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

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Dominique Manchon, Univ. Clermont-Auvergne
Gilles Vilmart, Univ. Geneva

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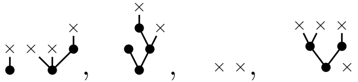
UNIVERSITÉ DE GENÈVE
FACULTY OF SCIENCE
Mathematics Section

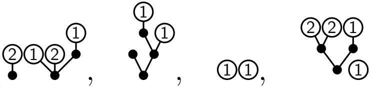
We consider the overdamped Langevin equation:

$$dX(t) = f(X(t))dt + \sqrt{2}dW(t), \quad W(t), X(t) \in \mathbb{R}^d,$$

where $f = -\nabla V$, noise is additive, and $W(t)$ is a std. Wiener process. We use grafted forests:

$$F_g := \{$$

$$, \dots \},$$

and exotic forests, which are grafted forests with paired grafted vertices:

$$EF := \{$$

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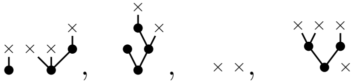
$F_g := \{$  $, \ldots\},$

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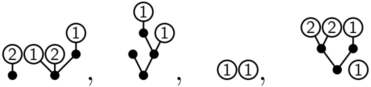
$EF := \{$  $, \ldots\},$

to represent differential operators, for example:

$\mathcal{F}_{hf}($  $) = 2h^2 \sum \xi^i \xi^j f_{ij}^k \partial_k, \quad \mathcal{F}_{hf}($  $) = 2h^2 \sum f_{ii}^k \partial_k.$

We note that $\mathcal{F}_f($  $)$ is a random variable, since $\xi \sim \mathcal{N}(0, I)$.

Related: Laurent and Vilmart [2019].

Preliminaries

$$\text{Deterministic case:} \quad \frac{dy}{dt} = f(y),$$

with $y(0) \in y_0$, $y(t) \in \mathbb{R}^d$, $f : \mathbb{R}^d \to \mathbb{R}^d$ is a smooth vector field.

We can use Runge-Kutta methods:

$$\begin{aligned} Y_i &= y_0 + h \sum_{j=1}^{s} a_{ij} f(Y_j), \\ y_1 &= y_0 + h \sum_{i=1}^{s} b_i f(Y_i), \end{aligned} \qquad \text{with} \qquad \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}.$$

We can Taylor expand $f(Y_i)$ around y_0 to obtain

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i f(y_0) + h^2 \sum_{i=1}^{s} b_i c_i f'(y_0) f(y_0) + \cdots .$$

Consider rooted non-planar trees $T := \{\bullet,$ , , , $\dots\}$.

Let $a : T \to \mathbb{R}$, then a B-series is a formal sum $B(a) : \mathbb{R}^d \to \mathbb{R}^d$:

$B(a) := \mathrm{Id} + a(\bullet) hf + a($$)h^2 f' f +$

$\dfrac{a(\;)}{2}$  $h^3 f''(f, f) + a($$)h^3 f' f' f + \cdots$

where all $f, f'f, f''(f, f), \dots : \mathbb{R}^d \to \mathbb{R}^d$.

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where all $f, f'f, f''(f,f), \cdots : \mathbb{R}^d \to \mathbb{R}^d$.

Exact solution and Runge-Kutta methods are B-series.

$$a(\bullet) = \sum b_i = 1,$$

$a($$) = \sum b_i c_i = \frac{1}{2},$

$a($$) = \sum b_i a_{ij} c_j = \frac{1}{6},$

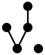
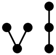
$a($$) = \sum b_i c_i^2 = \frac{1}{3},$

$$a(\tau) = \cdots = \frac{1}{\tau!}.$$

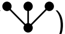
Related: Butcher [1963], Hairer and Wanner [1974], Hairer et al. [1993], Connes and Kreimer [1998], Butcher [2021].

S-series and the symmetry coefficient

B-series are based on trees, while S-series are based on forests:

$F := \{\varnothing,$ $\bullet,$ , , , $\dots\}.$

The symmetry coefficient of trees and forests:

$\sigma($$) = 2, \quad \sigma($$) = 2, \quad \sigma($$) = 3!.$

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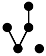
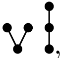
$F := \{\varnothing,$  $,$  $,$  $,$  $, \dots\}.$

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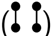
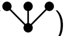
$\sigma($  $) = 2, \quad \sigma($  $) = 2, \quad \sigma($  $) = 3!.$

S-series were introduced to study first integrals. Chartier and Murua [2006]

Given a map $\phi : \mathbb{R}^d \to \mathbb{R}$, S-series are defined as

$$\phi \circ B(a) = S(a)[\phi] = \sum_{\pi \in F} \frac{a(\pi)}{\sigma(\pi)} \mathcal{F}_{hf}(\pi)[\phi].$$

We consider B-series in the stochastic context. We study $\mathbb{E}[\phi(B(a))]$, and, thus, we use and extend the concept of S-series for our needs.

Order conditions for invariant measure sampling

We consider an ergodic integrator $\{X_0, X_1, X_2, \dots\}$ for an ergodic problem:

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

For overdamped Langevin, we have $d\mu(x) = Ze^{-V(x)}dx$.

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Definition (Weak order q and order p for inv. measure)

Given an ergodic integrator $X_n \mapsto X_{n+1}$, we have

$$\text{weak order:} \quad |\mathbb{E}[\phi(X_N)] - \mathbb{E}[\phi(X(T))]| \leq Ch^q,$$

$$\text{inv. measure:} \quad \left|\lim_{N\to\infty} \frac{1}{N+1}\sum_{k=0}^{N} \phi(X_k) - \int_{\mathbb{R}^d} \phi(x)d\mu(x)\right| \leq Ch^p,$$

where C is independent of h assumed small enough. Generally, $p \geq q$.

Order 3 conditions: 15 for weak order **vs** 9 for inv. measure.

Related: Talay and Tubaro [1990], Debussche and Faou [2011], Abdulle et al. [2014], Laurent and Vilmart [2019]

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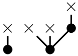
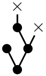
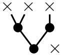
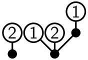
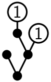
Reference: B. "Exotic B-series and S-series: algebraic structures and order conditions for invariant measure sampling", preprint 2022.

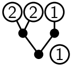
Part 1: Exotic S-series

Overdamped Langevin: $dX(t) = -\nabla V(X(t))dt + \sqrt{2}dW(t)$,

Grafted forests: $F_g := \{$ , , , $\dots\}$,

Exotic forests: $EF := \{$ 

, 

, 

, $\dots\}$.

S-series and exotic S-series

Define S-series over grafted forests and exotic S-series over exotic forests:

$$S(a) := \sum_{\pi \in F_g} \frac{a(\pi)}{\sigma(\pi)} \mathcal{F}_{hf}(\pi), \quad ES(a) = \sum_{\pi \in EF} \frac{a(\pi)}{\sigma(\pi)} \mathcal{F}_{hf}(\pi),$$

with $\sigma(\pi)$ being a symmetry coefficient.
We prove that $ES(a) = \mathbb{E}\left[S(a)\right]$ and describe the composition law.

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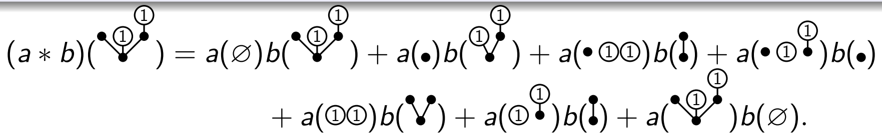
Theorem (Composition law)

Let $a, b : EF \to \mathbb{R}$ and let $\Delta_{CK} : \mathcal{EF} \to \mathcal{EF} \otimes \mathcal{EF}$ denote the Connes-Kreimer coproduct, then

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

where $(a * b)(\pi) = (m_{\mathbb{R}} \circ (a \otimes b) \circ \Delta_{CK})(\pi)$ for all exotic forests $\pi \in EF$.



Idea of the proof of $ES(a * b) = ES(a)[ES(b)]$

The exotic S-series can be written as

$$ES(a) = (\mathcal{F}_{hf} \circ A_\sigma^{-1} \circ \delta^{-1})(a),$$

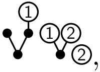
where $\delta^{-1}(a) = \sum_{\pi \in EF} a(\pi)\pi$ and $A_\sigma^{-1}(\pi) = \frac{\pi}{\sigma(\pi)}$.

We define Grossman-Larson product $\diamond$ on exotic forests as

$$\mathcal{F}_{hf}(\pi_1 \diamond \pi_2) = \mathcal{F}_{hf}(\pi_1)[\mathcal{F}_{hf}(\pi_2)]. \tag{1}$$

We analyse how $*$ changes as it passes through ES:

$$* \xrightarrow{\delta^{-1}} \circledast \xrightarrow{\color{red}{A_\sigma^{-1}}} \diamond \xrightarrow{\mathcal{F}_{hf}} [\;]$$

Difficulty: exotic trees can have multiple roots, e.g. , , ...

Part 2: Order conditions for invariant measure sampling

$$\Omega(\bullet) = \Sigma b_i - 1 = 0,$$

$$\Omega(\bullet\ \bullet) = \frac{1}{2}\Sigma b_i b_j + \frac{1}{2} - \Sigma b_i = 0,$$

$$\Omega(\overset{\bullet}{\bullet}) = \Sigma b_i c_i - \frac{1}{2} + \Sigma b_i - 2\Sigma b_i d_i = 0,$$

$$\Omega(\overset{\textcircled{0}\textcircled{0}}{\bullet}) = \frac{1}{2}\Sigma b_i d_i^2 - \frac{1}{4} + \frac{1}{2}\Sigma b_i - \Sigma b_i d_i = 0.$$

Order conditions for invariant measure sampling

We present a theoretical algorithm that generates order conditions for invariant measure for arbitrary high order systematically.

$$\Omega(\pi) = 0 \quad \text{for exotic forests} \quad \pi \in \widetilde{EF} \quad \text{with} \quad |\pi| \leq p.$$

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Let $\sqcup_\sigma$ denote a renormalized concatenation product of exotic forests.

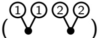
Theorem (Multiplicative property of Ω for stochastic RK)

For stochastic Runge-Kutta methods, the order condition map Ω satisfies:

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

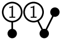
We see that $\Omega($  $) = \frac{1}{2}\Omega($  $)\Omega($  $)$ with  $\sqcup_\sigma$  $= 2$  and

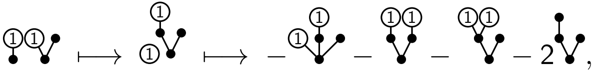
$\Omega($  $) = \frac{1}{2}\Sigma b_i d_i^2 - \Sigma b_i d_i + \frac{1}{2}\Sigma b_i - \frac{1}{4},$

$\Omega($  $) = \frac{1}{8}\Sigma b_i b_j d_i^2 d_j^2 + \frac{1}{4}\Sigma b_i b_j d_i^2 - \frac{1}{2}\Sigma b_i b_j d_i d_j^2 + \frac{1}{2}\Sigma b_i b_j d_i d_j - \frac{1}{2}\Sigma b_i b_j d_i + \frac{1}{8}\Sigma b_i b_j - \frac{1}{8}\Sigma b_i d_i^2 + \frac{1}{4}\Sigma b_i d_i - \frac{1}{8}\Sigma b_i + \frac{1}{32}.$

Labeled Transformation Chains (LTC)

We define LTC to trace the action of the algorithm on the exotic forests.

For example, the action of the algorithm on  is



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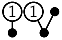
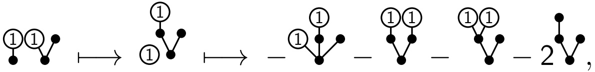
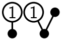
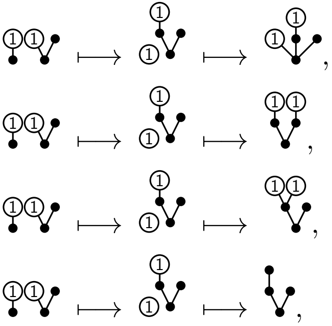
For example, the action of the algorithm on  is



and the list of labeled transformation chains (LTC) from  is



Each exotic tree has a single root.

Idea of the proof

The main ingredients used to prove the multipicative property are:

1. we can split and combine LTC,
2. the algorithm generating order conditions defines a linear map,
3. the stochastic Runge-Kutta methods form exotic S-series $ES(a)$ with

$$a(\pi_1 \sqcup \pi_2) = a(\pi_1)a(\pi_2).$$

We use them to prove the multiplicative property:

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

The following order conditions are satisfied automatically:

$$\Omega(\bullet\ \bullet) = 0, \quad \Omega(\overset{\bullet}{\underset{\bullet}{|}}\ \bullet) = 0, \quad \Omega(\overset{①\,①}{\vee}\ \bullet) = 0, \quad \Omega(\bullet\ \bullet\ \bullet) = 0.$$

The number of order 3 conditions for inv. measure drops from 13 to 9. This property of order 3 conditions was noticed in Laurent and Vilmart [2019] through manual computation.

Conclusion

Summary:

1. we defined exotic S-series with new symmetry coefficient, proved their relationship to S-series, and proved the composition law;
2. we introduced a theoretical algorithm to generate order conditions for invariant measure sampling and proved the multiplicative property of the generated order conditions.

Ongoing work:

1. description of the substitution law for exotic S-series;
2. 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.

Thank you for your attention!

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