{jj} f^k f^k \partial_i$
				$(\mathbf{0},\mathbf{1})(\mathbf{2},1)(2,3)$		$f^j_{ij} f^k f^k \partial_i$
				$(\mathbf{0},2)(\mathbf{1},1)(\mathbf{2},3)$		$f^i f^j_{jk} f^k \partial_i$
				$(\mathbf{0},3)(\mathbf{1},\mathbf{2})(1,2)$		$f^i f^j f^j_{kk} \partial_i$

Exotic aromatic trees of order 3

$\lvert\kappa\rvert$	κ	$\boldsymbol{\kappa}'$	τ	σ	γ	$\mathcal{F}(\gamma)(f)$
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)		$(\mathbf{0},1)(2,3)(4,5)$		$f^i f^j f^j f^k f^k \partial_i$

Combinatorics:

Order	Trees	Aromatic trees	Exotic aromatic trees
1	1	1	1
2	1	2	6
3	2	6	35
4	4	16	
5	9	45	