

Exotic aromatic B-series for the study of long time integrators of a class of ergodic SDEs.

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- 1 Numerical schemes for the overdamped Langevin equation
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Take N particles moving in a fluid (with $N \simeq 10^{24}$). Let $q(t)$ be their positions and $p(t)$ their velocities, then

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

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

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

where $f = -\nabla V$.

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Classical tools for the weak convergence

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

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

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

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

Classical tools for the weak convergence

We develop the exact solution in Taylor series:

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

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

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

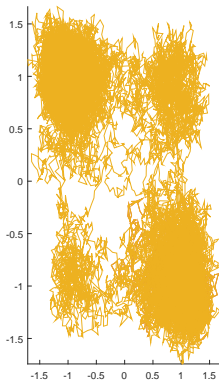
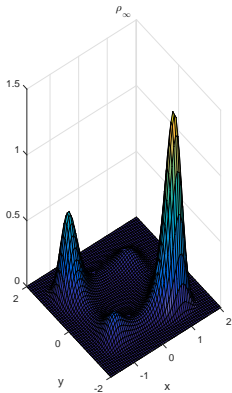
⇒ Tree formalism of B-series for deterministic problems: Butcher (1972) and Hairer, Wanner (1974),...

⇒ Tree formalism for strong and weak errors on finite time: Burrage 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

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



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 $\rho_\infty(x) = Z e^{-V(x)}$.

Order of convergence for the invariant measure

Definition (Convergence for the invariant measure)

We call error of the invariant measure the quantity

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

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

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 ,*

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

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

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

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 .

- $F(\bullet)(\phi) = \phi$

- $F(\begin{array}{c} \bullet \\ | \\ \bullet \end{array})(\phi) = \phi' f$

- $F(\begin{array}{c} \bullet \\ / \quad \backslash \\ \bullet \quad \bullet \end{array})(\phi) = \phi''(f, f' f)$

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

$$F(\begin{array}{c} \bullet \\ \circlearrowleft \\ \bullet \end{array})(\phi) = \text{div}(f) \times \left(\sum \partial_i f_j \partial_j f_i \right) \times \phi' f$$

Grafted aromatic forests

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

$$F(\begin{array}{c} \times \\ | \quad \backslash \\ \bullet \quad \bullet \\ | \quad / \\ \bullet \end{array})(\phi) = \phi''(f' \xi, \xi) \quad \text{and} \quad F(\begin{array}{c} \times \quad \times \\ \backslash \quad / \\ \bullet \end{array})(\phi) = \phi' f''(\xi, \xi).$$

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

$$\begin{aligned} \mathcal{A}_1\phi &= \mathbb{E}\left[\theta\phi'f'f + \frac{1}{2}\phi''(f, f) + \frac{\theta\sigma^2}{2}\phi'f''(\xi, \xi) + \theta\sigma^2\phi''(f'\xi, \xi) \right. \\ &\quad \left. + \frac{\sigma^2}{2}\phi^{(3)}(f, \xi, \xi) + \frac{\sigma^4}{24}\phi^{(4)}(\xi, \xi, \xi, \xi)\right] \\ &= \mathbb{E}\left[F\left(\theta \begin{array}{c} \bullet \\ | \\ \bullet \end{array} + \frac{1}{2} \begin{array}{c} \bullet \\ \diagdown \quad \diagup \\ \bullet \end{array} + \frac{\theta\sigma^2}{2} \begin{array}{c} \times \\ \diagdown \quad \diagup \\ \bullet \end{array} + \theta\sigma^2 \begin{array}{c} \times \\ | \\ \bullet \end{array} \right. \\ &\quad \left. + \frac{\sigma^2}{2} \begin{array}{c} \bullet \\ \diagdown \quad \diagup \\ \times \end{array} + \frac{\sigma^4}{24} \begin{array}{c} \times \\ \diagdown \quad \diagup \\ \times \end{array} \right) (\phi)\right]. \end{aligned}$$

New exotic aromatic forests : adding lianas

We add **lianas** to the aromatic forests.

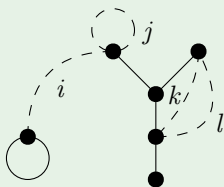
Examples

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

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

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

If γ is the following forest



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

Remark: our forests do not depend on the dimension.

Computing the expectation using lianas

$$\begin{aligned}\mathbb{E} \left[F \left(\begin{array}{c} \times \quad \times \\ \diagdown \quad / \\ \bullet \\ | \\ \bullet \end{array} \right) (\phi) \right] &= \mathbb{E}[\phi' f''(\xi, \xi)] = \sum_{i,j,k} \partial_i \phi \cdot \partial_{jk} f_i \cdot \mathbb{E}[\xi_j \xi_k] \\ &= \sum_{i,j} \partial_i \phi \cdot \partial_{jj} f_i = \phi' \Delta f \\ &= F \left(\begin{array}{c} (\times) \\ \diagdown \quad / \\ \bullet \\ | \\ \bullet \end{array} \right) (\phi)\end{aligned}$$

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.

$$\begin{aligned}\mathbb{E}\left[F\left(\begin{array}{c} \times \quad \times \quad \times \quad \times \\ \diagdown \quad \diagup \\ \bullet \\ \diagup \quad \diagdown \\ \times \quad \times \quad \times \quad \times \end{array}\right)(\phi)\right] &= \mathbb{E}[\phi^{(4)}(\xi, \xi, \xi, \xi)] = \sum_{ijkl} \partial_{ijkl} \phi \mathbb{E}[\xi_i \xi_j \xi_k \xi_l] \\ &= \sum_i \partial_{iiii} \phi \mathbb{E}[\xi_i^4] + 3 \sum_{\substack{i,j \\ i \neq j}} \partial_{iijj} \phi \mathbb{E}[\xi_i^2] \mathbb{E}[\xi_j^2] \\ &= 3 \sum_{i,j} \partial_{iijj} \phi = 3F\left(\begin{array}{c} \times \quad \times \\ \diagdown \quad \diagup \\ \bullet \\ \diagup \quad \diagdown \\ \times \quad \times \end{array}\right)(\phi).\end{aligned}$$

Explicit formula for \mathcal{A}_1

The operator \mathcal{A}_1 given by

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

is now convenient to write with exotic aromatic trees.

$$\begin{aligned} \mathcal{A}_1\phi &= \mathbb{E}\left[\theta\phi'f'f + \frac{1}{2}\phi''(f, f) + \frac{\theta\sigma^2}{2}\phi'f''(\xi, \xi) + \theta\sigma^2\phi''(f'\xi, \xi) \right. \\ &\quad \left. + \frac{\sigma^2}{2}\phi^{(3)}(f, \xi, \xi) + \frac{\sigma^4}{24}\phi^{(4)}(\xi, \xi, \xi, \xi)\right] \\ &= \mathbb{E}\left[F\left(\theta \begin{array}{c} \bullet \\ | \\ \bullet \end{array} + \frac{1}{2} \begin{array}{c} \bullet \quad \bullet \\ \diagdown \quad \diagup \\ \bullet \end{array} + \frac{\theta\sigma^2}{2} \begin{array}{c} \times \quad \times \\ \diagdown \quad \diagup \\ \bullet \end{array} + \theta\sigma^2 \begin{array}{c} \times \\ | \\ \bullet \end{array} \begin{array}{c} \times \\ \diagdown \\ \bullet \end{array} \begin{array}{c} \times \\ \diagup \\ \bullet \end{array} \right. \\ &\quad \left. + \frac{\sigma^2}{2} \begin{array}{c} \times \quad \times \\ \diagdown \quad \diagup \\ \bullet \end{array} + \frac{\sigma^4}{24} \begin{array}{c} \times \quad \times \quad \times \quad \times \\ \diagdown \quad \diagup \\ \bullet \end{array}\right)(\phi) \\ &= F\left(\theta \begin{array}{c} \bullet \\ | \\ \bullet \end{array} + \frac{1}{2} \begin{array}{c} \bullet \quad \bullet \\ \diagdown \quad \diagup \\ \bullet \end{array} + \frac{\theta\sigma^2}{2} \begin{array}{c} \circ \\ | \\ \bullet \end{array} + \theta\sigma^2 \begin{array}{c} \circ \\ | \\ \bullet \end{array} \begin{array}{c} \circ \\ \diagdown \\ \bullet \end{array} + \frac{\sigma^2}{2} \begin{array}{c} \circ \\ | \\ \bullet \end{array} + \frac{\sigma^4}{8} \begin{array}{c} \circ \\ | \\ \bullet \end{array} \begin{array}{c} \circ \\ \diagdown \\ \bullet \end{array} \begin{array}{c} \circ \\ \diagup \\ \bullet \end{array}\right)(\phi). \end{aligned}$$

Integrating by parts exotic aromatic forests

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

$$\begin{aligned} \int_{\mathbb{R}^d} F(\overset{\bullet}{\cdot}) (\phi) \rho_\infty dy &= \sum_{i,j} \int_{\mathbb{R}^d} \frac{\partial^3 \phi}{\partial x_i \partial x_j \partial x_j} f_i \rho_\infty dy \\ &= - \sum_{i,j} \left[\int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} \frac{\partial f_i}{\partial x_j} \rho_\infty dy + \int_{\mathbb{R}^d} \frac{\partial \phi}{\partial x_i \partial x_j} f_i \frac{\partial \rho_\infty}{\partial x_j} dy. \right] \end{aligned}$$

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

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

We write

$$\overset{\bullet}{\curvearrowright} \sim - \overset{\bullet}{\curvearrowleft} - \frac{2}{\sigma^2} \curvearrowright.$$

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

$$\text{Forest with liana} \sim -\frac{2}{\sigma^2} \text{Forest with liana at root} \sim \frac{2}{\sigma^2} \text{Forest with liana at node} + \frac{4}{\sigma^4} \text{Forest with liana at new node} \sim -\frac{2}{\sigma^2} \text{Forest with liana unpluged} - \frac{4}{\sigma^4} \text{Forest with liana at node} + \frac{4}{\sigma^4} \text{Forest with liana at new node}$$

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

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

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

$$\gamma_0 \sim \tilde{\gamma}_0 = \left(a \left(\begin{array}{c} \bullet \\ | \\ \bullet \end{array} \right) - \frac{2}{\sigma^2} a \left(\begin{array}{c} \bullet \\ | \\ \circ \end{array} \right) \right) \begin{array}{c} \bullet \\ | \\ \bullet \end{array},$$

and

$$\begin{aligned} \gamma_1 \sim \tilde{\gamma}_1 = & \left(a \left(\begin{array}{c} \bullet \\ | \\ \bullet \end{array} \right) - \frac{2}{\sigma^2} a \left(\begin{array}{c} \bullet \\ | \\ \bullet \end{array} \right) + \frac{2}{\sigma^2} a \left(\begin{array}{c} \bullet \\ | \\ \circ \end{array} \right) - \frac{4}{\sigma^4} a \left(\begin{array}{c} \bullet \\ | \\ \circ \end{array} \right) \right) \begin{array}{c} \bullet \\ | \\ \bullet \end{array} + \left(a \left(\begin{array}{c} \bullet \\ | \\ \bullet \end{array} \right) - a \left(\begin{array}{c} \bullet \\ | \\ \bullet \end{array} \right) \right. \\ & \left. + a \left(\begin{array}{c} \bullet \\ | \\ \bullet \end{array} \right) - \frac{2}{\sigma^2} a \left(\begin{array}{c} \bullet \\ | \\ \circ \end{array} \right) \right) \begin{array}{c} \bullet \\ | \\ \circ \end{array} + \left(a \left(\begin{array}{c} \bullet \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \end{array} \right) - \frac{2}{\sigma^2} a \left(\begin{array}{c} \bullet \\ | \\ \bullet \end{array} \right) + \frac{4}{\sigma^4} a \left(\begin{array}{c} \bullet \\ | \\ \circ \end{array} \right) \right) \begin{array}{c} \bullet \\ \diagdown \quad \diagup \\ \bullet \quad \bullet \end{array}. \end{aligned}$$

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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:

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

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

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),

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

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

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

Theorem (Vilmart (2015))

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

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

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

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)





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

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		$\phi' f_1' f_1$	$\sum b_i c_i - 2 \sum b_i d_i - 2 \sum \bar{b}_i + 2 \bar{d}_0^2 = -\frac{1}{2}$
		$\phi' f_1' f_2$	$\sum b_i \hat{c}_i - 2 \sum b_i d_i - \sum \bar{b}_i - \sum \hat{\bar{b}}_i + 2 \bar{d}_0^2 = -\frac{1}{2}$

Partitioned methods

Examples (Two methods of order 2)

$$\begin{aligned}X_{n+1} &= X_n + \frac{h}{2}f_1(X_{n+1} + \frac{1}{2}\sigma\sqrt{h}\xi_n) + \frac{h}{2}f_1(X_{n+1} + \frac{3}{2}\sigma\sqrt{h}\xi_n) \\ &\quad + hf_2(X_n + \frac{1}{2}\sigma\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \\ \overline{X}_n &= X_n + \frac{1}{2}\sigma\sqrt{h}\xi_n.\end{aligned}$$

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:

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





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

$$\begin{aligned}X_{n+1} &= X_n + hf_1(X_{n+1} + \frac{1}{2}\sigma\sqrt{h}\chi_n) + hf_2(X_n + \frac{1}{2}\sigma\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \\ \overline{X}_n &= X_n + \frac{1}{2}\sigma\sqrt{h}\xi_n.\end{aligned}$$

Non-reversible perturbation

Idea: If $dX = f_1(X)dt + \sigma dW$ has the invariant measure ρ_∞ , and if $f = f_1 + f_2$ where $\text{div}(f_2\rho_\infty) = 0$, then $dX = f(X)dt + \sigma dW$ has the invariant measure ρ_∞ . Adding a non-reversible perturbation f_2 can improve the rate of convergence to equilibrium (Lelièvre, Nier and Pavliotis (2013)), and can also reduce the variance (Duncan, Lelièvre and Pavliotis (2016)).

Theorem

Order	Tree τ	Order condition
1		$\sum b_i = 1$
2		$\sum b_i c_i - 2 \sum b_i d_i - 2 \sum \bar{b}_i + 2\bar{d}_0^2 = -\frac{1}{2}$
		$\sum b_i \hat{c}_i + \sum \bar{b}_i - \sum \hat{\bar{b}}_i = 0$
		$\sum \hat{b}_i c_i - 2 \sum \hat{b}_i d_i + \sum \hat{b}_i - \sum \bar{b}_i - \sum \hat{\bar{b}}_i + 2\bar{d}_0^2 = 0$

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.