Application of the Hopf algebra structures of exotic aromatic series to stochastic numerical analysis

Adrien Laurent - INRIA Rennes
Joint work with Eugen Bronasco

Stochastic Numerics with Applications to Sampling, SciCADE, 2024

Main reference of this talk:

E. Bronasco, A. Laurent. Hopf algebra structures for the backward error analysis of ergodic stochastic differential equations. *arxiv:2407.07451*.

Backward error analysis

Given a numerical integrator $y_{n+1} = \Phi_h^f(y_n)$ for solving $y' = f(y)$, there exists a (formal) modified vector field $h\tilde{f}$ such that
"The integrator is the exact solution of the modified ODE $\tilde{y}'(t) = \tilde{f}(\tilde{y}(t))$."

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Theorem (see Hairer, Lubich, Wanner, 2006)

The properties of the integrator are read on $\tilde{f}$:

- *if $\tilde{f} = f + \mathcal{O}(h^p)$, the scheme has order p.*
- *if $f = J\nabla H$ and the scheme is symplectic, the scheme preserves a modified Hamiltonian and $\tilde{f} = J\nabla\tilde{H}$.*
- *if $\operatorname{div}(\tilde{f}) = \operatorname{div}(f) = 0$, the scheme is volume-preserving.*

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Remark on modified equations: there also exists a modified vector field $h\tilde{f}$ such that: **"The integrator applied to $\tilde{y}'(t) = \tilde{f}(\tilde{y}(t))$ is exact for $y' = f(y)$."**

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The modified vector field $\tilde{f}$ can be conveniently computed with Butcher series:

$$h\tilde{f} = hf - \frac{h^2}{2} f'f + h^3\Big[\frac{1}{12} f''(f,f) + \frac{1}{3} f'f'f\Big] + \dots,$$
$$= hF_f(\bullet) - \frac{h^2}{2} F_f([\bullet]) + h^3\Big[\frac{1}{12} F_f([\bullet,\bullet]) + \frac{1}{3} F_f([[\bullet]])\Big] + \dots$$

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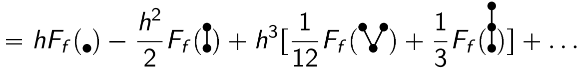


Question: do backward error analysis and the Butcher tree interpretation extend to the stochastic context?

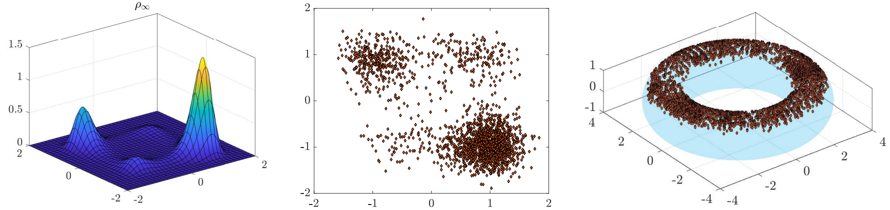
Ergodicity of overdamped Langevin dynamics

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

$$dX(t) = (\Pi_{\mathcal{M}} f)(X(t))dt + \Pi_{\mathcal{M}}(X(t)) \circ dW(t), \quad f = -\nabla V,$$

Euler-Maruyama method:

$$X_{n+1} = X_n + hf(X_n) + \Delta W_n.$$



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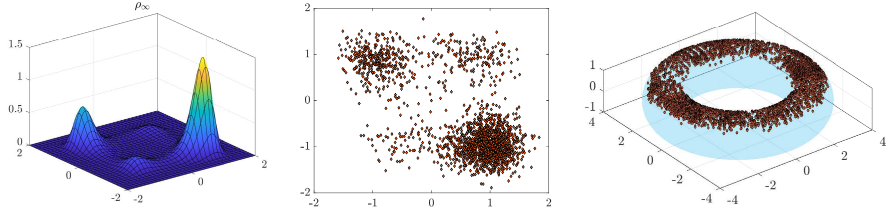

Different types of convergence:

- Strong (approximation of a single trajectory for a realization of $W(t)$),
- Weak (approximation of the law of $X(t)$),
- Invariant measure (approximation of the law of $X(t)$ at equilibrium).

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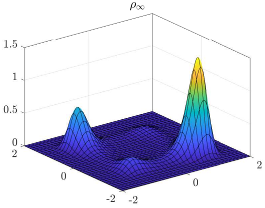

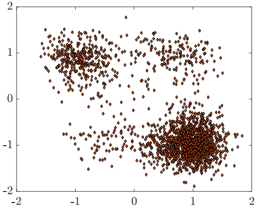

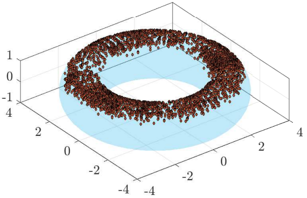

Ergodicity properties:

$$\lim_{T\to+\infty} \frac{1}{T}\int_0^T \phi(X(s))ds = \int_{\mathcal{M}} \phi(y)d\mu_\infty(y) \quad \text{almost surely,}$$

$$\lim_{N\to+\infty} \frac{1}{N+1}\sum_{n=0}^{N} \phi(X_n) = \int_{\mathcal{M}} \phi(y)d\mu^h(y)(y) \quad \text{almost surely.}$$

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BUT, for ergodic dynamics, the measure μ^h is the invariant measure of a modified SDE with a formal modified vector field $\tilde{f}$:

$$d\widetilde{Y}(t) = \widetilde{f}(\widetilde{Y}(t))dt + dW(t), \quad \mu^h = \widetilde{\mu_\infty} = \mu_\infty + h\mu^{[1]} + h^2\mu^{[2]} + \dots$$

Remark: a method is invariant-measure-preserving if

$$\mathrm{div}(\widetilde{f}) + \langle f, \widetilde{f} \rangle = \mathrm{div}(f) + \langle f, f \rangle.$$

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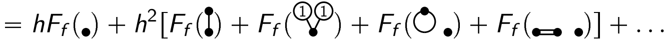
• L., Vilmart, 2020 & 2022:
The modified vector field $\tilde{f}$ can be conveniently computed with exotic aromatic series up to order 3 in $\mathbb{R}^d$ and order 2 on $\mathcal{M}$:

$$h\tilde{f} = hf + h^2[f'f + \Delta f + \mathrm{div}(f)f + \langle f, f \rangle f] + \dots$$



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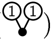
Main result:

Theorem (Bronasco, L., 2024)

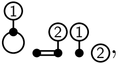
Under mild algebraic assumptions on the integrator, its modified vector field $\tilde{f}$ writes as an exotic aromatic B-series at any order and is given by an explicit formula.

Exotic aromatic series[1]

Prototypes of exotic aromatic forests EAF:

$F_f($$) = f'f$, $F_f($$) = \mathrm{div}(f)$, $F_f($$) = \langle f, f\rangle$, $F_f($$) = \Delta f$.

Example:

$\pi =$ , $$F_f(\pi)[\phi] = \sum_{i,j,s,l_1,l_2=1}^{d} f^i_{il_1} f^s f^s_{l_2} f^j_{l_1} \phi_{jl_2}.$$

Given $a \in EAF^*$, an exotic aromatic S-series is a formal series indexed by exotic aromatic forests:

$$S^h_f(a) = \sum_{\pi\in EAF} h^{|\pi|} \frac{a(\pi)}{\sigma(\pi)} F_f(\pi).$$

Example: exact flow of $dX = f(X) + dW$:

$$\mathbb{E}[\phi(X(h))] = \phi(x) + h\Big[\phi' f + \frac{1}{2}\Delta\phi\Big] + h^2\Big[\frac{1}{2}\phi' f' f + \frac{1}{4}\phi'\Delta f + \frac{1}{2}\phi''(f,f) + \dots$$

$= \mathbb{1} + h\Big[\bullet + \frac{1}{2}$ ①① $\Big] + h^2\Big[\frac{1}{2}$  $+ \frac{1}{4}$  $+ \frac{1}{2}\bullet\ \bullet + \dots$

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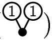
$F_f($$) = f'f$, $F_f($$) = \mathrm{div}(f)$, $F_f($$) = \langle f, f\rangle$, $F_f($$) = \Delta f$.

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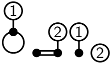
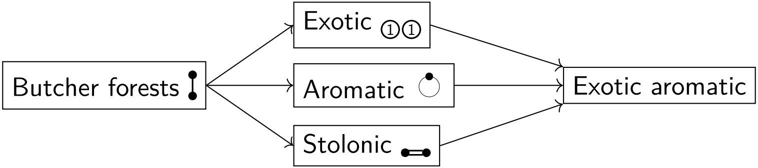
$\pi =$ , $$F_f(\pi)[\phi] = \sum_{i,j,s,l_1,l_2=1}^{d} f^i_{il_1} f^s f^s_{l_2} f^j_{l_1} \phi_{jl_2}.$$



[1] Aromatic B-series: Iserles, Quispel, Tse, 2007 ; Chartier, Murua, 2007 ; ...

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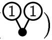
$F_f($$) = f'f$, $F_f($$) = \mathrm{div}(f)$, $F_f($$) = \langle f, f\rangle$, $F_f($$) = \Delta f$.

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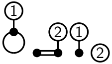
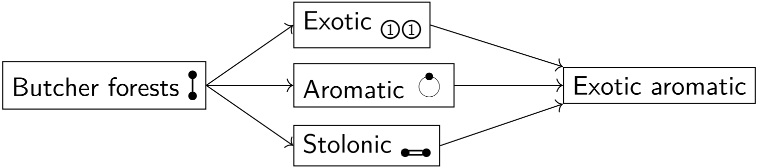
$\pi =$ , $\quad F_f(\pi)[\phi] = \sum_{i,j,s,l_1,l_2=1}^{d} f^i_{il_1} f^s f^s_{l_2} f^j_{l_1} \phi_{jl_2}.$



Proposition (L., Munthe-Kaas, 2024)

Exotic aromatic B-series are exactly the smooth local orthogonal equivariant maps.

[1] Aromatic B-series: Iserles, Quispel, Tse, 2007 ; Chartier, Murua, 2007 ; ...

New algebraic tools for backward error analysis

Idea of stochastic backward error analysis: consider

- the exact flow $\mathbb{E}[\phi(X(h))] = S_f^h(e)[\phi] = \phi + h\mathcal{L}\phi + \frac{h^2}{2}\mathcal{L}^2\phi + \dots,$
- the numerical flow $\mathbb{E}[\phi(X_1)] = S_f^h(a)[\phi] = \phi + h\mathcal{A}_1\phi + h^2\mathcal{A}_2\phi + \dots,$
- a flow $\varphi^h[\phi]$ preserves the invariant measure if

$$\int \varphi^h[\phi] d\mu_\infty = \int \phi d\mu_\infty.$$

Then, we want $h\tilde{f} = B_f^h(b)$ written as an exotic aromatic B-series such that **"the exact flow of the modified problem has the same invariant measure as the integrator"**.

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Difficulties:

1. Compute the exact flow $\mathbb{E}[\phi(\tilde{X}(h))]$ of the modified problem

$$d\tilde{X} = \tilde{f}(\tilde{X}) + dW, \quad h\tilde{f} = B_f^h(b) = hf + h^2\alpha f'f + h^2\beta\Delta f + \dots$$

2. Find $\tilde{f}$ such that $\mathbb{E}[\phi(\tilde{X}(h))]$ and $\mathbb{E}[\phi(X_1)]$ have same invariant measure.
3. the aromas (Bogfjellmo, 2019). (idea of clumping)

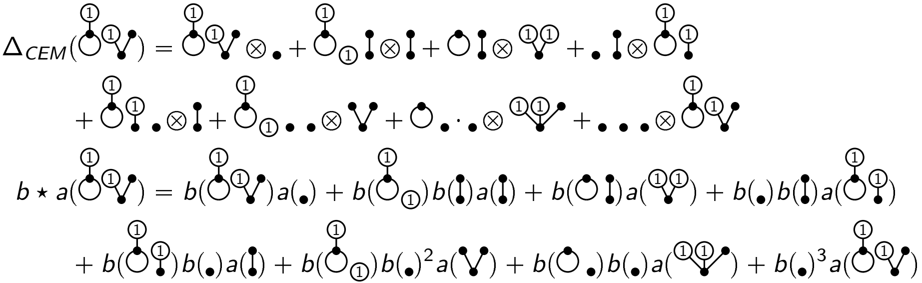
Tool 1: Hopf algebra for the substitution[2]

Characters satisfy $b(\pi_1 \cdot \pi_2) = b(\pi_1)b(\pi_2)$.

Theorem (Bronasco, L., 2024)

The substitution $hf \leftarrow B_f^h(b)$ in $S_f^h(a)$ is $S_f^h(b \star a)$, with $b \star a = (b \otimes a) \circ \Delta_{CEM}$,

$$\Delta_{CEM}(\pi) := \sum_{p \subset \pi} p \otimes \pi/_p.$$



[2] see also Chartier, Hairer, Vilmart, 2010; Calaque, Ebrahimi-Fard, Manchon, 2011; Bogfjellmo, 2019

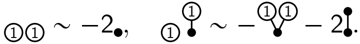
Tool 2: The integration by parts

Goal: reduce operators to **order one** differential operators

$$\int S_f^h(a)[\phi]d\mu_\infty = \int \phi' \widetilde{f} d\mu_\infty, \quad \widetilde{f} = B_f^h(b).$$

Integration by parts (L., Vilmart, '20-'22):

$$\int \Delta\phi d\mu_\infty = -\int \phi' f d\mu_\infty,$$

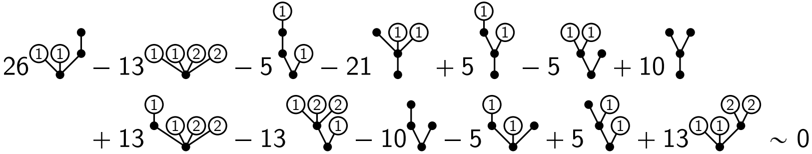


Proposition (Bronasco, 2023)

If a is a character over exotic forests, there exists an exotic B-series $h\widetilde{f} = B_f^h(b)$ such that $\int S_f^h(a)[\phi]d\mu_\infty = \int(\phi + h\phi'\widetilde{f})d\mu_\infty$.

Remark 1: the extension in the manifold case is open.

Remark 2: $\sim$ has a kernel:



Exotic aromatic series for backward error analysis

Theorem (Bronasco, L., 2024)

Consider a consistent method $S_f^h(a)$ for solving Langevin dynamics with $a \in Char(\mathcal{EF}, \cdot)$, then, there exists a modified vector field $h\widetilde{f} = B_f^h(b)$ with $b\colon \mathcal{ET} \to \mathbb{R}$ satisfying $b(\bullet) = 1$, $b_c \star e \sim a$, and given by an explicit formula.

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Application: The constrained Euler scheme on the sphere:

$$X_{n+1} = X_n + hf(X_{n+1}) + \sqrt{h}\xi_n + \lambda_n X_{n+1}, \quad |X_{n+1}| = 1.$$

has order 2 for the invariant measure when applied with the modified vector field

$$\begin{aligned}\widetilde{f} = f + h\Big[& -\frac{1}{2}f'f - \frac{1}{4}\Delta f + \frac{3}{4}f - \frac{1}{4}\operatorname{div}(n)f - \frac{1}{2}\langle n, f\rangle f - \frac{1}{4}f'n - \frac{1}{4}\operatorname{div}(n)f'n \\ & - \frac{1}{2}\langle n, f\rangle f'n - \frac{1}{4}f''(n,n) + \frac{1}{2}\langle n, f\rangle\langle n, f'n\rangle n + \frac{1}{4}\langle n, f''(n,n)\rangle n - \frac{1}{4}\operatorname{div}(f)'nn \\ & - \frac{1}{2}\langle n, f'f\rangle n + \frac{1}{4}\langle n, f'n\rangle n + \frac{1}{4}\operatorname{div}(n)(n, f'n\rangle n + \frac{1}{2}\langle n, f\rangle^2 n - \frac{3}{4}\langle n, f\rangle n \\ & + \frac{1}{4}\operatorname{div}(n)\langle n, f\rangle n\Big].\end{aligned}$$

Conclusion and outlooks

Summary:

- The concept of backward error analysis extends to the stochastic context through the approximation of the invariant measure of ergodic systems.
- We introduced the exotic aromatic formalism. It provides an algebraic framework for the calculations of order conditions.
- We present the Hopf algebra structures of composition and substitution of exotic aromatic S-series and apply them to provide an explicit algebraic description of stochastic backward error analysis at any order.
- The exotic aromatic series are natural objects that satisfy universal geometric and algebraic properties.

Outlooks and future works:

- Understanding of $\sim$ and backward error analysis for projection methods.
- Creation of discretisations that preserve the invariant measure exactly, in the spirit of volume-preserving methods (see L., MacLachlan, Munthe-Kaas, Verdier).
- Creation of high-order intrinsic methods on manifolds (see Bharath, Lewis, Sharma, Tretyakov, 2024).
- Study of exotic aromatic rough paths, algebraic structure of clumping,. . .

S-series, characters and primitive elements

Exact flow of $y' = f(y)$:

$$y(h) = y_0 + hf + \frac{h^2}{2} f'f + \frac{h^3}{6}[f''(f,f) + f'f'f] + \dots$$

$$= y_0 + hF_f(\bullet) + \frac{h^2}{2} F_f([\bullet]) + \frac{h^3}{6}[F_f([\bullet,\bullet]) + F_f([[\bullet]])] + \dots$$

Numerical flow $y_1 = y_0 + \sum_i b_i f(Y_i),\ Y_i = y_0 + \sum_j a_{ij} f(Y_j)$:

$$y_1 = y_0 + h\sum_i b_i f + h^2 \sum_i b_i c_i f'f + h^3[\frac{1}{2}\sum_i b_i c_i^2 f''(f,f) + \sum_i b_i a_{ij} c_j f'f'f] + \dots$$

$$= y_0 + h\sum_i b_i F_f(\bullet) + h^2 \sum_i b_i c_i F_f([\bullet]) + h^3[\frac{1}{2}\sum_i b_i c_i^2 F_f([\bullet,\bullet]) + \sum_i b_i a_{ij} c_j F_f([[\bullet]])] + \dots$$

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$$= \phi(y_0) + h\bullet + h^2[\frac{1}{2}[\bullet] + \frac{1}{2}\bullet\,\bullet] + h^3[\frac{1}{6}[\bullet,\bullet] + \frac{1}{6}[[\bullet]] + \frac{1}{2}\bullet\,[\bullet] + \frac{1}{6}\bullet\,\bullet\,\bullet] + \dots$$

Numerical flow $y_1 = y_0 + \sum_i b_i f(Y_i)$, $Y_i = y_0 + \sum_j a_{ij} f(Y_j)$:

$$\phi(y_1) = \phi(y_0) + h\sum_i b_i \bullet + h^2[\sum_i b_i c_i [\bullet] + \frac{1}{2}(\sum_i b_i)^2 \bullet\,\bullet]$$
$$+ h^3[\frac{1}{2}\sum_i b_i c_i^2 [\bullet,\bullet] + \sum_i b_i a_{ij} c_j [[\bullet]] + (\sum_i b_i)(\sum_i b_i c_i)\bullet\,[\bullet] + \frac{1}{6}(\sum_i b_i)^3 \bullet\,\bullet\,\bullet] + \dots$$

S-series, characters and primitive elements

Exact flow of $y' = f(y)$:

$$\phi(y(h)) = \phi(y_0) + h\phi' f + \frac{h^2}{2}[\phi' f' f + \phi''(f,f)] + \dots$$

$$= \phi(y_0) + h\bullet + h^2[\frac{1}{2}[\bullet] + \frac{1}{2}\bullet\,\bullet] + h^3[\frac{1}{6}[\bullet,\bullet] + \frac{1}{6}[[\bullet]] + \frac{1}{2}\bullet\,[\bullet] + \frac{1}{6}\bullet\,\bullet\,\bullet] + \dots$$

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Characters satisfy $a(\pi_1 \cdot \pi_2) = a(\pi_1)a(\pi_2)$

Primitive elements = elements that cannot be split

$$a(\bullet\,[\bullet]\,[\bullet,\bullet]) = a(\bullet)a([\bullet])a([\bullet,\bullet])$$

Problem: In stochastic, ①① is primitive!

Exotic aromatic series for backward error analysis

Theorem (Bronasco, L., 2024)

Consider a consistent method $S_f^h(a)$ for solving Langevin dynamics with $a \in Char(\mathcal{EF}, \cdot)$, then, there exists a modified vector field $h\widetilde{f} = B_f^h(b)$ with $b\colon \mathcal{ET} \to \mathbb{R}$ satisfying $b(\bullet) = 1$, $b_c \star e \sim a$, and given by

$$b = \delta_\bullet + A\Big(\sum_{k=0}^{\infty} (-1)^k A_{\tilde{\star}e}^k (a-e)\Big),$$

where $A_{\tilde{\star}e}(x) = A(x)\tilde{\star}e$ and for all $\tau \in ET$ such that $|\tau| > 1$, we define

$$\tilde{\Delta}_{CEM}(\tau) = \Delta_{CEM}(\tau) - \bullet \otimes \tau - \tau \otimes \bullet, \quad \text{and} \quad b_{n-1,c}\tilde{\star}e = (b_{n-1,c} \otimes e) \circ \tilde{\Delta}_{CEM}.$$

Theorem (Bronasco, L., 2024)

- $(\mathcal{EAF}, \mathbf{1}, \diamond, \epsilon_{\mathcal{EA}}, \Delta_{\mathcal{EA}}, S_\diamond)$ *forms a Grossman-Larson Hopf algebroid.*
- $(\mathcal{CEF}, \mathbf{1}, \diamond, \epsilon, \Delta, S_\diamond^C)$ *forms a Grossman-Larson Hopf algebra.*
- $(\mathcal{CEF}, \mathbf{1}, \cdot, \mathbf{1}^*, \Delta_{CEM}, S)$ *forms a Hopf algebra.*

Composition of exotic aromatic S-series

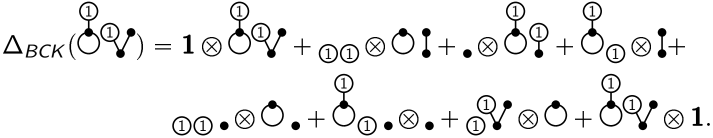
Theorem (Bronasco, 2023)

Let $S(a)$ and $S(b)$ be two exotic aromatic S-series. Then,

$$S(a)[S(b)[\phi]] = S(a * b)[\phi], \quad \textit{with } a * b = (a \otimes b) \circ \Delta_{BCK},$$

with $\Delta_{BCK}(\pi) := \sum_{\pi_0 \subset \pi} (\pi \backslash \pi_0) \otimes \pi_0$.

Example:



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Application: The exact flow in $\mathbb{R}^d$ is

$$S^h(e)[\phi], \quad e = \exp^*(l) := \sum_{n=0}^{\infty} \frac{1}{n!} l^{*n}, \quad \delta_\sigma(l) = \bullet + \frac{1}{2} \textcircled{1}\textcircled{1}.$$

The first terms of e in $\mathbb{T}^d$ are

$\delta_\sigma(e) = \mathbf{1} + \bullet + \frac{1}{2}\textcircled{1}\textcircled{1} + \frac{1}{2}$  $+ \frac{1}{2}\bullet\ \bullet + \frac{1}{2}\bullet\ \textcircled{1}\textcircled{1} + \frac{1}{4}$  $+ \frac{1}{2}$  $+ \frac{1}{8}\textcircled{1}\textcircled{1}\textcircled{2}\textcircled{2} + \dots$

Applications to the calculation of weak order conditions, postprocessors (see Vilmart, 2015),...

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Problem: the S-series of the exact flow is not the exponential of a combination of trees, but the exponential of a combination of forests. The primitive elements of exotic forests do not reduce to exotic trees:

$$\mathcal{ET} \subsetneq \mathrm{Prim}(\mathcal{EF}), \quad \mathcal{T} = \mathrm{Prim}(\mathcal{F}).$$

Intrinsic numerical integration

Consider the overdamped Langevin dynamics on a Riemannian manifold $(\mathcal{M}, g)$,

$$dX(t) = -\nabla V(X(t))dt + dB^{\mathcal{M}}(t).$$

In local coordinates, it is given by

$$dX^i = [-g^{ij}(X(t))\partial_j V(X(t)) + -\frac{1}{2}g^{kj}(X(t))\Gamma^i_{kj}(X(t))]dt + g^{1/2,ij}(X(t))dW_j(t).$$

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Consider the overdamped Langevin dynamics on a Riemannian manifold $(\mathcal{M}, g)$,

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Motivations for finding new methods:

- Projection methods are not intrinsic and they rely on an embedding.
- A variety of manifolds are already implemented in some packages (for instance, Manifolds.jl), with the geodesics, the parallel transport,...
- The high order theory of projection methods is difficult and no exact formula exists for the moment.
- There is no proof that sampling projection methods of order more than 2 exist on manifolds.

Intrinsic numerical integration

Consider the overdamped Langevin dynamics on a Riemannian manifold $(\mathcal{M}, g)$,

$$dX(t) = -\nabla V(X(t))dt + dB^{\mathcal{M}}(t).$$

Nomizu classification of manifolds with invariant connections (1954):

	$R = 0$	$\nabla R = 0$
$T = 0$	Euclidean space	Symmetric space
$\nabla T = 0$	Lie group	Reductive homogeneous space

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Example (Lie-group approach)

New method of weak order 1 and order 2 for the invariant measure on a Lie group with a bi-invariant metric (following Celledoni, Marthinsen, Owren, 2003).

$$\begin{aligned} H_n &= \exp\Big(-h\nabla V(Y_n) + \sqrt{h}\hat{\xi}_n\Big) Y_n \\ Y_{n+1} &= \exp\Big(-\tfrac{h}{2}\nabla V(H_n)\Big) \exp\Big(-\tfrac{h}{2}\nabla V(Y_n) + \sqrt{h}\hat{\xi}_n\Big) Y_n \end{aligned}$$

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Example (From Bharath, Lewis, Sharma, Tretyakov, 2023)

The geodesic Euler/Riemannian Langevin method has weak order one:

$$X_{n+1} = \exp_{X_n}(-\nabla V(X_n)dt + \sqrt{h}\xi_n)$$

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Ongoing/future works:

- High order theory for stochastic Lie-group and geodesic methods,
- Backward error analysis and modified equations on manifolds,
- Geometric characterization of (exotic) planar B-series,
- Machine learning techniques and modified equations,
- Creation of exact sampling methods, with variational calculus and Noether theory.