Algebraic structure of exotic Lie-Butcher series for the foundations of stochastic geometric integration

Adrien Busnot Laurent - INRIA Rennes
Joint work with Eugen Bronasco, Baptiste Huguet, and Sébastien Macé

Université de Rennes IRMAR ENS rennes Inria

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Contents

References of this talk:

• E. Bronasco, A. BL, Hopf algebra structures for the backward error analysis of ergodic stochastic differential equations, *In revision in Numerische Matematikk*.
• E. Bronasco, A. BL, B. Huguet, High order integration of stochastic dynamics on Riemannian manifolds with frozen flow methods, *arXiv:2503.21855*.
• A. BL, S. Macé, Efficient sampling of the invariant measure of Riemannian Langevin dynamics with frozen flow methods, *In preparation*.

Contents

Riemannian stochastic dynamics

Consider a Riemannian manifold $(\mathcal{M}, \nabla^{\mathrm{LC}})$. Let $E_1, \dots, E_D$ be a smooth frame:

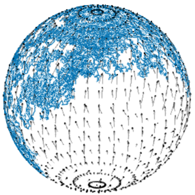
$$\mathrm{Span}_{\mathbb{R}}(E_1(p), \dots, E_D(p)) = T_p\mathcal{M}, \quad y \in \mathcal{M}.$$

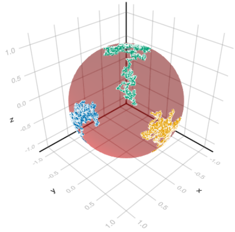
Given a vector field $F(x) = \sum_{d=1}^{D} f^d(x) E_d(x)$, we consider (see Hsu)

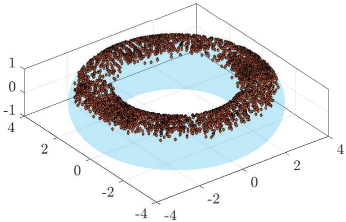
$$dX(t) = F(X(t))dt + \sqrt{2} \sum_{d=1}^{D} E_d(X(t)) \circ dW_d(t).$$

Riemannian Langevin dynamics for E_d orthonormal basis:

$$dX(t) = -\sum_{d=1}^{D} (E_d[V]E_d + \nabla^{\mathrm{LC}}_{E_d} E_d)(X(t))dt + \sqrt{2} \sum_{d=1}^{D} E_d(X(t)) \circ dW_d(t)$$







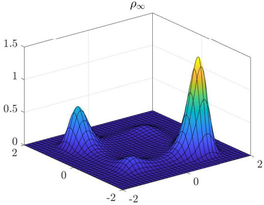
Ergodicity and applications

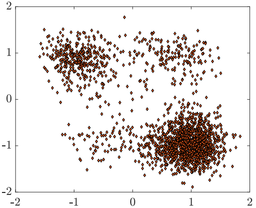
Weak approximations: Given a test function $\phi \in \mathcal{C}_P^\infty(\mathcal{M})$, an integrator is of weak order p if

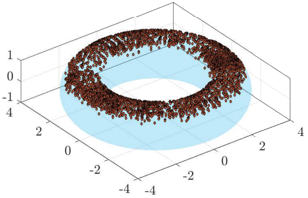
$$|\mathbb{E}[\phi(X_n)] - \mathbb{E}[\phi(X(t_n))]| \leqslant Ch^p, \quad n = 0, \ldots, N.$$

Ergodicity property:

$$\lim_{T \to +\infty} \frac{1}{T} \int_0^T \phi(X(s))ds = \int_{\mathcal{M}} \phi(y)\rho_\infty(y)d\,\mathrm{vol}(y) \quad \text{almost surely}, \quad \rho_\infty \propto e^{-V}.$$







Applications of sampling on manifolds: geometric statistics, molecular dynamics, machine learning, PINNs, ...

The idea of geometric integration

Dynamics on a manifold $\mathcal{M}$: .

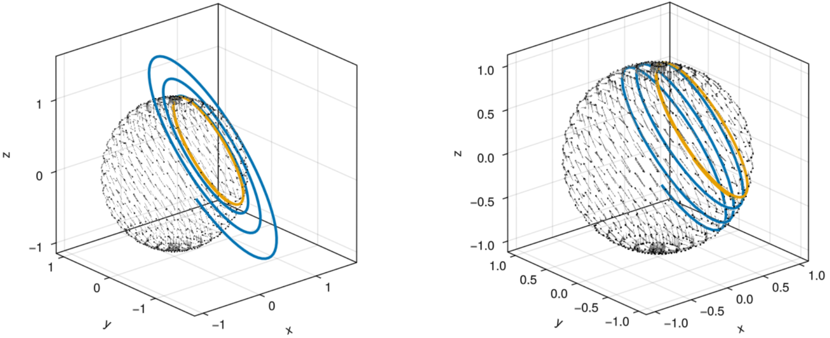


Figure: Non-geometric versus geometric methods.

The idea of geometric integration

Figure: Numerical simulations of a Brownian motion on the sphere.

Idea: **numerical methods should try to preserve the geometry as much as possible**.

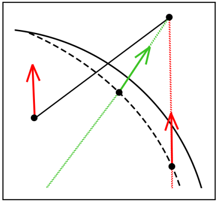
Challenge: a geometry is not "just a manifold". The numerical approaches have to satisfy that **their definition, convergence analysis, and implementation all rely on the same geometric framework as the model.**

Existing stochastic integrators on manifolds

Motivations for finding new methods:

• Projection methods rely on an embedding in a bigger space, are expensive and unstable.

• The high order theory of projection methods is difficult (BL, 2021 - 7 pages of calculations, **no straightforward algebraic structure**, $\sim$ 25 order conditions for order 2).



Example (Euler projection integrator)

The most popular integrator is the Euler scheme with explicit projection direction[a]

$$X_{n+1} = X_n + hf(X_n) + \sqrt{2h}\xi_n + \lambda\nabla\zeta(X_n),\ \zeta(X_{n+1}) = 0.$$

[a] Ciccotti, Kapral, Vanden-Eijnden, 2005; Lelièvre, Le Bris, Vanden-Eijnden, 2008; Lelièvre, Rousset, Stolz, 2010; ...

Example (From Bharath, Lewis, Sharma, Tretyakov, 2024)

The Riemannian Langevin method has order one:

$$X_{n+1} = \exp^{\text{Riem}}_{X_n}(hf(X_n) + \sqrt{2h}g^{-1/2}(X_n)\xi_n)$$

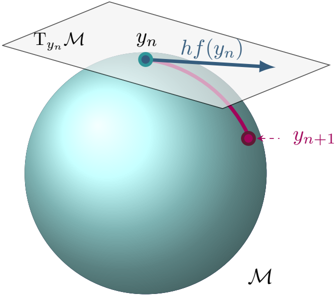
Contents

Connection and geodesic exponential

An affine **connection** $\rhd\colon \mathfrak{X}(\mathcal{M}) \times \mathfrak{X}(\mathcal{M}) \to \mathfrak{X}(\mathcal{M})$ encodes the geometric structure we equip the manifold with.
A **geodesic** $\gamma(t) = \exp(tv)p$ is a curve on $\mathcal{M}$ satisfying

$$\gamma'(t) \rhd \gamma'(t) = 0, \quad \gamma(0) = p \in \mathcal{M}, \quad \gamma'(0) = v \in T_p\mathcal{M}.$$

Example: the geodesic Euler method for $y' = F(y)$ is $y_{n+1} = \exp(hF(y_n))y_n$.



Example

Euclidean case:

$$g \rhd f(p) = f'(p)g(p),$$

$$\exp(tv)p = p + tv.$$

Matrix Lie group:

$$\exp(tv)p = \mathrm{Exp}(tv)p.$$

Frame and connection

Let $E_1, \dots, E_D$ be a frame basis (for simplicity):

$$\mathrm{Span}_{\mathbb{R}}(E_1(p), \dots, E_D(p)) = T_p\mathcal{M}, \quad p \in \mathcal{M}.$$

Define the Weitzenböck connection

$$G \rhd F = \sum_{d=1}^{D} G[f^d] E_d, \quad F(x) = \sum_{d=1}^{D} f^d E_d,$$

and the bracket

$$[F, G] = [\![F, G]\!]_J - F \rhd G + G \rhd F,$$

where $[\![F, G]\!]_J$ is the Jacobi bracket.

Proposition (Ebrahimi-Fard, Lundervold, Munthe-Kaas, '12)

If the frame spans a Lie algebra, the space $(\mathfrak{X}(\mathcal{M}), [-,-], \rhd)$ *is a post-Lie algebra:*

$$F \rhd [G, H] = [F \rhd G, H] + [G, F \rhd H],$$
$$[F, G] \rhd H = F \rhd (G \rhd H) - (F \rhd G) \rhd H - G \rhd (F \rhd H) + (G \rhd F) \rhd H.$$

In particular, $\rhd$ *has* ***constant torsion and vanishing curvature****.*

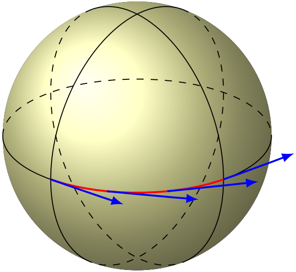
Frozen flows

A **frozen vector field** is

$$F_x(p) = \sum_{d=1}^{D} f^d(x) E_d(p).$$

The **frozen-flow** $\exp(tF_x)p$ is the solution of

$$y'(t) = F_x(y(t)), \quad y(0) = p.$$



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Proposition

The frozen-flow Euler method for

$$dX = F(X)dt + \sqrt{2} E_d(X) \circ dW_d$$

is of weak order one and is given by

$$Y_{n+1} = \exp\left(\sum_{d=1}^{D} \left(hf^d(Y_n) + \sqrt{2h}\xi_n^d \right) E_d \right) Y_n, \quad \xi_n \sim \mathcal{N}(0, I_D)$$

Frozen-flow methods

New frozen-flow integrators[1]

$$H_n^i = \exp\Big(\sum_{d=1}^{D} \Big(h \sum_{j=1}^{s} Z_{i,j,K}^0 f^d(H_n^j) + \sqrt{h} Z_{i,K}^d \Big) E_d \Big) \dots$$

$$\dots \exp\Big(\sum_{d=1}^{D} \Big(h \sum_{j=1}^{s} Z_{i,j,1}^0 f^d(H_n^j) + \sqrt{h} Z_{i,1}^d \Big) E_d \Big) Y_n,$$

$$Y_{n+1} = \exp\Big(\sum_{d=1}^{D} \Big(h \sum_{i=1}^{s} z_{i,K}^0 f^d(H_n^i) + \sqrt{h} z_K^d \Big) E_d \Big) \dots$$

$$\dots \exp\Big(\sum_{d=1}^{D} \Big(h \sum_{i=1}^{s} z_{i,1}^0 f^d(H_n^i) + \sqrt{h} z_1^d \Big) E_d \Big) Y_n.$$

where the coefficients are Gaussian.

Remark: the frozen-flow methods work on ANY smooth Riemannian manifold.

[1] in the spirit of Crouch-Grossman and commutator-free Lie group methods, see Celledoni, Marthinsen, Owren and also Iserles, Munthe-Kaas, Quispel, Zanna, $\sim$ 1990's-2006

Convergence theorem

Theorem (Bronasco, BL, Huguet)

Consider a vector field F and a frame E_d that are Lipschitz continuous, $2p+2$-times continuously differentiable, satisfy technical polynomial growth estimates for their derivatives[a]. Denote the Taylor-Talay-Tubaro expansions

$$\mathbb{E}[\phi(X_1)|X_0 = x] = \phi(x) + \sum_{j=1}^{p} h^j \mathcal{A}_j \phi(x) + h^{p+1} R_p^h(\phi, x),$$

$$\mathbb{E}[\phi(X(h))|X_0 = x] = \phi(x) + \sum_{j=1}^{p} \frac{h^j}{j!} \mathcal{L}^j \phi(x) + h^{p+1} R_p^h(\phi, x).$$

Then, if the operators satisfy

$$\mathcal{A}_j = \frac{1}{j!}\mathcal{L}^j, \quad j = 1, \dots p, \quad \mathcal{L}\phi = F[\phi] + \sum_{d=1}^{D} E_d[E_d[\phi]],$$

then the integrator has global weak order p.

[a] in the spirit of the Bakry-Émery criterion $\mathrm{Ric} + \mathrm{Hess}(V) \geqslant \kappa$.

New second order intrinsic method

Equation: $dX(t) = F(X(t))dt + \sqrt{2}\sum_{d=1}^{D} E_d(X(t)) \circ dW_d(t)$, $F = f^d E_d$

New explicit frozen flow integrator of weak order two:

$$H_n = \exp\Big(\sum_{d=1}^{D}\Big(\frac{1}{2}hf^d(Y_n) + \sqrt{h}\xi_n^{d,1}\Big)E_d\Big)Y_n$$

$$\begin{aligned}Y_{n+1} = \exp\Big(\sum_{d=1}^{D}\Big((\frac{\sqrt{2}}{2} - 1\Big)hf^d(Y_n) + (2-\sqrt{2})hf^d(H_n) \\ + (1-\sqrt{2})\sqrt{h}\xi_n^{d,1} + \sqrt{h}\xi_n^{d,2}\Big)E_d\Big) \\ \exp\Big(\sum_{d=1}^{D}\Big((1-\frac{\sqrt{2}}{2})hf^d(Y_n) + (\sqrt{2}-1)hf^d(H_n) + \sqrt{2h}\xi_n^{d,1}\Big)E_d\Big)Y_n.\end{aligned}$$

Notes on the implementation:

- On homogeneous spaces, exp is the matrix exponential.
- The frozen-flow exponential can be replaced by high-order retractions.
- The geometric operations are already implemented in a handful of packages (see, for instance, Manifolds.jl)

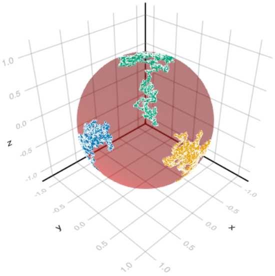
Brownian dynamics on SO

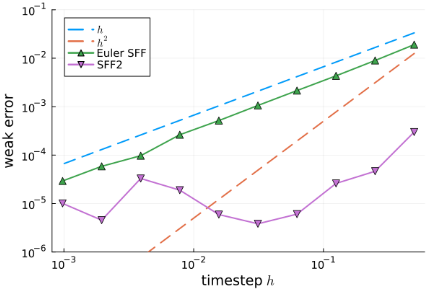
Frame: $E_d(y) = A_d y$ with (A_d) an orthonormal basis of the Lie algebra $\mathfrak{so}_d$.
Brownian dynamics:

$$dX(t) = \sum_{d=1}^{D} E_d(X(t)) \circ dW_d(t), \quad D = \dim(\mathfrak{so}_p) = \frac{p(p-1)}{2}.$$

The new method becomes

$$Y_{n+1} = \operatorname{Exp}\left(\sum_{d=1}^{D}\Big(\big(\frac{\sqrt{2}}{2}-1\big)\sqrt{h}\xi_n^{d,1} + \frac{\sqrt{2}}{2}\sqrt{h}\xi_n^{d,2}\Big)A_d\right)\operatorname{Exp}\left(\sum_{d=1}^{D}\sqrt{h}\xi_n^{d,1}A_d\right)Y_n.$$



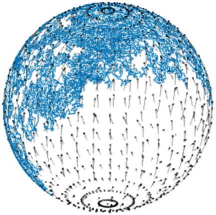


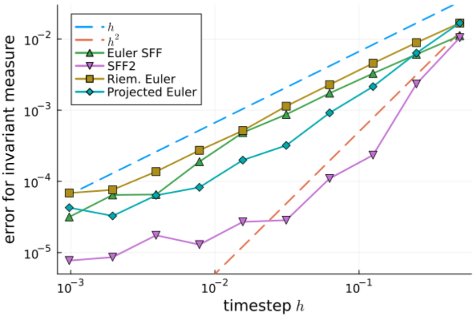
Remark: There is no timestep restriction for the new methods.

Ergodic dynamics on the sphere

We now have **3 numerical approaches**:

- Projection: $X_{n+1} = X_n + hF(X_n) + \sqrt{2h}\xi_n + \lambda g(X_n), \quad \zeta(X_{n+1}) = 0,$
- Riemannian: $X_{n+1} = \exp^{\mathrm{Riem}}_{X_n}(hF(X_n) + \sqrt{2h}\xi_n),$
- Frozen-flow : $X_{n+1} = \exp(hF(X_n) + \sqrt{2h}\xi_n^d E_d)X_n.$





The new second order methods outperforms the other integrators in accuracy for a similar cost. It is the **first high-order intrinsic integrator of the literature**.

Contents

Tensor algebra of vector fields

Let the frozen composition in $T(\mathfrak{X}(\mathcal{M}))$ be the differential operator

$$(G \cdot F) \rhd \phi = \sum_{i,j} g^j f^i E_j[E_i[\phi]].$$

Similarly, define the Grossman-Larson product (extend by Guin-Oudom)

$$(G * F) \rhd \phi = \sum_{i,j} g^j E_j[f^i E_i[\phi]] = G \rhd (F \rhd \phi) = (G \rhd F) \rhd \phi + (G \cdot F) \rhd \phi.$$

In $\mathbb{R}^d$, we have

$$(G \cdot F) \rhd \phi = \phi''(G, F), \quad (G * F) \rhd \phi = (\phi' F)' G.$$

Then, $(T(\mathfrak{X}(\mathcal{M})), \cdot, \Delta_{\sqcup\!\sqcup}, \rhd)$ and $(T(\mathfrak{X}(\mathcal{M})), *, \Delta_{\sqcup\!\sqcup})$ are (post-)Hopf algebras.

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Proposition

The Taylor expansions of the geodesic and exact flow exponentials are

$$\phi(\exp(F_p)p) = \exp^{\cdot}(F) \rhd \phi(p), \quad \phi(\exp(F)p) = \exp^{*}(F) \rhd \phi(p),$$

where $\exp^*(F) = \mathrm{id} + F + \frac{1}{2!} F * F + \frac{1}{3!} F * F * F + \dots.$

Example of the Euler method

The Taylor expansion of the Euler frozen-flow method is

$$\phi(\exp(hF_p + \sqrt{2h}\xi^d E_d)p) = \exp^\cdot(hF + \sqrt{2h}\xi^d E_d) \rhd \phi$$

[2] see Isserlis-Wick theorem.

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$$\phi(\exp(hF_p+\sqrt{2h}\xi^d E_d)p) = \exp^{\cdot}(hF+\sqrt{2h}\xi^d E_d) \rhd \phi$$
$$= \Big(\mathrm{id} + h^{1/2}\sqrt{2}\xi^d E_d + h(F+\xi^{d_2}\xi^{d_1}E_{d_2}\cdot E_{d_1})$$
$$+ h^{3/2}(\frac{\sqrt{2}}{2}\xi^d F\cdot E_d + \frac{\sqrt{2}}{2}\xi^d E_d\cdot F + \frac{\sqrt{2}}{3}\xi^{d_3}\xi^{d_2}\xi^{d_1}E_{d_3}\cdot E_{d_2}\cdot E_{d_1}) + \dots\Big) \rhd \phi.$$

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$$\begin{aligned}
&\phi(\exp(hF_p+\sqrt{2h}\xi^d E_d)p) = \exp^{\cdot}(hF+\sqrt{2h}\xi^d E_d)\rhd\phi\\
&=\Big(\mathrm{id}+h^{1/2}\sqrt{2}\xi^d E_d + h(F+\xi^{d_2}\xi^{d_1}E_{d_2}\cdot E_{d_1})\\
&+h^{3/2}(\frac{\sqrt{2}}{2}\xi^d F\cdot E_d+\frac{\sqrt{2}}{2}\xi^d E_d\cdot F+\frac{\sqrt{2}}{3}\xi^{d_3}\xi^{d_2}\xi^{d_1}E_{d_3}\cdot E_{d_2}\cdot E_{d_1})+\dots\Big)\rhd\phi.
\end{aligned}$$

Then, the expectation pairs the Gaussians together[2] and yields

$$\begin{aligned}
\mathbb{E}[\phi(\exp(hF_p+\sqrt{2h}\xi^d E_d)p)] &= \Big(\mathrm{id}+h(F+E_d\cdot E_d)\\
&+h^2(\frac{1}{2}F\cdot F+\frac{1}{3}F\cdot E_d\cdot E_d+\frac{1}{3}E_d\cdot F\cdot E_d+\frac{1}{3}E_d\cdot E_d\cdot F\\
&+\frac{1}{6}E_{d_2}\cdot E_{d_2}\cdot E_{d_1}\cdot E_{d_1}+\frac{1}{6}E_{d_2}\cdot E_{d_1}\cdot E_{d_2}\cdot E_{d_1}+\frac{1}{6}E_{d_1}\cdot E_{d_2}\cdot E_{d_2}\cdot E_{d_1})\\
&+\dots\Big)\rhd\phi.
\end{aligned}$$

[2] see Isserlis-Wick theorem.

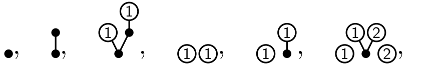
Planar exotic forests[3]

Definition

A planar exotic forest is an ordered list of planar trees decorated by $\mathbb{N}$ s.t.
- $\bullet$ stands for the decoration 0,
- the other decorations only appear 0 or 2 times, and only on leaves.

Examples of exotic planar forests:

$$\mathcal{E}\mathcal{F} = \text{Span}_{\mathbb{R}}(\mathbf{1}, \ \ldots)$$



[3] see L., Vilmart, 2020-2022; L., Munthe-Kaas, 2024

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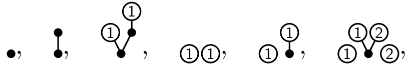

$$\dots)$$

Difficulty: An exotic forest is NOT a concatenation of exotic trees in general:

$$ⓛ① \neq ① \cdot ①.$$

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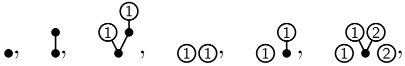
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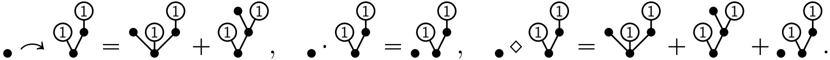
$\mathcal{EF}$ is equipped with grafting $\curvearrowright$, concatenation $\cdot$, and Grossman-Larson $\diamond$:



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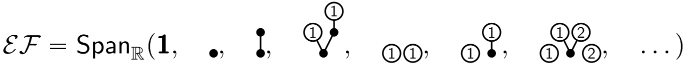

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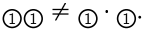

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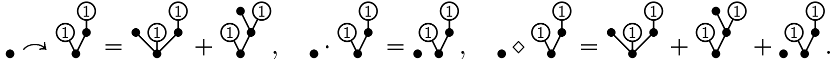

Theorem

$(\mathcal{EF}, \cdot, \Delta_{\sqcup\!\sqcup})$ and $(\mathcal{EF}, \diamond, \Delta_{\sqcup\!\sqcup})$ are Hopf algebras. $(\mathcal{EF}, \cdot, \Delta_{\sqcup\!\sqcup})$ is NOT post-Hopf.

[3] see L., Vilmart, 2020-2022; L., Munthe-Kaas, 2024

Elementary differential map

The elementary differential map $\mathbb{F}\colon \mathcal{EF} \to T(\mathfrak{X}(\mathcal{M}))$ translates from exotic forests to differential operators:

$$\mathbb{F}(\bullet) = F, \quad \mathbb{F}\left(\begin{smallmatrix}\bullet\\ |\\ \bullet\end{smallmatrix}\right) = F \rhd F, \quad \mathbb{F}\left(_{\textcircled{1}}\begin{smallmatrix}\textcircled{1}\\ |\\ \bullet\end{smallmatrix}\right) = E_d \cdot (E_d \rhd F), \quad \mathbb{F}\left(\begin{smallmatrix}\textcircled{1}\\ |\\ \bullet\end{smallmatrix}_{\textcircled{1}}\right) = (E_d \rhd F) \cdot E_d.$$

Proposition

$\mathbb{F}$ *is a morphism:* $\mathbb{F}(\pi_1 \curvearrowright \pi_2) = \mathbb{F}(\pi_1) \rhd \mathbb{F}(\pi_2)$,

$$\mathbb{F}(\pi_1 \cdot \pi_2) = \mathbb{F}(\pi_1) \cdot \mathbb{F}(\pi_2), \quad \mathbb{F}(\pi_1 \diamond \pi_2) = \mathbb{F}(\pi_1) * \mathbb{F}(\pi_2).$$

Example (frozen-flow Euler method)

$$\begin{aligned}
\mathbb{E}[\phi(\exp(hF_p + \sqrt{2h}\xi^d E_d)p)] &= \mathbb{F}\Big(\mathbf{1} + h(\bullet + \textcircled{1}\textcircled{1}) + h^2(\frac{1}{2}\bullet\ \bullet + \frac{1}{3}\bullet\ \textcircled{1}\textcircled{1} \\
&\quad + \frac{1}{3}\textcircled{1}\bullet\textcircled{1} + \frac{1}{3}\textcircled{1}\textcircled{1}\bullet + \frac{1}{6}\textcircled{2}\textcircled{2}\textcircled{1}\textcircled{1} + \frac{1}{6}\textcircled{2}\textcircled{1}\textcircled{2}\textcircled{1} + \frac{1}{6}\textcircled{1}\textcircled{2}\textcircled{2}\textcircled{1}) + \dots\Big) \rhd \phi(p) \\
&= \Big(\mathrm{id} + h(F + E_d \cdot E_d) + h^2(\frac{1}{2}F \cdot F + \frac{1}{3}F \cdot E_d \cdot E_d + \frac{1}{3}E_d \cdot F \cdot E_d \\
&\quad + \frac{1}{3}E_d \cdot E_d \cdot F + \frac{1}{6}E_{d_2} \cdot E_{d_2} \cdot E_{d_1} \cdot E_{d_1} + \frac{1}{6}E_{d_2} \cdot E_{d_1} \cdot E_{d_2} \cdot E_{d_1} + \dots\Big) \rhd \phi(p).
\end{aligned}$$

Exotic Lie-Butcher series

Exotic Lie-Butcher series are formal series indexed by exotic forests with $a \in \mathcal{EF}^*$:

$$S_h(a)[\phi] = \sum_{\pi \in EF} h^{|\pi|} a(\pi)\mathbb{F}(\pi)[\phi], \quad B_h(a) = \sum_{\tau \in ET} h^{|\tau|} a(\tau)\mathbb{F}(\tau).$$

Theorem (Bronasco, BL, Huguet)

The Taylor expansion of the exact flow is the exotic Lie series

$$\mathbb{E}[\phi(X(h))] = \exp(h\mathcal{L})[\phi] = S_h(e) \rhd \phi, \quad e = \exp^*(\delta_{\bullet} + \delta_{\textcircled{1}\textcircled{1}}).$$

The numerical flow is also given by an exotic Lie series.

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Proposition (in the spirit of Owren, 2006)

Let $\varphi\colon \mathcal{M} \to \mathcal{M}$ with $\phi(\varphi(p)) = (S(a) \rhd \phi)(p)$, then the ***frozen vector field*** *$F_\varphi\colon p \to F_{\varphi(p)}(p)$ satisfies*

$$F_\varphi \rhd \phi = (S(a) \rhd hF) \rhd \phi = B(\tilde{a}) \rhd \phi, \quad \tilde{a}(\tau) = a(B^-(\tau)), \quad \tilde{a} \in \mathcal{ET}^*.$$

Frozen flow : $\phi(\exp(B_p(\tilde{a}))) = S(a) \rhd \phi, \quad a(\tau_1 \cdots \tau_n) = \frac{1}{n!}\tilde{a}(\tau_1)\ldots\tilde{a}(\tau_n).$

Frozen composition:

$$\phi(\varphi^1 \cdot \varphi^2) = (S(a^2) \cdot S(a^1)) \rhd \phi = S(a^2 \cdot a^1) \rhd \phi, \quad a^2 \cdot a^1 = \mu \circ (a^2 \otimes a^1) \circ \Delta..$$

Composition *(see Munthe-Kaas, Wright, 2008):*

$$\phi(\varphi^1 \circ \varphi^2) = S(a^2) \rhd (S(a^1) \rhd \phi) = S(a^2 * a^1) \rhd \phi, \quad a^2 * a^1 = \mu \circ (a^2 \otimes a^1) \circ \Delta_{MKW}.$$

Order conditions

Exotic forest π	Differential $\mathbb{F}(\pi)[\phi]$	Order condition $a(\pi) = e(\pi)$
•	$f^i E_i[\phi]$	$z^0_{i,k_1} = 1$
①①	$E_{d_1}[E_{d_1}[\phi]]$	$\sum^!_{k_1 \geqslant k_2} \mathbb{E}[z^{d_1}_{k_2} z^{d_1}_{k_1}] = 1$
	$f^j E_j[f^i] E_i[\phi]$	$z^0_{i,k_2} Z^0_{i,j,k_1} = \frac{1}{2}$
	$E_{d_1}[E_{d_1}[f^i]] E_i[\phi]$	$\sum^!_{k_2 \geqslant k_3} \mathbb{E}[Z^{d_1}_{i,k_3} Z^{d_1}_{i,k_2}] z^0_{i,k_1} = \frac{1}{2}$
• •	$f^j f^i E_j[E_i[\phi]]$	$\sum^!_{k_1 \geqslant k_2} z^0_{j,k_2} z^0_{i,k_1} = \frac{1}{2}$
	$E_{d_1}[f^i] E_i[E_{d_1}[\phi]]$	$\sum^!_{k_1 \geqslant k_2} z^0_{i,k_2} \mathbb{E}[Z^{d_1}_{i,k_3} z^{d_1}_{k_1}] = 0$
	$E_{d_1}[f^i] E_{d_1}[E_i[\phi]]$	$\sum^!_{k_2 \geqslant k_1} z^0_{i,k_2} \mathbb{E}[Z^{d_1}_{i,k_3} z^{d_1}_{k_1}] = 1$
• ①①	$f^i E_i[E_{d_1}[E_{d_1}[\phi]]]$	$\sum^!_{k_1 \geqslant k_2 \geqslant k_3} z^0_{i,k_3} \mathbb{E}[z^{d_1}_{k_2} z^{d_1}_{k_1}] = \frac{1}{2}$
① • ①	$f^i E_{d_1}[E_i[E_{d_1}[\phi]]]$	$\sum^!_{k_1 \geqslant k_3 \geqslant k_2} z^0_{i,k_3} \mathbb{E}[z^{d_1}_{k_2} z^{d_1}_{k_1}] = 0$
①① •	$f^i E_{d_1}[E_{d_1}[E_i[\phi]]]$	$\sum^!_{k_3 \geqslant k_1 \geqslant k_2} z^0_{i,k_3} \mathbb{E}[z^{d_1}_{k_2} z^{d_1}_{k_1}] = \frac{1}{2}$
②②①①	$E_{d_2}[E_{d_2}[E_{d_1}[E_{d_1}[\phi]]]]$	$\sum^!_{k_1 \geqslant k_2 \geqslant k_3 \geqslant k_4} \mathbb{E}[z^{d_2}_{k_4} z^{d_2}_{k_3}] \mathbb{E}[z^{d_1}_{k_2} z^{d_1}_{k_1}] = \frac{1}{2}$
②①②①	$E_{d_2}[E_{d_1}[E_{d_2}[E_{d_1}[\phi]]]]$	$\sum^!_{k_1 \geqslant k_2 \geqslant k_3 \geqslant k_4} \mathbb{E}[z^{d_2}_{k_4} z^{d_2}_{k_2}] \mathbb{E}[z^{d_1}_{k_3} z^{d_1}_{k_1}] = 0$
①②②①	$E_{d_1}[E_{d_2}[E_{d_2}[E_{d_1}[\phi]]]]$	$\sum^!_{k_1 \geqslant k_2 \geqslant k_3 \geqslant k_4} \mathbb{E}[z^{d_2}_{k_3} z^{d_2}_{k_2}] \mathbb{E}[z^{d_1}_{k_4} z^{d_1}_{k_1}] = 0$

Primitive elements and shuffle relations

Shuffle product:

$$\bullet \sqcup\!\sqcup \text{①①} = \bullet\,\text{①①} + \text{①}\bullet\text{①} + \text{①①}\,\bullet,$$
$$\text{②②} \sqcup\!\sqcup \text{①①} = 2\,\text{②②①①} + 2\,\text{②①②①} + 2\,\text{②①①②},$$

The coefficient maps of numerical flows are characters of $(\mathcal{EF}, \sqcup\!\sqcup)$:

$$a(\pi_1 \sqcup\!\sqcup \pi_2) = a(\pi_1)a(\pi_2).$$

Following Owren, '06, we have shuffle relations:

$$a(\bullet)^2 = 2a(\bullet\ \bullet),$$
$$a(\bullet)a(\text{①①}) = a(\bullet\,\text{①①}) + a(\text{①①}\,\bullet) + a(\text{①}\bullet\text{①}),$$
$$a(\text{①①})^2 = 2a(\text{②②①①}) + 2a(\text{②①②①}) + 2a(\text{①②②①}).$$

Proposition

The order conditions are indexed by the exotic forests, modulo the shuffle relations. In particular, there are 2, 8, and 73 conditions for order 1,2, and 3 (against 2, 11, and 95 exotic forests).

Conclusion

Summary:

- We provide a brand new class of intrinsic high-order methods for solving stochastic dynamics on manifolds.
- We give a convergence analysis and the Talay-Tubaro methodology.
- The order theory relies on a new formalism of planar exotic forests, which extends the existing deterministic works.

Outlooks:

- The analysis and implementation rely on an artificial connection. Ongoing extension of Lie-group methods to geodesic methods.
- Creation of efficient high-order sampling method (PhD thesis of Sébastien Macé).
- Geometric universal characterisation of planar exotic series, algebraic study of the evenly decorated/aromatic exotic series and applications.
- Implementation of the new methods in the Julia package Manifolds.jl (with P. Navaro and R. Bergmann).
- **Available ANR postdoc position** starting Sept. 2026 in Rennes (2 years).

Exotic MKW structure

Theorem

Let the Munthe-Kaas-Wright coproduct:

$$\Delta_{MKW}(\tau) := \sum_{\text{adm. cut } c} P^c(\tau) \otimes R^c(\tau), \quad \Delta_{MKW}(\pi) := (id \otimes B^-)\Delta_{MKW}(B^+(\pi)).$$

Then, $(\mathcal{EF}, ⧢, \Delta_{MKW})$ is a Hopf algebra dual to $(\mathcal{EF}, \diamond, \Delta_{⧢})$. Its convolution product represents the composition of exotic series:

$$S(a) \circ S(b) = S(a * b), \quad a * b = \mu_{\mathbb{R}} \circ (a \otimes b) \circ \Delta_{MKW},$$

Example