A new tree formalism for the numerical study of the overdamped Langevin equation.

Adrien Laurent
Joint work with Gilles Vilmart

University of Geneva

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Contents

1. Modelling particles with the overdamped Langevin equation
2. Numerical schemes for the overdamped Langevin equation
3. Exotic aromatic trees for the study of invariant measure order conditions
4. Application to the construction of high order integrators

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The beginning of molecular dynamics

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$f(x,t)$: density of particles at x and time t,
$\rho_x(y,\tau)$: probability that a particle in x moves to $x+y$ in a time τ.

$$f(x,t+\tau) = \int_{-\infty}^{+\infty} f(x-y,t)\rho_x(y,\tau)dy$$

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A Taylor expansion gives:

$$f(x,t+\tau)=f(x,t)\int_{-\infty}^{+\infty}\rho_x(y,\tau)dy+\frac{\partial f}{\partial x}(x,t)\int_{-\infty}^{+\infty} y\rho_x(y,\tau)dy$$
$$+\frac{1}{2}\frac{\partial^2 f}{\partial x^2}(x,t)\int_{-\infty}^{+\infty} y^2\rho_x(y,\tau)dy+\dots$$

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$$+\frac{1}{2}\frac{\partial^2 f}{\partial x^2}(x,t)\int_{-\infty}^{+\infty}y^2\rho_x(y,\tau)dy+\dots$$

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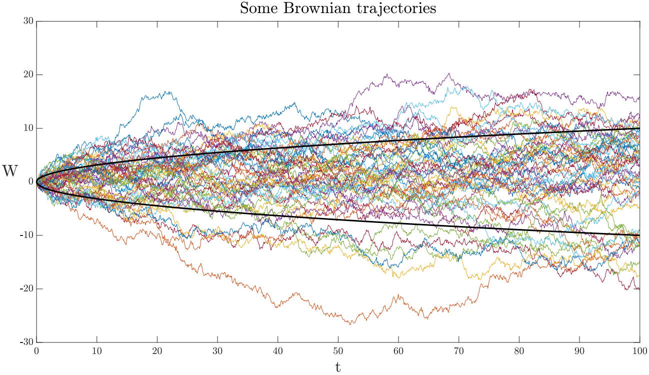
The solution is $f(x,t)=\frac{1}{\sqrt{2\pi Dt}}e^{-\frac{x^2}{2Dt}}$, i.e. the probability distribution of a Gaussian random variable $\mathcal{N}(0,Dt)$

The definition of Brownian motion

Definition

A stochastic process W is a Brownian motion if

- $W(0) = 0$ a.e.
- $\forall 0 \leqslant s \leqslant t,\ W(t) - W(s) \sim \mathcal{N}(0, t-s)$
- $\forall 0 < t_1 < t_2 < \ldots < t_n,\ W(t_1),\ W(t_2) - W(t_1),\ \ldots,\ W(t_n) - W(t_n - 1)$ are independent random variables.



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

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

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

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

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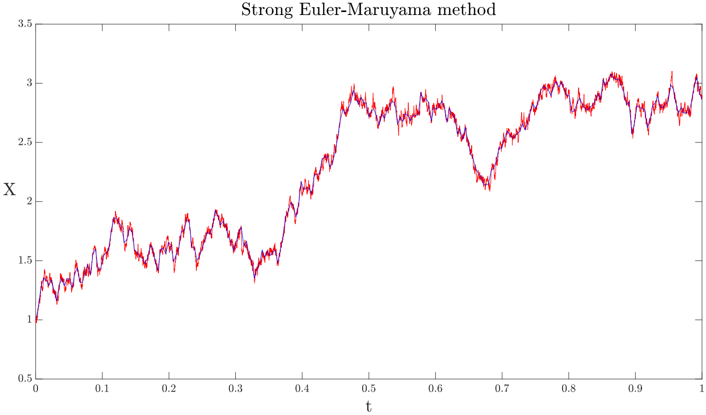
First schemes: the strong Euler-Maruyama method

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.

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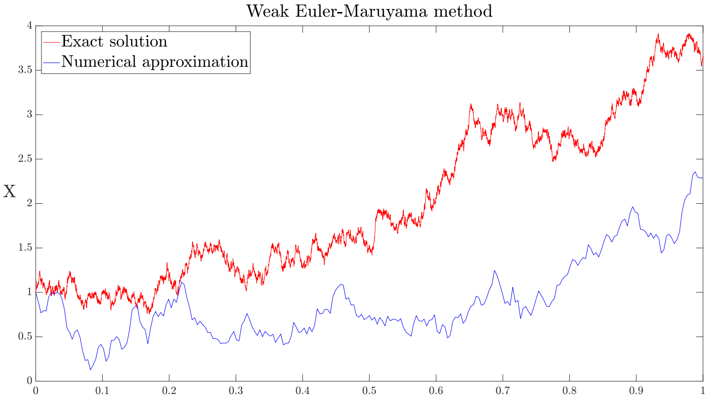

The weak convergence: definition and tools

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:

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

We compare with the Taylor series of the numerical approximation:

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

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

Under assumptions, the scheme is of weak order p if

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

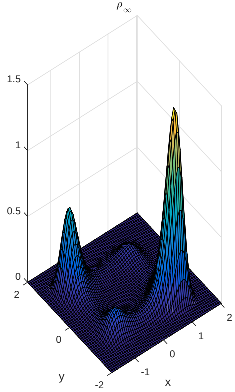
⇒ Tree formalism of B-series for deterministic problems: Butcher (1972) and Hairer, Wanner (1974),...

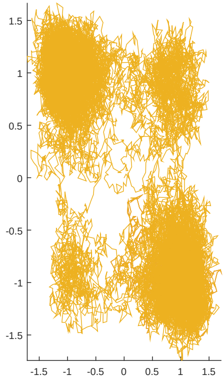
⇒ Tree formalism for strong and weak errors on finite time: Burrage K., Burrage P.M. (1996); Komori, Mitsui, Sugiura (1997); Rößler (2004/2006), ...

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.

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

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

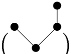
It yields $\mathbb{E}[\phi(X_1)|X_0 = x] = \phi(x) + h\mathcal{L}\phi(x) + h^2\mathcal{A}_1\phi(x) + \dots$, where

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

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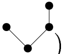
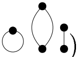
- $F($$)(\phi) = \phi''(f, f'f)$

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

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

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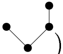
- $F($$)(\phi) = \phi''(f, f'f)$

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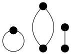
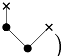
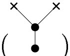
$F($$)(\phi) = \mathrm{div}(f) \times \left(\sum \partial_i f_j \partial_j f_i\right) \times \phi' f$

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)$.

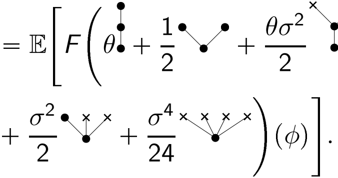
Grafted forests for the θ-method

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.

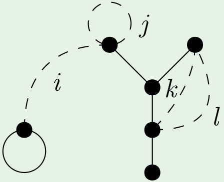
Examples

$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))$.

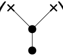
If γ is the following forest



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

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

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

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

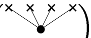
$$= F \left(\right.$$

$$\left. \right) (\phi)$$

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.

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

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

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

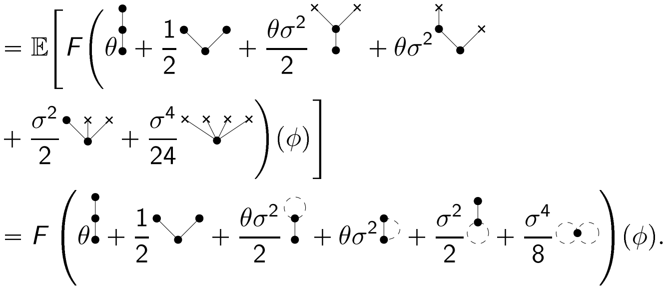
Explicit formula for $\mathcal{A}_1$

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

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

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 $\int_E \phi'(\widetilde{f}) \rho_\infty dy$.

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

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

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

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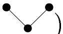
$$\int_{\mathbb{R}^d} F($$  $$)(\phi)\rho_\infty dy = \sum_{i,j} \int_{\mathbb{R}^d} \frac{\partial^3 \phi}{\partial x_i \partial x_j \partial x_j} f_i \rho_\infty dy$$

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

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

 $\sim -$  $- \frac{2}{\sigma^2}$  .

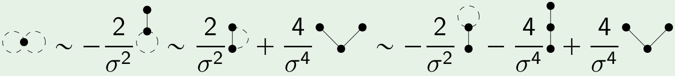
Main tool 2: integration by parts

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

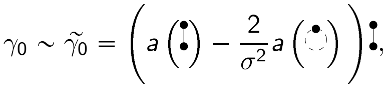
Take a method of order p. If $\mathcal{A}_p = F(\gamma_p)$ for a certain linear combination of exotic aromatic forests γ_p, if $\gamma_p \sim \tilde{\gamma}_p$ and $F(\tilde{\gamma}_p) = 0$, then the method is at least of order $p+1$ for the invariant measure.

Order conditions using exotic aromatic forests

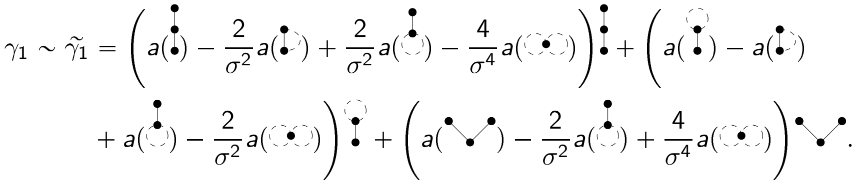
In particular, if

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

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



and



Contents

1 Modelling particles with the overdamped Langevin equation

2 Numerical schemes for the overdamped Langevin equation

3 Exotic aromatic trees for the study of invariant measure order conditions

4 Application to the construction of high order integrators

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:

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

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

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

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

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		$\phi' f_1$	$\sum b_i = 1$
		$\phi' f_2$	$\sum \widehat{b}_i = 1$
2		$\phi' f_1' f_1$	$\sum b_i c_i - 2\sum b_i d_i - 2\sum \overline{b_i} + 2\overline{d_0}^2 = -\frac{1}{2}$
		$\phi' f_1' f_2$	$\sum b_i \hat{c}_i - 2\sum b_i d_i - \sum \overline{b_i} - \sum \overline{\widehat{b}_i} + 2\overline{d_0}^2 = -\frac{1}{2}$
	...	...	...

Partitioned methods

Examples (Two methods of order 2)

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

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:

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

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.