Exotic B-series and S-series: algebraic structures and order conditions for invariant measure sampling

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Abstract

B-series and generalizations are a powerful tool for the analysis of numerical integrators. An extension named exotic S-series permits us to study the order conditions for sampling the invariant measure of ergodic SDEs. We study the natural composition laws on exotic S-series and apply this algebraic framework to the derivation of order conditions for a class of stochastic Runge-Kutta methods.

1. Setting: invariant measure sampling with Runge-Kutta methods

We consider the overdamped Langevin equation

$$dX(t) = f(X(t))dt + \sqrt{2}dW(t), \qquad (1.1)$$

where $X(t) \in \mathbb{R}^d$ is a stochastic process with d being arbitrarily large and $f = -\nabla V$ being a gradient of a smooth potential V. Langevin dynamics are widely used in molecular dynamics and are ergodic under appropriate assumptions.

1.1 Approximation of invariant measure

We say that a problem is *ergodic* if there exists a unique invariant measure μ satisfying for all deterministic initial conditions X_0 and all smooth test functions ϕ,

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \phi(X(s))ds = \int_{\mathbb{R}^d} \phi(x)d\mu(x), \quad \text{almost surely.}$$

We are interested in studying the numerical integrators that approximate the invariant measure of the overdamped Langevin equation. The accuracy of the approximation is characterized by the order of the integrator with respect to the invariant measure. For example, order p w.r.t. invariant measure μ is

$$\left|\lim_{N\to\infty} \frac{1}{N+1}\sum_{n=0}^{N} \phi(X_n) - \int_{\mathbb{R}^d} \phi(x)d\mu(x)\right| \le Ch^p,$$

where C is independent of h assumed small enough.

1.2 Stochastic Runge-Kutta (SRK) methods

Let $a_{ij}, b_i, d_i^{(k)}$ be the coefficients defining the stochastic Runge-Kutta scheme, and $\xi_n^{(k)} \sim \mathcal{N}(0, I_d)$ be independent Gaussian random vectors. Then, the stochastic Runge-Kutta scheme has the form:

$$Y_i = X_n + h\sum_{j=1}^{s} a_{ij} f(Y_j) + \sum_{k=1}^{l} d_i^{(k)}\sqrt{h}\sqrt{2}\xi_n^{(k)}, \quad i = 1,\dots,s,$$

$$X_{n+1} = X_n + h\sum_{i=1}^{s} b_i f(Y_i) + \sqrt{h}\sqrt{2}\xi_n^{(1)}.$$

We shall assume for simplicity that $l = 1$.

1.3 Order conditions w.r.t. invariant measure

Given an SRK method $X_1 = \Psi(X_0)$, we have

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

where $\mathcal{A}_i$, $i = 1, 2, \dots$, are linear differential operators.

Theorem 1. [4] (related work in $\mathbb{T}^d$: [2])

Under technical assumptions, if for every test function ϕ,

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

then the scheme has order p for the invariant measure.

Remark. The scheme has weak order q if $\mathcal{A}_j = \frac{\mathcal{L}^{(j)}}{j!}$ where

$$\mathcal{L}\phi = f\cdot\nabla\phi + \Delta\phi, \quad \text{with } \Delta\phi = \sum_{i=1}^{d}\frac{\partial^2\phi}{\partial x_i^2}.$$

Moreover, we have $p \ge q$.

2. B-series and S-series framework: new normalization and the extension of Connes-Kreimer coproduct on trees

We generalize the B-series framework [3] and obtain *grafted B-series* by Taylor expanding the SRK methods.

$$X_1 = B(a, X_0) = X_0 + \sum_{\tau\in T_g} h^{|\tau|}\frac{a(\tau)}{\sigma(\tau)}F(\tau)(X_0)$$

$$= X_0 + F\Big(\sqrt{h}\times + h\sum_{i=0}^{s} b_i\bullet + h\sqrt{h}\sum_{i=0}^{s} b_i d_i + \cdots\Big)(X_0)$$

with T_g being the set of grafted trees, $|\tau|$ the size of τ, $\sigma(\tau)$ the symmetry coefficient of τ, and $a : T_g \to \mathbb{R}$ is an appropriately defined functional. Some values are listed in the following Table 1.

tree τ	size $\lvert\tau\rvert$	symmetry $\sigma(\tau)$	functional $a(\tau)$	elem. differential $F(\tau)$
$\times$	0.5	1	1	$\sqrt{2}\xi$
$\bullet$	1	1	$\sum_{i=1}^s b_i$	f
	1.5	1	$\sum_{i=1}^s b_i d_i$	$\sqrt{2}f'\xi$
	2	1	$\sum_{i,j=1}^s b_i a_{i,j}$	$f'f$
	2	2	$\sum_{i=1}^s b_i d_i^2$	$2f''(\xi,\xi)$
	2.5	1	$\sum_{i,j=1}^s b_i a_{ij} d_i$	$\sqrt{2}f''(f,\xi)$
	2.5	1	$\sum_{i,j=1}^s b_i a_{ij} d_j$	$\sqrt{2}f'f'\xi$
	2.5	6	$\sum_{i=1}^s b_i d_i^3$	$2\sqrt{2}f'''(\xi,\xi,\xi)$

Table 1: Grafted trees with correspondent constants, functionals, and elementary differentials

2.1 Exotic forests and exotic S-series

We are interested in the order of SRK methods w.r.t. invariant measure, therefore, we take the expectation of Taylor expansion of $\phi(X_1)$ to obtain an exotic S-series

$$\mathbb{E}[\phi(X_1)] = ES(a, X_0)[\phi]$$

$$= \phi(X_0) + \sum_{\pi\in EF} h^{|\pi|}\frac{a(\pi)}{\sigma(\pi)}F(\pi)[\phi](X_0)$$

$$= \phi(X_0) + F\Big(h\sum_{i=0}^{s} b_i\bullet + h^2\sum_{i=1}^{s} b_i d_i^2 + \cdots\Big)[\phi](X_0),$$

where EF is the set of exotic forests and $F(\pi)$ is a differential operator, for example,

$$F(\ )[\phi] = 4\sum_{i_1,i_2=1}^{d}\phi''\big(\partial_{i_1}f, (\partial_{i_1}f)'(\partial_{i_2 i_2}f)\big).$$

Some values of $a(\pi)$, $|\pi|$, and $\sigma(\pi)$ are listed in the Table 2.

tree τ	size $\lvert\tau\rvert$	symmetry $\sigma(\tau)$	functional $a(\tau)$	elem. differential $F(\tau)$
$\bullet$	1	1	$\sum_{i=1}^s b_i$	f
	2	1	$\sum_{i,j=1}^s b_i a_{i,j}$	$f'f$
	2	2	$\sum_{i=1}^s b_i d_i^2$	$2\sum_{i=1}^d \partial_{ii}f$
	3	2	$\sum_{i,j,k=1}^s b_i a_{ij} a_{ik}$	$f''(f,f)$
	3	2	$\sum_{i,j=1}^s b_i a_{ij} d_i^2$	$2\sum_{i=1}^d(\partial_{ii}f)'f$
	3	1	$\sum_{i,j=1}^s b_i a_{ij} d_i d_j$	$2\sum_{i=1}^d(\partial_i f)'(\partial_i f)$
	3	2	$\sum_{i,j=1}^s b_i a_{ij} d_j^2$	$2\sum_{i=1}^d f'(\partial_{ii}f)$

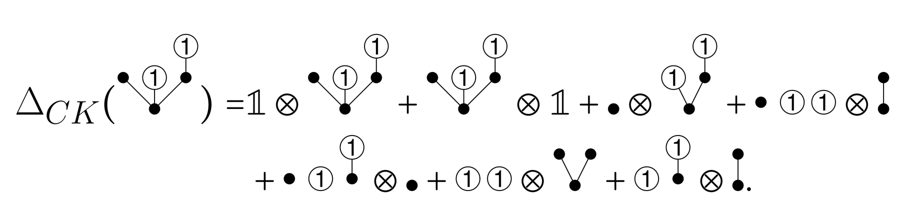
Table 2: Exotic trees with correspondent constants, functionals, and elementary differentials

2.2 Composition of exotic S-series

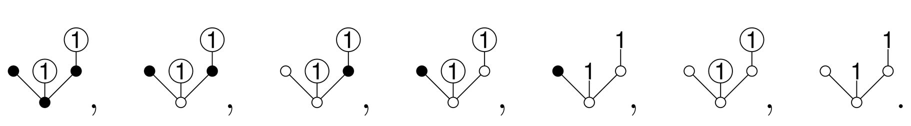
Define Connes-Kreimer coproduct $\Delta_{CK} : \mathcal{EF} \to \mathcal{EF}\otimes\mathcal{EF}$ as

$$\Delta_{CK}(\pi) := \sum_{\pi_s\in\mathcal{S}(\pi)} \pi\setminus\pi_s \otimes \pi_s,$$

where $\mathcal{S}(\pi)$ is the set of all ordered rootes subforests of π. For example,



We list the ordered rooted subforests below.



The ordered rooted subforests are denoted by white vertices and borderless number vertices. We prove the composition law for exotic S-series using new normalization σ.

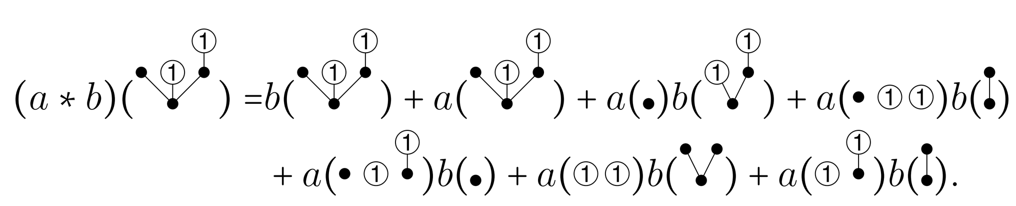
Theorem 2. [1] Composition law

Let $a, b : EF \to \mathbb{R}$, then

$$ES(a)[ES(b)] = ES(a * b),$$

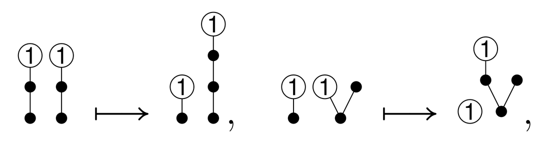
where $(a * b)(\pi) = ((a\otimes b)\circ\Delta_{CK})(\pi)$ for $\pi \in EF$.

For example,

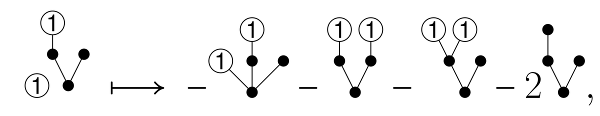


3. Generating order conditions w.r.t. invariant measure: a new systematic algorithm

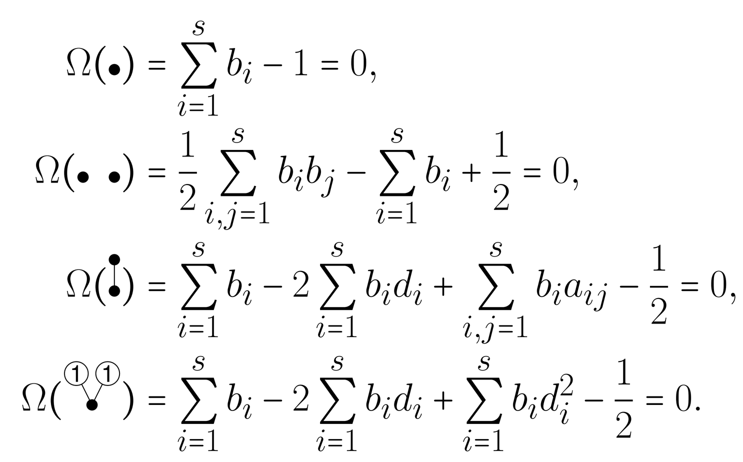
We use Theorem 1 and B-series framework to describe a theoretical algorithm (omitted for brevity) that performs transformations on exotic forests. The possible transformations include: the edge-liana inversion, for example,



which uses the fact that $f = -\nabla V$, and integration by parts,



which uses the integral formula from Theorem 1. We apply the algorithm to the exotic S-series obtained from SRK methods to generate order conditions w.r.t. invariant measure. Every order condition corresponds to an exotic forest $\pi \in EF$ and the condition is satisfied when $\Omega(\pi) = 0$. Some of the generated conditions are:



3.1 Multiplicative property of order conditions

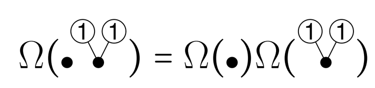
Let $\sqcup_\sigma$ denote a renormalized concatenation product of exotic forests. We note that $\sqcup_\sigma$ is the dual of the deshuffle coproduct. For example,

Theorem 3. [1] Multiplicative property of Ω for SRK

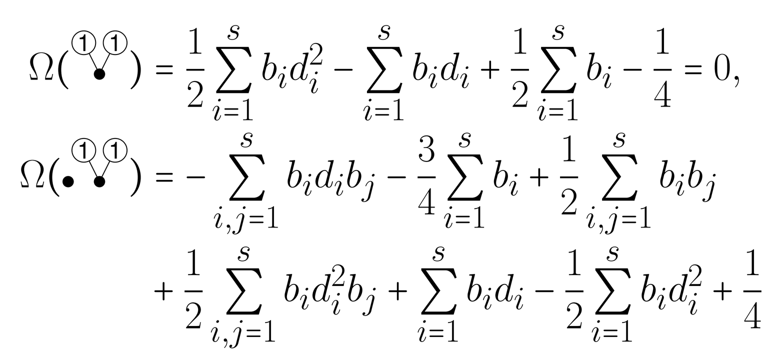
The order condition map Ω satisfies:

$$\Omega(\pi_1\sqcup_\sigma\pi_2) = \Omega(\pi_1)\Omega(\pi_2).$$

For example, we see that $\Omega(\bullet\ \bullet) = \frac{1}{2}\Omega(\bullet)^2$ and



with the corresponding order conditions being



The multiplicative property of the map Ω implies that the order conditions w.r.t. invariant measure corresponding to exotic forests mith more than one tree are satisfied automatically if all lower order conditions are satisfied.

4. Ongoing works

- Analysis of the **substitution law** for exotic aromatic S-series;
- Development of a **symbolic package** for manipulation of forest-like structures. In collaboration with Jean-Luc Falcone from the Comp. Science Dep. of Univ. Geneva.

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