Order conditions for sampling the invariant measure of ergodic SDEs in $\mathbb{R}^d$ and on manifolds

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Joint work with Gilles Vilmart

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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. *Submitted*, 39 pages.

Contents

The overdamped Langevin equation in molecular dynamics

Take N particles moving in a fluid. Then, the positions $q(t)$ and the velocities $p(t)$ of the particles satisfy the underdamped Langevin equation:

$$\begin{cases} dq(t) = p(t)dt \\ dp(t) = (-\nabla V(q(t)) - \gamma p(t))dt + \sqrt{\frac{2\gamma}{\beta}} dW(t) \end{cases}$$

In a high friction regime, we obtain the following simplified equation in $\mathbb{R}^d$ called the overdamped Langevin equation, where $f = -\nabla V$:

$$dX(t) = f(X(t))dt + \sigma dW(t), \quad X(0) = X_0 \in \mathbb{R}^d.$$

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If there are constraints $\zeta(X) = 0$ (e.g. strong covalent bonds between atoms, or fixed angles in molecules), the solution lies on the manifold $\mathcal{M} = \{x \in \mathbb{R}^d, \zeta(x) = 0\}$ and we get the constrained Langevin dynamics:

$$dX(t) = \Pi_{\mathcal{M}}(X(t))f(X(t))dt + \sigma \Pi_{\mathcal{M}}(X(t)) \circ dW(t), \quad X(0) = X_0 \in \mathcal{M},$$

where $\Pi_{\mathcal{M}} : \mathbb{R}^d \to \mathbb{R}^{d \times d}$ is the projection operator on the tangent bundle of $\mathcal{M}$.

Classical tools for the weak convergence

A numerical scheme is said to have local weak order p if for all test functions ϕ,

$$|\mathbb{E}[\phi(X_1)|X_0 = x] - \mathbb{E}[\phi(X(h))|X(0) = x]| \leqslant C(x,\phi)h^{p+1}.$$

Let $u(x,t) = \mathbb{E}[\phi(X(t))|X(0) = x]$, $t \geqslant 0$, then under certain assumptions, u satisfies the following backward Kolmogorov equation:

$$\frac{\partial u}{\partial t}(x,t) = \mathcal{L}u(x,t), \quad t > 0, \quad u(x,0) = \phi(x).$$

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On $\mathcal{M} = \zeta^{-1}(\{0\})$, we write $g = \nabla\zeta$ and $G = g^T g = \|g\|^2$, then $\mathcal{L}$ is given by

$$\begin{aligned}\mathcal{L}\phi = \phi' f + \frac{\sigma^2}{2}\Delta\phi - \frac{\sigma^2}{2}G^{-1}\operatorname{div}(g)\phi' g \\ - G^{-1}(g,f)\phi' g + \frac{\sigma^2}{2}G^{-2}(g,g'g)\phi' g - \frac{\sigma^2}{2}G^{-1}\phi''(g,g).\end{aligned}$$

Classical tools for the weak convergence

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$$- G^{-1}(g, f)\phi' g + \frac{\sigma^2}{2}G^{-2}(g, g'g)\phi' g - \frac{\sigma^2}{2}G^{-1}\phi''(g, g).$$

$\rightarrow$ From now on, $\mathcal{M}$ is either $\mathbb{R}^d$ or a compact smooth manifold of codimension one such that $G(x) \neq 0$, for all $x \in \mathcal{M}$.

Classical tools for the weak convergence

We develop the exact solution in Taylor series:

$$\mathbb{E}[\phi(X(h))|X(0)=x] = \phi(x) + h\mathcal{L}\phi(x) + \frac{h^2}{2!}\mathcal{L}^2\phi(x) + \frac{h^3}{3!}\mathcal{L}^3\phi(x) + \dots$$

We compare with the Taylor series of the numerical approximation:

$$\mathbb{E}[\phi(X_1)|X_0=x] = \phi(x) + h\mathcal{A}_0\phi(x) + h^2\mathcal{A}_1\phi(x) + h^3\mathcal{A}_2\phi(x) + \dots$$

Theorem (Talay, Tubaro (1990) and Milstein, Tretyakov (2004))

Under assumptions, the scheme is of weak order p if

$$\frac{1}{j!}\mathcal{L}^j = \mathcal{A}_{j-1}, \quad j = 1, \dots, p.$$

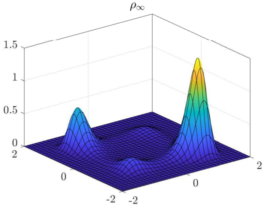
→ Tree formalism of B-series for deterministic problems: Butcher (1972) and Hairer, Wanner (1974),...
→ Tree formalism for strong and weak errors on finite time: Burrage, Burrage (1996); Komori, Mitsui, Sugiura (1997); Rößler, Debrabant, Kværnø, ...

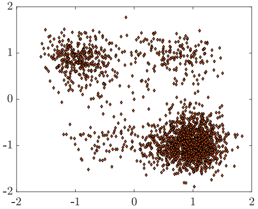
Ergodicity, invariant measure

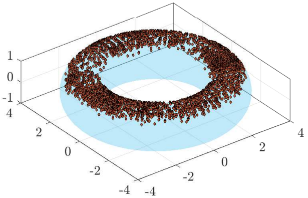
Ergodicity: there exists a unique invariant measure $d\mu_\infty = \rho_\infty d\sigma_\mathcal{M}$ such that

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

for all test functions ϕ and with the Euclidean canonical measure $d\sigma_\mathcal{M}$ on $\mathcal{M}$.
The Gibbs density ρ_∞ satisfies $\mathcal{L}^*\rho_\infty = 0$ and $\rho_\infty(x) = Z\exp(-\frac{2}{\sigma^2}V(x))$.







Order of convergence for the invariant measure

Definition (Convergence for the invariant measure)

We call error of the invariant measure the quantity

$$e(\phi, h) = \left| \lim_{N \to +\infty} \frac{1}{N+1} \sum_{n=0}^{N} \phi(X_n) - \int_{\mathbb{R}^d} \phi(y) \rho_\infty(y) d\sigma_{\mathcal{M}}(y) \right|.$$

The scheme is of order p if for all test function ϕ, $e(\phi, h) \leqslant C(\phi) h^p$.

Remark: a scheme of weak order p automatically has at least order p for the invariant measure. One can build high order scheme for the invariant measure with low weak order (see, e.g., Bou-Rabee, Owhadi, 2010 and Leimkuhler, Matthews, 2013).

Example (first introduced in Leimkuhler, Matthews, 2013)

$$X_{n+1} = X_n + hf(X_n) + \sigma\sqrt{h}\frac{\xi_n + \xi_{n+1}}{2}$$

The scheme has weak order 1 and order 2 for the invariant measure in $\mathbb{R}^d$.

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The scheme is of order p if for all test function ϕ, $e(\phi, h) \leqslant C(\phi) h^p$.

Theorem (L., V., 2020 on a compact smooth manifold $\mathcal{M}$ Abdulle, V., Zygalakis, 2014 in $\mathbb{R}^d$ Related work: Debussche, Faou, 2012; Kopec, 2013)

Under technical assumptions, if $\mathcal{A}_j^* \rho_\infty = 0$ in $L^2(d\sigma_{\mathcal{M}})$, $j = 2, \dots p-1$, i.e. for all test functions ϕ,

$$\int_{\mathcal{M}} \mathcal{A}_j \phi(y) \rho_\infty(y) d\sigma_{\mathcal{M}}(y) = 0, \qquad j = 2, \dots, p-1,$$

then the numerical scheme has order p for the invariant measure.

Contents

Example: the θ-method

Overdamped Langevin equation in $\mathbb{R}^d$:

$$dX = f(X)dt + \sigma dW, \quad f = -\nabla V$$

The θ-method:

$$X_{n+1} = X_n + h(1-\theta)f(X_n) + h\theta f(X_{n+1}) + \sigma\sqrt{h}\xi_n,$$

where $\xi_n \sim \mathcal{N}(0, I_d)$ are independent standard Gaussian variables.

Methodology:

1. Compute the Taylor expansion of X_1,
2. Compute the Taylor expansion of $\phi(X_1)$,
3. Compute $\mathbb{E}[\phi(X_1)]$ and deduce the $\mathcal{A}_j\phi$,
4. Simplify $\int_{\mathbb{R}^d} \mathcal{A}_j\phi(y)\rho_\infty(y)dy$.

Example: the θ-method

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$$X_{n+1} = X_n + h(1-\theta)f(X_n) + h\theta f(X_{n+1}) + \sigma\sqrt{h}\xi_n,$$

where $\xi_n \sim \mathcal{N}(0, I_d)$ are independent standard Gaussian variables.
An expansion in h yields, for $\xi \sim \mathcal{N}(0, I_d)$,

$$X_1 = x + \sqrt{h}\sigma\xi + hf + h\sqrt{h}\theta\sigma f'\xi + h^2\theta f'f + h^2\frac{\theta\sigma^2}{2}f''(\xi,\xi) + \dots$$

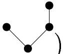
We deduce $\mathbb{E}[\phi(X_1)|X_0 = x] = \phi(x) + h\mathcal{L}\phi(x) + h^2\mathcal{A}_1\phi(x) + \dots$, where

$$\mathcal{A}_1\phi = \mathbb{E}[\theta\phi'f'f + \frac{1}{2}\phi''(f,f) + \frac{\theta\sigma^2}{2}\phi'f''(\xi,\xi) + \theta\sigma^2\phi''(f'\xi,\xi) + \frac{\sigma^2}{2}\phi^{(3)}(f,\xi,\xi) + \frac{\sigma^4}{24}\phi^{(4)}(\xi,\xi,\xi,\xi)].$$

Grafted aromatic forests

Differential trees and B-series used for numerical analysis: Butcher (1972) and Hairer, Wanner (1974) (See also Hairer, Wanner, Lubich (2006) and Butcher (2008))

We use trees as a powerful notation for our differentials. We denote $F(\gamma)(\phi)$ the elementary differential of a tree γ.

- $F(\bullet)(\phi) = \phi$
- $F($$)(\phi) = \phi' f = \sum_i \partial_i \phi f_i$
- $F($$)(\phi) = \phi''(f, f'f) = \sum_{i,j,k} \partial_{ij} \phi f_i \partial_k f_j f_k$

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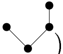
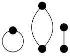
- $F($$)(\phi) = \phi''(f, f'f) = \sum_{i,j,k} \partial_{ij}\phi f_i \partial_k f_j f_k$

Aromatic forests: introduced by Chartier, Murua (2007) (See also Bogfjellmo (2015))

$F($$)(\phi) = \left(\sum \partial_i f_i\right) \times \left(\sum \partial_i f_j \partial_j f_i\right) \times \phi' f$

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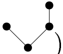
- $F($  $)(\phi) = \phi''(f, f'f) = \sum_{i,j,k} \partial_{ij}\phi f_i \partial_k f_j f_k$

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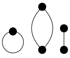
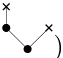
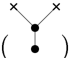
$F($  $)(\phi) = \left(\sum \partial_i f_i\right) \times \left(\sum \partial_i f_j \partial_j f_i\right) \times \phi' f$

Grafted aromatic forests: ξ is represented by crosses (in the spirit of P-series)

$F($  $)(\phi) = \sigma^2 \phi''(f'\xi, \xi)$ and $F($  $)(\phi) = \sigma^2 \phi' f''(\xi, \xi)$.

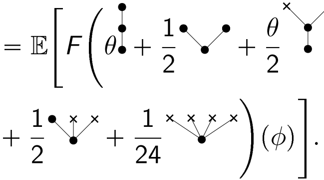
Grafted forests for the θ-method

For the θ method,

$$\mathbb{E}[\phi(X_1)|X_0 = x] = \phi(x) + h\mathcal{L}\phi(x) + h^2\mathcal{A}_1\phi(x) + \ldots$$

and $\mathcal{A}_1$ is given by

$$\begin{aligned}\mathcal{A}_1\phi = \mathbb{E}[&\theta\phi' f' f + \frac{1}{2}\phi''(f,f) + \frac{\theta\sigma^2}{2}\phi' f''(\xi,\xi) + \theta\sigma^2\phi''(f'\xi,\xi)\\ &+ \frac{\sigma^2}{2}\phi^{(3)}(f,\xi,\xi) + \frac{\sigma^4}{24}\phi^{(4)}(\xi,\xi,\xi,\xi)]\end{aligned}$$



Exotic aromatic forests: adding lianas (Math. Comp. 2020)

We add lianas to the aromatic forests.

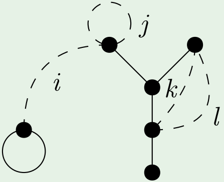
Examples

$F($$) = \sigma^2 \sum_i \phi''(f'(e_i), e_i)$.

$F($$) = \sigma^2 \sum_i \phi''(e_i, e_i) = \sigma^2 \Delta\phi$.

$F($$) = \sigma^4 \sum_{i,j} \phi''(e_i, f'''(e_j, e_j, e_i)) = \sigma^4 \sum_i \phi''(e_i, (\Delta f)'(e_i))$.

If γ is the following forest



then $F(\gamma)(\phi) = \sigma^8 \sum_{i,j,k=1}^{d} \operatorname{div}(\partial_i f) \times \phi'((\partial_{kl} f)'(f''(\partial_{ijj} f, \partial_{kl} f)))$.

Remark: the forests do not depend on the dimension of the problem.

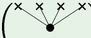
Main tool 1: expectation of a grafted exotic aromatic forest

The following result is a consequence of the Isserlis theorem.

Theorem

If γ is a grafted exotic aromatic rooted forest with an even number of crosses, $\mathbb{E}[F(\gamma)(\phi)]$ is the sum of all possible forests obtained by linking the crosses of γ pairwise with lianas.

Example

$\mathbb{E}\left[F\left(\right.\right.$  $\left.\left.\right)(\phi)\right]$

$$= \sigma^4 \mathbb{E}[\phi^{(4)}(\xi,\xi,\xi,\xi)] = \sigma^4 \sum_{ijkl} \partial_{ijkl}\phi \mathbb{E}[\xi_i\xi_j\xi_k\xi_l]$$

$$= \sigma^4 \sum_{i} \partial_{iiii}\phi \mathbb{E}[\xi_i^4] + 3\sigma^4 \sum_{\substack{i,j \\ i\neq j}} \partial_{iijj}\phi \mathbb{E}[\xi_i^2]\mathbb{E}[\xi_j^2]$$

$= 3\sigma^4 \sum_{i,j} \partial_{iijj}\phi = 3F\left(\right.$  $\left.\right)(\phi).$

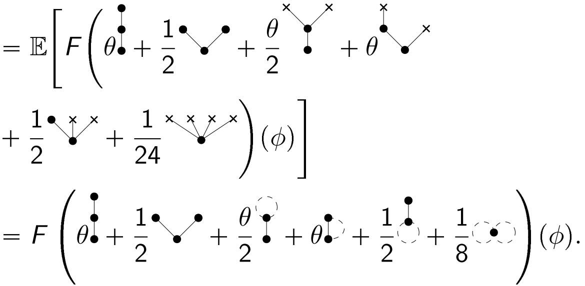
Explicit formula for $\mathcal{A}_1$

The operator $\mathcal{A}_1$ given by

$$\mathbb{E}[\phi(X_1)|X_0 = x] = \phi(x) + h\mathcal{L}\phi(x) + h^2\mathcal{A}_1\phi(x) + \ldots$$

is now convenient to write with exotic aromatic trees.

$$\mathcal{A}_1\phi = \mathbb{E}[\theta\phi' f' f + \frac{1}{2}\phi''(f,f) + \frac{\theta}{2}\phi' f''(\xi,\xi) + \theta\phi''(f'\xi,\xi) + \frac{1}{2}\phi^{(3)}(f,\xi,\xi) + \frac{1}{24}\phi^{(4)}(\xi,\xi,\xi,\xi)]$$



Integrating by parts exotic aromatic forests

Goal: simplify $\int_{\mathbb{R}^d} \mathcal{A}_j \phi \rho_\infty dy$, i.e. write it as $\int_{\mathbb{R}^d} \phi'(\widetilde{f}) \rho_\infty dy$.

$$\int_{\mathbb{R}^d} F(\cdot)(\phi)\rho_\infty dy = \sigma^2 \sum_{i,j} \int_{\mathbb{R}^d} \frac{\partial^3 \phi}{\partial x_i \partial x_j \partial x_j} f_i \rho_\infty dy$$

$$= -\sigma^2 \sum_{i,j} \left[\int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} \frac{\partial f_i}{\partial x_j} \rho_\infty dy + \int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} f_i \frac{\partial \rho_\infty}{\partial x_j} dy. \right]$$

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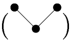
$\int_{\mathbb{R}^d} F($  $)(\phi)\rho_\infty dy$

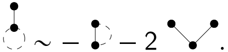
$$= \sigma^2 \sum_{i,j} \int_{\mathbb{R}^d} \frac{\partial^3 \phi}{\partial x_i \partial x_j \partial x_j} f_i \rho_\infty dy$$

$$= -\sigma^2 \sum_{i,j} \Big[\int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} \frac{\partial f_i}{\partial x_j} \rho_\infty dy + \int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} f_i \frac{\partial \rho_\infty}{\partial x_j} dy. \Big]$$

If $f = -\nabla V$, $\rho_\infty(x) = Ze^{-2V(x)/\sigma^2}$ and $\nabla \rho_\infty = \frac{2}{\sigma^2} f \rho_\infty$. Then

$\int_{\mathbb{R}^d} F($  $)(\phi)\rho_\infty dy = -\int_{\mathbb{R}^d} F($  $)(\phi)\rho_\infty dy - 2\int_{\mathbb{R}^d} F($  $)(\phi)\rho_\infty dy.$

We write

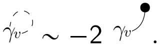


Main tool 2: integration by parts

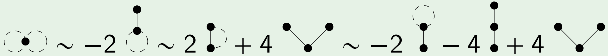
Theorem

Integrating by part an exotic aromatic forest γ amounts to unplug a liana from the root, and to plug it either to another node of γ or to connect it to a new node, transform the liana in an edge and multiply by 2.

For a node v of the exotic aromatic forest γ, it rewrites in



Example



Theorem

Take a method of order p. If $\mathcal{A}_p = F(\gamma_p)$ for a certain linear combination of exotic aromatic forests γ_p, if $\gamma_p \sim \widetilde{\gamma}_p$ and $F(\widetilde{\gamma}_p) = 0$, then the method is at least of order $p+1$ for the invariant measure.

Application to the construction of high order integrators

Theorem (Conditions for order p for the invariant measure in $\mathbb{R}^d$)

Order conditions for a class of stochastic Runge-Kutta methods:

$$Y_i^n = X_n + h\sum_{j=1}^{s} a_{ij} f(Y_j^n) + d_i\sigma\sqrt{h}\xi_n, \qquad i = 1, \dots, s,$$

$$X_{n+1} = X_n + h\sum_{i=1}^{s} b_i f(Y_i^n) + \sigma\sqrt{h}\xi_n,$$

Order	*Tree* τ	$F(\tau)(\phi)$	*Order condition*
1		$\phi' f$	$\sum b_i = 1$
2		$\phi' f' f$	$\sum b_i c_i - 2\sum b_i d_i = -\frac{1}{2}$
		$\sigma^2\phi'\Delta f$	$\sum b_i d_i^2 - 2\sum b_i d_i = -\frac{1}{2}$
3	...	...	...

Postprocessors

Idea: extend to the context of ergodic SDEs the popular idea of effective order for ODEs from Butcher (1969),

$$y_{n+1} = \chi_h \circ K_h \circ \chi_h^{-1}(y_n), \qquad y_n = \chi_h \circ K_h^n \circ \chi_h^{-1}(y_0).$$

Postprocessing: $\overline{X}_n = G_n(X_n)$, with weak Taylor series expansion

$$\mathbb{E}(\phi(G_n(x))) = \phi(x) + h^p \overline{\mathcal{A}}_p \phi(x) + \mathcal{O}(h^{p+1}).$$

Theorem (V. (2015))

Under technical assumptions, assume that $X_n \mapsto X_{n+1}$ and $\overline{X}_n$ satisfy

$$\mathcal{A}_j^* \rho_\infty = 0, \quad j < p,$$

$$(\mathcal{A}_p + [\mathcal{L}, \overline{\mathcal{A}}_p])^* \rho_\infty = 0,$$

then the scheme has order $p+1$ for the invariant measure.

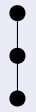
Remark: the postprocessing is needed only at the end of the time interval (not at each time step).

Postprocessors

Theorem

If we denote γ *the exotic aromatic B-series such that* $F(\gamma) = (\mathcal{A}_p + [\mathcal{L}, \overline{\mathcal{A}_p}])$ *and if* $\gamma \sim 0$, *then* $\overline{X_n}$ *is of order* $p+1$ *for the invariant measure.*

Theorem (Conditions for order p using postprocessors)

Order	*Tree* τ	*Order conditions*
2		$\sum b_i c_i - 2\sum b_i d_i - 2\sum \overline{b_i} + 2\overline{d_0}^2 = -\frac{1}{2}$
		$\sum b_i d_i^2 - 2\sum b_i d_i - \sum \overline{b_i} + \overline{d_0}^2 = -\frac{1}{2}$

Example (first introduced in Leimkhuler, Matthews, 2013)

$$X_{n+1} = X_n + hf(X_n + \frac{\sigma}{2}\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \qquad \overline{X_n} = X_n + \frac{1}{2}\sigma\sqrt{h}\overline{\xi_n}.$$

The scheme has order 1 of accuracy for the invariant measure, but $\overline{X}_n$ has order 2.

Contents

The Euler integrator for constrained Langevin dynamics

Constrained Langevin dynamics on the manifold $\mathcal{M} = \{x \in \mathbb{R}^d, \zeta(x) = 0\}$

$$dX = \Pi_{\mathcal{M}}(X) f(X) dt + \sigma \Pi_{\mathcal{M}}(X) \circ dW.$$

Example (Euler integrator)

Two widely used integrators are the Euler scheme with explicit projection direction, where $g = \nabla \zeta$

$$X_{n+1} = X_n + hf(X_n) + \sigma\sqrt{h}\xi_n + \lambda g(X_n), \quad \zeta(X_{n+1}) = 0,$$

and alternatively the Euler scheme with implicit projection direction

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

→ References: Ciccotti, Kapral, Vanden-Eijnden (2005); Lelièvre, Le Bris, Vanden-Eijnden (2008); Lelièvre, Rousset, Stolz (2010); ...

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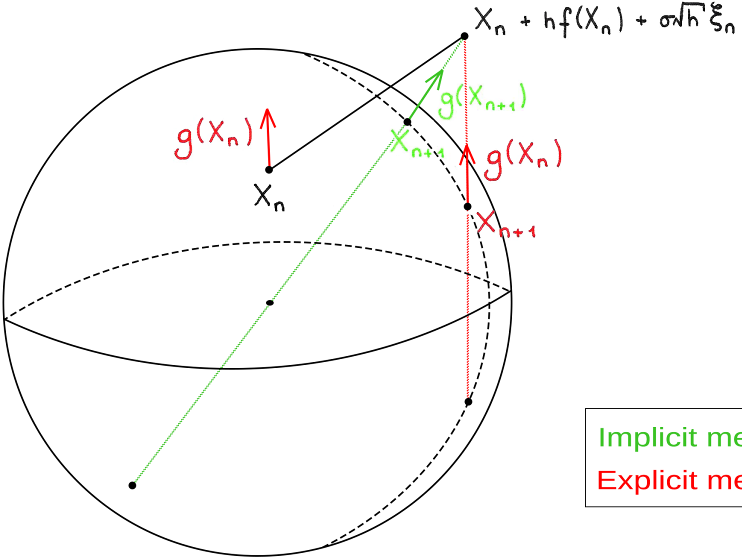
Issue: both Euler integrators have order 1 for the invariant measure.

The Euler integrator for constrained Langevin dynamics



Implicit method

Explicit method

A new class of RK methods for constrained Langevin

In the spirit of the methods RATTLE (Lelièvre, Rousset, Stolz (2019)) and SPARK (Jay (1998)), we use the following class of Runge-Kutta integrators:

$$Y_i = X_n + h\sum_{j=1}^{s} a_{ij} f(Y_j) + \sigma\sqrt{h} d_i \xi_n + \lambda_i \sum_{j=1}^{s} \widehat{a}_{ij} g(Y_j), \quad i = 1, \dots, s,$$

$$\zeta(Y_i) = 0 \quad \text{if} \quad \delta_i = 1, \quad i = 1, \dots, s,$$

$$X_{n+1} = Y_s,$$

Butcher tableau with $c = A\mathbb{1}$, $\delta = \widehat{A}\mathbb{1} \in \{0, 1\}$, $b = A_{s,:}$ and $\widehat{b} = \widehat{A}_{s,:}$

$$\begin{array}{c|c||c|c||c} c & A & \delta & \widehat{A} & d \\ \hline & b^T & & \widehat{b}^T & \end{array}$$

Example

The Euler integrator $X_{n+1} = X_n + hf(X_n) + \sigma\sqrt{h}\xi_n + \lambda g(X_{n+1})$, $\zeta(X_{n+1}) = 0$ has the following Butcher tableau

$$\begin{array}{c|cc||c|cc||c} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 1 \\ \hline & 1 & 0 & & 0 & 1 & \end{array}.$$

Order conditions for sampling Langevin dynamics on $\mathcal{M}$

Theorem (Runge-Kutta conditions)

- *Consistency conditions:* $c_s = d_s = 1$ *and* $\sum_{j=1}^{s} \widehat{b}_j d_j = \sum_{j=1}^{s} \widehat{b}_j \delta_j d_j$
- *22 cond. for order 2 for the invariant measure (resp. 11 cond. if* $\delta = \mathbb{1}$*):*

$$\sum_{j=1}^{s} b_j c_j = 2\sum_{j=1}^{s} b_j d_j - \frac{1}{2},\ \sum_{i,j=1}^{s} \widehat{b}_i d_i^2 \widehat{a}_{ij} d_j = \sum_{i,j=1}^{s} \widehat{b}_i d_i \widehat{a}_{ij} d_j + \frac{1}{2}\Big(\sum_{i=1}^{s} \widehat{b}_i d_i\Big)^2,\ \dots$$

- *25 cond. for weak order 2 (conditions do not have a solution if* $\delta = \mathbb{1}$*).*

Example

An integrator of order 2 for the invariant measure if $\mathcal{M}$ is the sphere

$$Y_1 = X_n + h\left(\frac{3}{2} - \sqrt{2}\right) f(Y_2) + \sigma\sqrt{h}\left(1 - \frac{\sqrt{2}}{2}\right)\xi_n + \lambda_1(2g(Y_1) - g(Y_2)),$$

$$Y_2 = X_n + hf(Y_1) + \sigma\sqrt{h}\xi_n + \lambda_2 g(Y_1), \quad \zeta(Y_1) = \zeta(Y_2) = 0,$$

$$X_{n+1} = Y_2.$$

Numerical experiments

- We introduce a 4-stages RK method of order 2 for the invariant measure that uses only 3 evaluations of f per step.

$$
\begin{aligned}
Y_1 &= X_n + \sigma\sqrt{h}d_1\xi_n + \lambda_1 g(Y_1),\\
Y_2 &= X_n + hc_2 f(Y_1) + \sigma\sqrt{h}d_2\xi_n + \lambda_2\left[\widehat{a}_{21}g(Y_1) + \widehat{a}_{22}g(Y_2)\right],\\
Y_3 &= X_n + hc_3 f(Y_2) + \sigma\sqrt{h}d_3\xi_n + \lambda_3\left[\widehat{a}_{31}g(Y_1) + \widehat{a}_{32}g(Y_2) + \widehat{a}_{33}g(Y_3)\right],
\end{aligned}
$$

$$
X_{n+1} = X_n + h\sum_{j=1}^{3}\widehat{a}_{4j}f(Y_j) + \sigma\sqrt{h}\xi_n + \lambda_4\sum_{j=1}^{3}\widehat{a}_{4j}g(Y_j),
$$

where $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ are such that $\zeta(Y_1) = \zeta(Y_2) = \zeta(Y_3) = \zeta(X_{n+1}) = 0$.

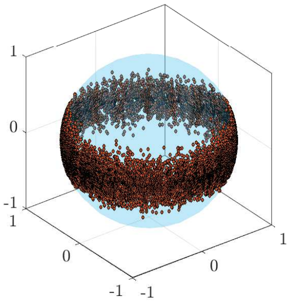
Butcher tableau:

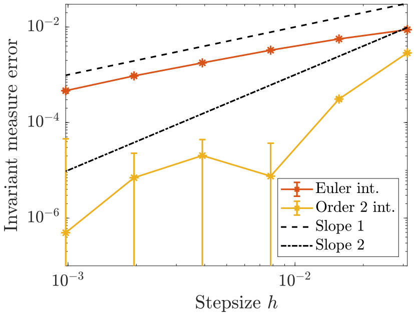
$$
\begin{array}{c|cccc||c|cccc||c}
0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & d_1\\
c_2 & c_2 & 0 & 0 & 0 & 1 & \widehat{a}_{21} & \widehat{a}_{22} & 0 & 0 & d_2\\
c_3 & 0 & c_3 & 0 & 0 & 1 & \widehat{a}_{31} & \widehat{a}_{32} & \widehat{a}_{33} & 0 & d_3\\
1 & \widehat{a}_{41} & \widehat{a}_{42} & \widehat{a}_{43} & 0 & 1 & \widehat{a}_{41} & \widehat{a}_{42} & \widehat{a}_{43} & 0 & 1\\
\hline
 & \widehat{a}_{41} & \widehat{a}_{42} & \widehat{a}_{43} & 0 & & \widehat{a}_{41} & \widehat{a}_{42} & \widehat{a}_{43} & 0 &
\end{array}
$$

Numerical experiments

• We introduce a 4-stages RK method of order 2 for the invariant measure that uses only 3 evaluations of f per step.

• We plot the invariant measure error versus the timestep h for the order 2 integrator and the Euler scheme when $\mathcal{M}$ is the unit sphere in $\mathbb{R}^3$, with the constraint $\zeta(x) = (\|x\|^2 - 1)/2$, the potential $V(x) = 25(1 - x_1^2 - x_2^2)$, the final time $T = 10$ and 10^7 trajectories.

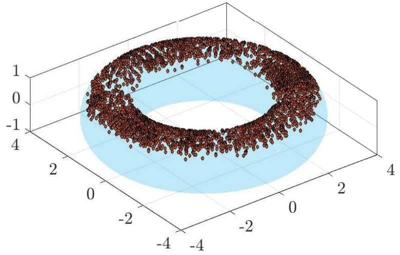


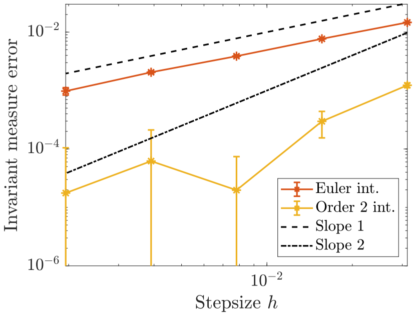


Numerical experiments

• We introduce a 4-stages RK method of order 2 for the invariant measure that uses only 3 evaluations of f per step.

• We plot the invariant measure error versus the timestep h for the order 2 integrator and the Euler scheme when $\mathcal{M}$ is a torus in $\mathbb{R}^3$, with the constraint $\zeta(x) = (\|x\|^2 + 8)^2 - 36(x_1^2 + x_2^2)$, the potential $V(x) = 25(x_3 - 1)^2$, the final time $T = 20$ and 10^7 trajectories.





Numerical experiments

• We introduce a 4-stages RK method of order 2 for the invariant measure that uses only 3 evaluations of f per step.

• We compare the approximations $\overline{I}_{\text{Euler}}$ and $\overline{I}_2$ given by the Euler scheme and the new order 2 Runge-Kutta integrator of $I(m)=\int_{\mathrm{SL}(m)} \mathrm{Tr}(x)d\mu_\infty(x)$ on the special linear group $\mathcal{M}=\mathrm{SL}(m)$ in $\mathbb{R}^{m^2}$ with the constraint $\zeta(x)=\det(x)-1$, the final time $T=10$ with the stepsize $h=T/2^{12}$, 10^6 trajectories and the potential

$$V(x)=25\,\mathrm{Tr}((x-I_{m^2})^T(x-I_{m^2})).$$

m	$\dim(\mathrm{SL}(m))$	$I(m)$	error for $\overline{I}_{\text{Euler}}$	error for $\overline{I}_2$
2	3	2.00967	$6.4\cdot10^{-4}$	$4.4\cdot10^{-5}$
3	8	3.01954	$1.1\cdot10^{-3}$	$2.0\cdot10^{-4}$
4	15	4.02930	$1.6\cdot10^{-3}$	$2.3\cdot10^{-4}$

Exotic aromatic forests: adding scalar product (Submitted. 2020)

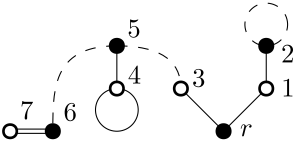
We use partitioned forests and we introduce a new kind of edge that represents the scalar product.

Examples

$F($$) = G^{-1}\sum_{i,j} g_i \partial_j f_i g_j = G^{-1}(g, f'g)$.

$F($$) = \sigma^2 G^{-2}\sum_{i,j,k} g_i \partial_{jk} g_i g_j g_k = \sigma^2 G^{-2}(g, g''(g,g))$.

In general, we can get forests of the form



where the associated differential is

$$F(\gamma)(\phi) = \sigma^8 G^{-2} \sum_{i_1,\dots,i_6=1}^{d} \sum_{j_1,\dots,j_3=1}^{d} \partial_{j_1 j_1} f_{i_2}\ \partial_{j_2 j_3} f_{i_5}\ \partial_{j_3} f_{i_6}\ \partial_{i_2} g_{i_1}\ \partial_{j_2} g_{i_3}\ \partial_{i_4 i_5} g_{i_4}\ g_{i_6}\ \partial_{i_1 i_3}\phi.$$

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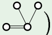
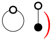
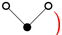
$F($$) = \sigma^2 G^{-2} \sum_{i,j,k} g_i \partial_{jk} g_i g_j g_k = \sigma^2 G^{-2}(g, g''(g,g)).$

On the manifold $\mathcal{M}$, the generator $\mathcal{L}$ is given by

$$\mathcal{L}\phi = \phi' f - G^{-1}(g,f)\phi' g - \frac{\sigma^2}{2} G^{-1} \operatorname{div}(g)\phi' g + \frac{\sigma^2}{2} G^{-2}(g, g'g)\phi' g + \frac{\sigma^2}{2}\Delta\phi - \frac{\sigma^2}{2} G^{-1}\phi''(g,g)$$

$= F($$)(\phi) - G^{-1}(g,f)\phi' g - \frac{1}{2}F($$)(\phi) + \frac{\sigma^2}{2} G^{-2}(g, g'g)\phi' g$

$+ \frac{\sigma^2}{2}\Delta\phi - \frac{1}{2}F($$)(\phi)$

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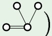
$F($$) = \sigma^2 G^{-2}\sum_{i,j,k} g_i \partial_{jk} g_i g_j g_k = \sigma^2 G^{-2}(g, g''(g,g)).$

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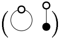
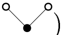
$= F($$)(\phi) - G^{-1}(g,f)\phi' g - \frac{1}{2}F($$)(\phi) + \frac{\sigma^2}{2}G^{-2}(g, g'g)\phi' g$

$+ \frac{1}{2}F($$)(\phi) - \frac{1}{2}F($$)(\phi)$

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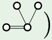
$F($$) = \sigma^2 G^{-2}\sum_{i,j,k} g_i \partial_{jk} g_i g_j g_k = \sigma^2 G^{-2}(g, g''(g,g)).$

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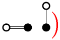
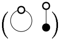
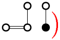
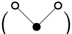
$= F($$)(\phi) - F($$)(\phi) - \frac{1}{2}F($$)(\phi) + \frac{1}{2}F($$)(\phi)$

$+ \frac{1}{2}F($$)(\phi) - \frac{1}{2}F($$)(\phi)$

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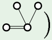
$F($$) = \sigma^2 G^{-2}\sum_{i,j,k} g_i \partial_{jk} g_i g_j g_k = \sigma^2 G^{-2}(g, g''(g,g)).$

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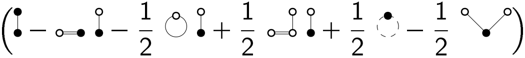
$= F\Big($  $\Big)(\phi).$

Similarly, we obtain an expansion in exotic aromatic forests of the operators $\mathcal{A}_j$.
Goal: find conditions such that $\mathcal{A}_j^* \rho_\infty = 0$ in $L^2(d\sigma_{\mathcal{M}})$.

Isometric equivariance of exotic aromatic B-series

Examples of aromatic forests:

$F($$) = f'f = \sum_i \partial_i f\, f_i$ $\qquad$ $F($$) = \mathrm{div}(f) = \sum_i \partial_i f_i$

Examples of exotic aromatic forests:

$F($$) = \Delta f = \sum_i \partial_{ii} f$ $\qquad$ $F($$) = \|f\|^2 = \sum_i f_i f_i$

Definition

Affine equivariant map: invariant under an affine coordinates map.
Isometric equivariant map: invariant under an isometric coordinates map.

Local affine equivariant maps are exactly aromatic B-series methods (see McLachlan, Modin, Munthe-Kaas, Verdier, 2016).

Proposition

Exotic aromatic B-series methods are isometric equivariant.

Converse: ongoing work with H. Munthe-Kaas and O. Verdier.

Integration by parts of exotic aromatic forests

Lemma (Integration by parts on $\mathcal{M}$)

If $\psi : \mathbb{R}^d \to \mathbb{R}$ and $H : \mathbb{R}^d \to \mathbb{R}^d$ are smooth functions, then we have

$$\int_{\mathcal{M}} (\nabla_{\mathcal{M}}\psi, H) d\sigma_{\mathcal{M}} = -\int_{\mathcal{M}} \psi \, \mathrm{div}_{\mathcal{M}}(\Pi_{\mathcal{M}} H) d\sigma_{\mathcal{M}},$$

where $\nabla_{\mathcal{M}}\psi := \Pi_{\mathcal{M}}\nabla\psi$ and $\mathrm{div}_{\mathcal{M}}(H) := \mathrm{div}(H) - G^{-1}(g, H'g)$.

Integration by parts of exotic aromatic forests

Lemma (Integration by parts on $\mathcal{M}$)

If $\psi : \mathbb{R}^d \to \mathbb{R}$ *and* $H : \mathbb{R}^d \to \mathbb{R}^d$ *are smooth functions, then we have*

$$\int_{\mathcal{M}} \Big[G^{-k}\psi' H - G^{-(k+1)}(g,H)\psi' g\Big] d\mu_\infty = \int_{\mathcal{M}} \Big[G^{-(k+1)}(g,H'g)\psi - (2k+1)G^{-(k+2)}(g,g'g)(g,H)\psi - G^{-k}\operatorname{div}(H)\psi + 2kG^{-(k+1)}(g,g'H)\psi + G^{-(k+1)}\operatorname{div}(g)(g,H)\psi + \frac{2}{\sigma^2}G^{-(k+1)}(g,f)(g,H)\psi - \frac{2}{\sigma^2}G^{-k}(f,H)\psi\Big] d\mu_\infty.$$

Integration by parts of exotic aromatic forests

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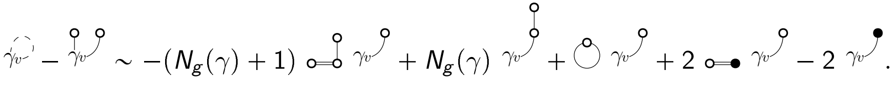
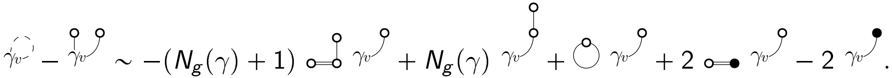
For integrating by parts an exotic aromatic forests in the direction of a liana, it rewrites into



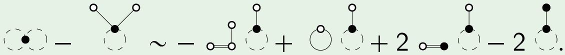
Integration by parts of exotic aromatic forests

Integration by parts of exotic aromatic forests:

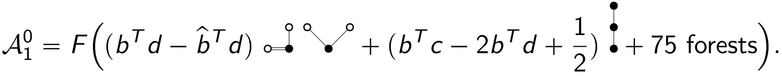


Example

For $\gamma =$  and $v = r$ the root, we get



Application: We have $\int_{\mathcal{M}} \mathcal{A}_1 \phi d\mu_\infty = \int_{\mathcal{M}} \mathcal{A}_1^0 \phi d\mu_\infty$ where



Choosing the coefficients such that $\mathcal{A}_1^0 = 0$ yields the order 2 conditions for the invariant measure.

Summary

• We introduced a new algebraic formalism of trees to study the order for the invariant measure of numerical integrators for the overdamped Langevin equation in $\mathbb{R}^d$ and on compact smooth manifolds of codimension one.

• The exotic aromatic forests formalism inherits the properties of the previously introduced tree formalisms, as a composition law and a universal geometric property.

• We recover efficient numerical methods, a systematic methodology to improve order and a formal simplification of any numerical method that can be developed in exotic aromatic B-series.

• Possible applications to partitioned problems or systems with perturbations, and extensions to more general SDEs where f is not a gradient, on manifolds of any codimension, or to SDEs with multiplicative noise of the form

$$dX = f(X)dt + \Sigma(X)dW.$$