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

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Abstract

We introduce a new algebraic framework based on a modification of aromatic Butcher-series for the systematic study of the accuracy of numerical integrators for a class of ergodic stochastic differential equations (SDEs) with additive noise. The proposed analysis includes the case of Runge-Kutta type schemes possibly with postprocessed integrators. Also the introduced exotic aromatic B-series satisfy an isometric equivariance property.

1. Long time integrators for overdamped Langevin

The *overdamped Langevin equation* is obtained from molecular dynamics, where $\sigma > 0$, $f = -\nabla V$ is a gradient and $dW(t)/dt$ is a d-dimensional white noise:

$$dX(t) = f(X(t))dt + \sigma dW(t). \qquad (1.1)$$

This equation stands in $\mathbb{R}^d$, where d is proportional to the number of particles.

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

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

With backward Kolmogorov equation, we get $\mathbb{E}[\phi(X(h))|X(0) = x] = \phi(x) + h\mathscr{L}\phi(x) + \frac{h^2}{2}\mathscr{L}^2\phi(x) + \dots$ where $\mathscr{L}\phi = \phi'(f) + \frac{\sigma^2}{2}\Delta\phi$ (see Milstein, Tretyakov, 2004).
We compare with the Talay-Tubaro development $\mathbb{E}[\phi(X_1)|X_0 = x] = \phi(x) + h\mathcal{A}_0\phi(x) + h^2\mathcal{A}_1\phi(x) + \dots$
Then the scheme has weak order p if $\forall j \leq p$, $\mathscr{L}^j = j!\mathcal{A}_{j-1}$.

► Tree formalism 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 property: there exists a probability density ρ_∞ such that $\lim_{T\to+\infty} \frac{1}{T}\int_0^T \phi(X(s))ds = \int_{\mathbb{R}^d} \phi(y)\rho_\infty(y)dy$ almost surely.
If $f = -\nabla V$, then $\rho_\infty(x) = Ze^{-\frac{2V(x)}{\sigma^2}}$.
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, $e(\phi, h) \leq C(x, \phi)h^p$.

Theorem 1.1 [1] (related work: Debussche, Faou, 2012; Kopec, 2013). *Under technical assumptions, if* $\mathcal{A}_j^*\rho_\infty = 0, j = 1, \dots p-1$, *i.e. for all test functions* ϕ,

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

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

2. Exotic aromatic B-series for the systematic study of a numerical method order

Trees have proven to be useful for the study and the construction of high order integrators: Butcher, 1972 and Hairer, Wanner, 1974 (See also Hairer, Wanner, Lubich, 2006 and Chartier, Hairer, Vilmart, 2010).
We rewrite our differentials with trees. We denote $F(\gamma)(\phi)$ the elementary differential of a tree γ.

$$F(\bullet)(\phi) = \phi, \quad F(\cdot)(\phi) = \phi' f, \quad F(\cdot)(\phi) = \phi''(f, f'f)$$

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

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

Grafted aromatic forests: $\xi \sim \mathcal{N}(0, I_d)$ is represented by crosses (in the spirit of P-series)

$$F(\cdot)(\phi) = \phi''(f'\xi, \xi) \quad \text{and} \quad F(\cdot)(\phi) = \phi' f''(\xi, \xi).$$

We also introduce lianas in our forests and call these exotic aromatic forests.

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

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

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

Example. *The* θ*-method for solving numerically* (1.1):

$$X_{n+1} = X_n + h(1-\theta)f(X_n) + h\theta f(X_{n+1}) + \sigma\sqrt{h}\xi_n, \quad (2.1)$$

where $\xi_n \sim \mathcal{N}(0, I_d)$ *are independent standard Gaussian random variables.* $\mathcal{A}_1$ *is given by*

$$\begin{aligned}\mathcal{A}_1\phi &= \mathbb{E}[\theta\phi' f' f + \frac{1}{2}\phi''(f, f) + \frac{\theta\sigma^2}{2}\phi' f''(\xi, \xi) + \theta\sigma^2\phi''(f'\xi, \xi) \\ &+ \frac{\sigma^2}{2}\phi^{(3)}(f, \xi, \xi) + \frac{\sigma^4}{24}\phi^{(4)}(\xi, \xi, \xi, \xi)] \\ &= \mathbb{E}\Big[F\Big(\theta\cdot + \frac{1}{2}\cdot + \frac{\theta\sigma^2}{2}\cdot + \theta\sigma^2\cdot \qquad (2.2) \\ &+ \frac{\sigma^2}{2}\cdot + \frac{\sigma^4}{24}\cdot\Big)(\phi)\Big]\end{aligned}$$

It is shown in [5] that affine equivariant maps are exactly aromatic B-series.

Theorem 2.1
Exotic aromatic B-series are isometric equivariant.

3. Analysis of invariant measure order conditions using exotic aromatic forests

The formalism previously defined greatly simplifies the computation of $\mathcal{A}_j^*\rho_\infty$. Firstly it gives the expectation of grafted aromatic forests.

Theorem 3.1 (Computing the expectation of grafted B-series). *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 *pairwisely with lianas.*

Example. *For the* θ*-method* (2.1) *(compare with* (2.2)*),*

$$\mathcal{A}_1 = F\Big(\theta\cdot + \frac{1}{2}\cdot + \frac{\theta\sigma^2}{2}\cdot + \theta\sigma^2\cdot + \frac{\sigma^2}{2}\cdot + \frac{\sigma^4}{8}\cdot\Big).$$

The integration by parts is also improved:

Theorem 3.2 (Integrating by parts exotic aromatic forests). *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*

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

If we can go from γ_1 *to* γ_2 *with this process, we write* $\gamma_1 \sim \gamma_2$.

Example. *The detailed calculus:*

$$\begin{aligned}\int_{\mathbb{R}^d} F(\cdot)(\phi)\rho_\infty dy &= \sum_{i,j}\int_{\mathbb{R}^d} \frac{\partial^3\phi}{\partial x_i\partial x_j\partial x_j} f_i\rho_\infty dy \\ &= -\sum_{i,j}\Big[\int_{\mathbb{R}^d} \frac{\partial\phi}{\partial x_i\partial x_j}\frac{\partial f_i}{\partial x_j}\rho_\infty dy + \int_{\mathbb{R}^d} \frac{\partial\phi}{\partial x_i\partial x_j} f_i\frac{\partial\rho_\infty}{\partial x_j}dy\Big] \\ &= -\int_{\mathbb{R}^d} F(\cdot)(\phi)\rho_\infty dy - \frac{2}{\sigma^2}\int_{\mathbb{R}^d} F(\cdot)(\phi)\rho_\infty dy.\end{aligned}$$

Another example:

$$\cdot \sim -\frac{2}{\sigma^2}\cdot \sim \frac{2}{\sigma^2}\cdot + \frac{4}{\sigma^4}\cdot \sim -\frac{2}{\sigma^2}\cdot - \frac{4}{\sigma^4}\cdot + \frac{4}{\sigma^4}\cdot.$$

Theorem 3.3
(Order conditions using exotic aromatic forests)
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 under technical assumptions, the method is at least of order $p+1$ for the invariant measure.

Example.

$$\int_{\mathbb{R}^d} \mathcal{A}_1\phi\rho_\infty dy = \int_{\mathbb{R}^d} \Big(\frac{1}{2} - \theta\Big)\phi'\Big(f'f + \frac{\sigma^2}{2}\Delta f\Big)\rho_\infty dy.$$

⇒ *If* $\theta = \frac{1}{2}$, $\mathcal{A}_1^*\rho_\infty = 0$ *and we recover that the* θ*-method* (2.1) *has order 2 for the invariant measure.*
⇒ *The* θ*-method* (2.1) *(with step* h*) applied to*

$$dX = \Big(f - h\Big(\frac{1}{2} - \theta\Big)\Big(f'f + \frac{\sigma^2}{2}\Delta f\Big)\Big)(X)dt + \sigma dW$$

is of order 2 for the invariant measure of (1.1).

4. Application to the construction of high order integrators for the invariant measure sampling

The previously introduced formalism naturally apply to the study of order conditions for numerical integrators.

• Order conditions for the invariant measure

Theorem 4.1 (Conditions for order p for the invariant measure). *Detailed conditions for order 2, 3 for stochastic Runge-Kutta methods:*

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

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		$\phi' f' f' f$	$\sum b_i a_{ij} c_j - 2\sum b_i a_{ij} d_j + \sum b_i c_i - (\sum b_i d_i)^2 = 0$
	...	...	...

• Order conditions for postprocessed integrators

Theorem 4.2 (related work: [6]). *Under technical assumptions, 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 4.3
(Conditions for order p using postprocessors)
Conditions for order 2, 3 for stochastic Runge-Kutta methods with Runge-Kutta postprocessor:

$$\begin{aligned}\overline{Y_i^n} &= X_n + h\sum_{j=1}^{s} \overline{a_{ij}} f(\overline{Y_j^n}) + \overline{d_i}\sigma\sqrt{h}\xi_n, \qquad i = 1, \dots, s, \\ \overline{X_n} &= X_n + h\sum_{i=1}^{s} \overline{b_i} f(\overline{Y_i^n}) + \overline{d_0}\sigma\sqrt{h}\xi_n.\end{aligned}$$

Order	Tree τ	Order condition
2		$\sum b_i c_i - 2\sum b_i d_i - 2\sum \overline{b_i} + 2\overline{d_0}^2 = -\frac{1}{2}$
		$\sum b_i d_i^2 - 2\sum b_i d_i - \sum \overline{b_i} + \overline{d_0}^2 = -\frac{1}{2}$
3	...	...

• Order conditions for partitioned methods

We study the equation $dX = (f_1 + f_2)dt + \sigma dW$ where f_1 and f_2 are gradients. We introduce appropriate Runge-Kutta integrators and give a systematic method to study their order.

Example. *Under technical assumptions, the following IMEX (implicit-explicit) method with postprocessor* $\overline{X_n}$ *has order 2 for the invariant measure (where* χ_n *are independent standard Gaussian variables independent of* ξ_n*):*

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

• High order integrators with non-reversible perturbation

An interesting modification of (1.1) is to introduce a non gradient perturbation f_2 that preserves the invariant measure. It permits for some classes of problems to improve the rate of convergence to equilibrium, and it can also reduce the variance (see [3, 4]). We give order conditions to obtain high order consistent methods for this particular type of problems.

Example. *Under technical assumptions, the following consistent postprocessed scheme* $\overline{X_n}$ *has order 2 for the invariant measure:*

$$\begin{aligned}X_{n+1} &= X_n + hf_1(X_n + \tfrac{\sigma}{2}\sqrt{h}\xi_n) + \tfrac{5}{4}hf_2(X_n + \tfrac{\sigma}{2}\sqrt{h}\xi_n) \\ &-\tfrac{1}{4}hf_2(X_n - 2hf_2(X_n + \tfrac{\sigma}{2}\sqrt{h}\xi_n) - \tfrac{\sigma}{2}\sqrt{h}\xi_n) + \sigma\sqrt{h}\xi_n, \\ \overline{X_n} &= X_n + \tfrac{\sigma}{2}\sqrt{h}\xi_n.\end{aligned}$$

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