Un nouveau type de B-series pour l'étude d'intégrateurs numériques pour la mesure invariante de l'équation de Langevin overdamped.

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Contents

The Langevin equation

Take N particles moving in a fluid (with $N \simeq 10^{24}$). Let $q(t)$ be their positions and $p(t)$ their velocities. The particles are submitted to

- a potential V and the associated force $-\nabla V$,
- a friction force $-\gamma p$,
- a collision term $\sqrt{\frac{2\gamma}{\beta}} dW$.

Then applying the fundamental principle of dynamic, we find the Langevin equation.

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

Friction limit

If $\gamma \to \infty$, we assume the acceleration is negligible. It is called the friction limit. It means the dynamic is dominated by collisions. Then

$$\left\{ \begin{array}{l} dq(t) = p(t)dt \\ 0 = (-\nabla V(q(t)) - \gamma p(t))dt + \sqrt{\frac{2\gamma}{\beta}} dW(t) \end{array} \right.$$

and finally

$$dq(t) = -\gamma^{-1} \nabla V(q(t))dt + \sqrt{\frac{2}{\gamma\beta}} dW(t).$$

In this talk, we focus on this following simplified equation called the overdamped Langevin equation:

$$dX(t) = f(X(t))dt + \sigma dW(t)$$

where $f = -\nabla V$.
This is a Stochastic Differential Equation (SDE). It means that X satisfies

$$X(t) = X(0) + \int_0^t f(X(s))ds + \sigma W(t).$$

Contents

Two methods for ODEs

Problem:

$$y' = f(y), \quad y(0) = y_0$$

Example of three numerical methods, with $t_n = nh \leqslant T = Nh$ and $y_n \simeq y(t_n)$:

- Explicit Euler: $y_{n+1} = y_n + hf(y_n)$
- RK2: $y_{n+1} = y_n + hf(y_n + \frac{h}{2} f(y_n))$
- RK4:

$$y_{n+1} = y_n + \frac{h}{6}\Big[f(y_n) + 2f(y_n + \frac{h}{2} f(y_n)) + 2f(y_n + \frac{h}{2} f(y_n + \frac{h}{2} f(y_n))) + f(y_n + hf(y_n + \frac{h}{2} f(y_n + \frac{h}{2} f(y_n))))\Big]$$

A scheme has local order p iif $|y(t_1) - y_1| \leqslant Ch^{p+1}$.

Deriving the order of a Runge-Kutta method

The equation $y' = f(y)$ gives $y'(0) = f(y_0)$.
The equation $y'' = f'(y)(y') = f'(y)(f(y))$ gives $y''(0) = f'(y_0)(f(y_0))$, etc...

Taylor expansion of the real solution:

$$y(t_1) = y_0 + hf(y_0) + \frac{h^2}{2} f'f(y_0) + \frac{h^3}{6}(f'f'f + f''(f,f))(y_0) + \dots$$

Taylor expansion of the numerical scheme: for RK2,

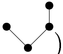
$$\begin{aligned} y_1 &= y_0 + hf(y_0 + \frac{h}{2} f(y_0)) \\ &= y_0 + hf(y_0) + \frac{h^2}{2} f'f(y_0) + \frac{h^3}{6} f''(f,f)(y_0) + \dots \end{aligned}$$

Remark

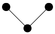
The performance of a method greatly depends of its order.

The magic of B-series

Define a set of trees representing differentials

- $F(\bullet)(f) = f$
- $F($$)(f) = f'f$
- $F($$)(f) = f''(f, f'f)$

Then

1. $y'(0) = f(y_0)$ becomes $y'(0) = F(\bullet)(f)(y_0)$.
2. $y''(0) = f'(y_0)(f(y_0))$ becomes $y''(0) = F($$)(f)(y_0)$.
3. $y'''(0) = (F($$) + F($$))(y_0)$.
4. $y^{(q)}(0) = \sum_{|\tau|=q} \alpha(\tau) F(\tau)(y_0)$ where α can be computed easily with a recursive formula.

A similar development can be obtained for all Runge-Kutta methods, allowing to obtain order conditions without tedious computations.

Contents

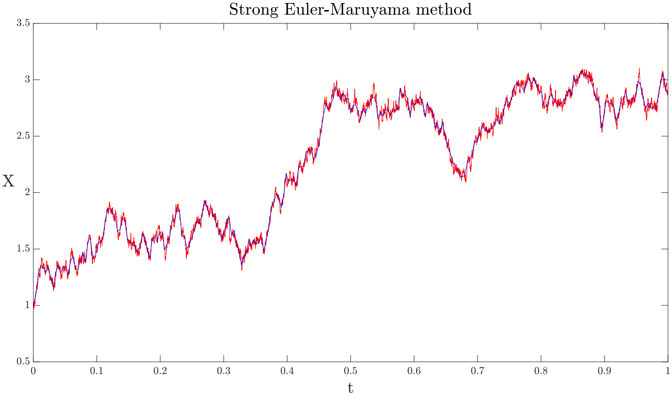
First schemes: the strong Euler-Maruyama method

Overdamped Langevin equation:

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

The strong Euler-Maruyama method:

$$X_{n+1} = X_n + hf(X_n) + \sigma(W((n+1)h) - W(nh)).$$



First schemes: the weak Euler-Maruyama method

Overdamped Langevin equation:

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

The Euler-Maruyama method:

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

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

First schemes: the weak Euler-Maruyama method

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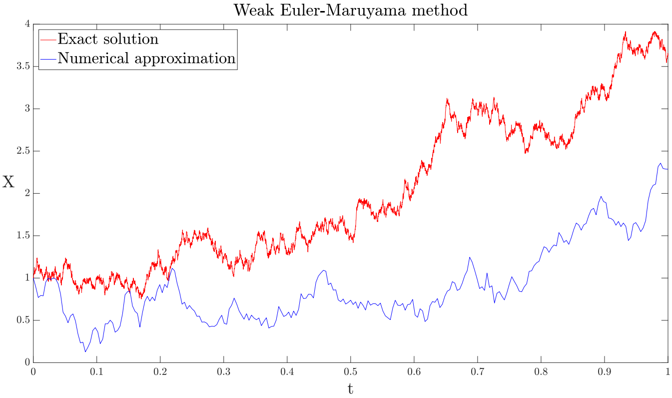

The weak convergence: definition and tools

Definition

A numerical scheme is said to have local weak order p if for all smooth ϕ with polynomial growth,

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

For example, the Euler-Maruyama method has weak order 1.

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For example, the Euler-Maruyama method has weak order 1.

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

$$\begin{cases} \frac{\partial u}{\partial t} = \nabla u.f + \frac{\sigma^2}{2}\Delta u = \mathscr{L}u, \\ u(x,0) = \phi(x). \end{cases}$$

Classical tools for the weak convergence

We develop the exact solution in Taylor series:

$$\mathbb{E}[\phi(X(h))|X(0)=x] = \phi(x) + h\mathscr{L}\phi(x) + \frac{h^2}{2}\mathscr{L}^2\phi(x) + \ldots$$

We compare with the Taylor series of the numerical approximation:

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

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

Under assumptions, the scheme is of weak order p if

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

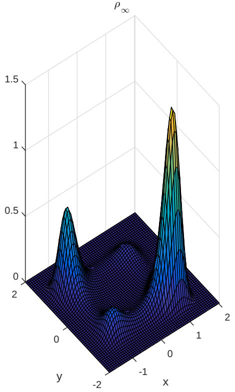
⇒ Tree formalism of B-series for deterministic problems: Butcher (1972) and Hairer, Wanner (1974),...

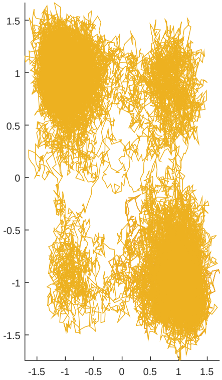
⇒ Tree formalism for strong and weak errors on finite time: Burrage K., Burrage P.M. (1996); Komori, Mitsui, Sugiura (1997); Rößler (2004/2006), ...

Ergodicity, invariant measure

Ergodicity property: there exists a (unique) invariant measure ρ_∞ such that

$$\lim_{T\to+\infty} \frac{1}{T}\int_0^T \phi(X(s))ds = \int_{\mathbb{R}^d} \phi(y)\rho_\infty(y)dy \quad \text{a.s..}$$





Under ergodicity assumption, ρ_∞ is a steady state of the Fokker-Planck equation, i.e.

$$\mathcal{L}^*\rho_\infty = 0.$$

For Brownian dynamics $dX = -\nabla V(X)dt + \sqrt{2}dW$, we have $\rho_\infty(x) = Ze^{-V(x)}$.

Order of convergence for the invariant measure

Definition (Convergence for the invariant measure)

We call error of the invariant measure the quantity

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

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

Theorem (Abdulle, Vilmart, Zygalakis (2014); Related work: Debussche, Faou (2012); Kopec (2013))

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

$$\int_{\mathbb{R}^d} \mathcal{A}_j \phi \rho_\infty dy = 0, \qquad j = 2, \dots, p-1,$$

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

Contents

Example: the θ-method

Overdamped Langevin equation:

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

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

We have (for $\xi \sim \mathcal{N}(0, I_d)$)

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

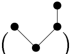
It yields $\mathbb{E}[\phi(X_1)|X_0 = x] = \phi(x) + h\mathcal{L}\phi(x) + h^2\mathcal{A}_1\phi(x) + \dots$, where

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

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($$)(\phi) = \phi' f$
- $F($$)(\phi) = \phi''(f, f'f)$

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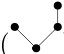
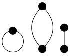
- $F($$)(\phi) = \phi''(f, f'f)$

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

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

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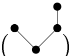
- $F($  $)(\phi) = \phi''(f, f'f)$

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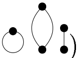
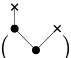
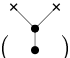
$F($  $)(\phi) = \mathrm{div}(f) \times \left(\sum \partial_i f_j \partial_j f_i\right) \times \phi' f$

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

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

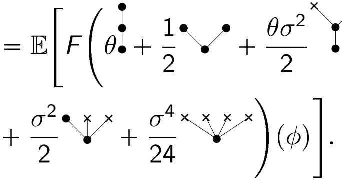
Grafted forests for the θ-method

For the θ method,

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

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

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



New exotic aromatic forests : adding lianas

We add lianas to the aromatic forests.

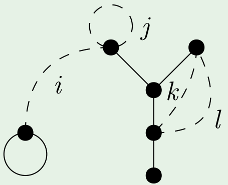
Examples

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

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

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

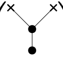
If γ is the following forest



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

Remark: our forests do not depend on the dimension.

Computing the expectation using lianas

$\mathbb{E}\Big[F\Big($  $\Big)(\phi)\Big] = \mathbb{E}[\phi' f''(\xi,\xi)] = \sum_{i,j,k} \partial_i\phi.\partial_{jk} f_i.\mathbb{E}[\xi_j\xi_k]$

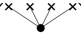
$$= \sum_{i,j} \partial_i\phi.\partial_{jj} f_i = \phi'\Delta f$$

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

Main tool 1: expectation of a grafted exotic aromatic forest

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.

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

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

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

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

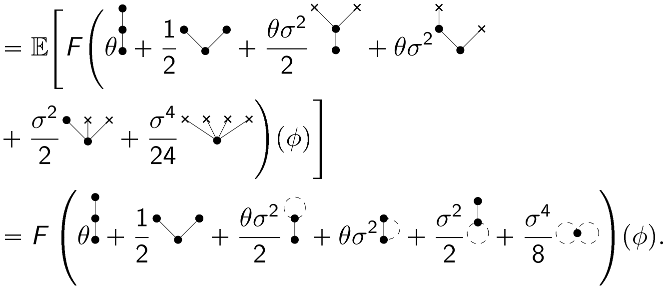
Explicit formula for $\mathcal{A}_1$

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.

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



Integrating by parts exotic aromatic forests

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

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

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

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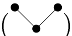
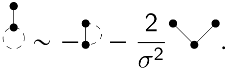
$$= -\sum_{i,j} \left[\int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} \frac{\partial f_i}{\partial x_j} \rho_\infty dy + \int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} f_i \frac{\partial \rho_\infty}{\partial x_j} dy. \right]$$

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

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

We write



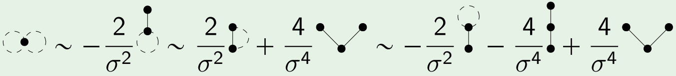
Main tool 2: integration by parts

Theorem

Integrating by part an exotic aromatic forest γ amounts to unplug a liana from the root, 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 $\frac{2}{\sigma^2}$. Then

$$\int_{\mathbb{R}^d} F(\gamma)(\phi)\rho_\infty dy = -\sum_{\tilde{\gamma}\in U(\gamma,e)} \int_{\mathbb{R}^d} F(\tilde{\gamma})(\phi)\rho_\infty dy.$$

Example



Theorem

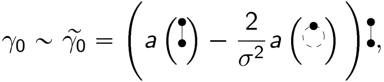
Take a method of order p. If $\mathcal{A}_p = F(\gamma_p)$ for a certain linear combination of exotic aromatic forests γ_p, if $\gamma_p \sim \tilde{\gamma}_p$ and $F(\tilde{\gamma}_p) = 0$, then the method is at least of order $p+1$ for the invariant measure.

Order conditions using exotic aromatic forests

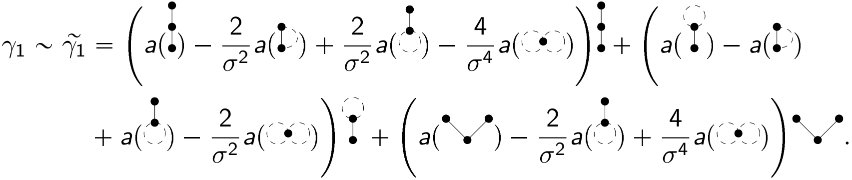
In particular, if

$$\mathbb{E}[\phi(X_1)|X_0 = x] = F(\bullet)(\phi) + \sum_{\substack{\gamma\in\mathcal{EAT} \\ 1\leqslant|\gamma|\leqslant p}} h^{|\gamma|} a(\gamma) F(\gamma)(\phi) + \dots,$$

and if $\mathcal{A}_p = F(\gamma_p)$ then



and



Contents

Order conditions for stochastic RK methods

Theorem (Conditions for order p for the invariant measure)

Conditions for consistency and order 2 for stochastic Runge-Kutta methods:

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

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

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

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

X_n has order 1 of accuracy for the invariant measure, but $\overline{X_n}$ has order 2.

Partitioned methods

Problem: solve $dX = f(X)dt + \sigma dW$ with $f = f_1 + f_2$ applying different numerical treatments for each f_i. For example, if f_1 is stiff and f_2 is non-stiff, we want to apply an implicit method to f_1 and an explicit one to f_2.

Theorem

Order	*Tree* τ	$F(\tau)(\phi)$	*Order condition*
1		$\phi' f_1$	$\sum b_i = 1$
		$\phi' f_2$	$\sum \hat{b}_i = 1$
2		$\phi' f_1' f_1$	$\sum b_i c_i - 2\sum b_i d_i - 2\sum \overline{b_i} + 2\overline{d_0}^2 = -\frac{1}{2}$
		$\phi' f_1' f_2$	$\sum b_i \hat{c}_i - 2\sum b_i d_i - \sum \overline{b_i} - \sum \overline{\hat{b}_i} + 2\overline{d_0}^2 = -\frac{1}{2}$
	...	...	...

Partitioned methods

Examples (Two methods of order 2)

$$
\begin{aligned}
X_{n+1} &= X_n + \tfrac{h}{2} f_1(X_{n+1} + \tfrac{1}{2}\sigma\sqrt{h}\xi_n) + \tfrac{h}{2} f_1(X_{n+1} + \tfrac{3}{2}\sigma\sqrt{h}\xi_n) \\
&\quad + h f_2(X_n + \tfrac{1}{2}\sigma\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \\
\overline{X_n} &= X_n + \tfrac{1}{2}\sigma\sqrt{h}\overline{\xi_n}.
\end{aligned}
$$

It can be put in Runge-Kutta form with $s = 0$ and $\overline{d_0} = \frac{1}{2}$ for the postprocessor and the following Butcher tableau:

$$
\begin{array}{c|c|c|c|c}
c & A & \widehat{c} & \widehat{A} & d \\
\hline
 & b & & \widehat{b} &
\end{array}
=
\begin{array}{c|ccc|c|ccc|c}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 \\
1 & 0 & 1/2 & 1/2 & 1 & 1 & 0 & 0 & 1/2 \\
1 & 0 & 1/2 & 1/2 & 1 & 1 & 0 & 0 & 3/2 \\
\hline
 & 0 & 1/2 & 1/2 & & 1 & 0 & 0 &
\end{array}
$$

If we add a family of independent noises $(\chi_n)_n$ independent of $(\xi_n)_n$, we get the following order 2 method:

$$
\begin{aligned}
X_{n+1} &= X_n + h f_1(X_{n+1} + \tfrac{1}{2}\sigma\sqrt{h}\chi_n) + h f_2(X_n + \tfrac{1}{2}\sigma\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \\
\overline{X_n} &= X_n + \tfrac{1}{2}\sigma\sqrt{h}\overline{\xi_n}.
\end{aligned}
$$

Isometric equivariance of exotic aromatic B-series

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

Theorem

Exotic aromatic B-series methods are isometric equivariant.

Remark: the converse is ongoing work.

Summary

• We introduced a new algebraic formalism of exotic aromatic trees to study the order for the invariant measure of numerical integrators for overdamped Langevin equation.

• 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 (up to order 3), systematic methodology to improve order and formal simplification of any numerical method that can be developed in exotic aromatic B-series.

• Possible applications and extensions to more general SDEs where f is not a gradient or to SDEs of the form

$$dX = f(X)dt + \Sigma^{1/2}dW.$$

Main reference 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. *Submitted*, arXiv:1707.02877, 2017.