Using exotic aromatic forests to construct order two scheme for the invariant measure sampling of Langevin dynamics with variable diffusion

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Abstract

Exotic aromatic forests, an extension of aromatic forests into the stochastic context, play a crucial role in generating order conditions for invariant measure sampling and in studying the algebraic properties of stochastic integrators. This work demonstrates practical benefits through a new method, a generalization of the Leimkuhler-Matthews method, which achieves order two for overdamped Langevin dynamics with variable diffusion.

1. Stochastic differential equations

Let ϕ denote a test function $\mathbb{R}^d \to \mathbb{R}$. Consider a stochastic differential equation with multiplicative noise with smooth vector field $F : \mathbb{R}^d \to \mathbb{R}^d$ and smooth diffusion $D : \mathbb{R}^d \to \mathbb{R}^{d\times d}$:

$$dX = F(X)dt + \sigma D(X)dW, \quad X(t) \in \mathbb{R}^d,$$

where $W(t) \in \mathbb{R}^d$ is a standard Wiener process. The weak Taylor expansion of the solution $X(t)$ is given by

$$\mathbb{E}[\phi(X(h))] = \phi(X_0) + h\mathcal{L}\phi(X_0) + \dots + \frac{h^k}{k!}\mathcal{L}^{\circ k}\phi(X_0) + \cdots,$$

with generator, using Hessian matrix $\nabla^2\phi$, given by

$$\mathcal{L}\phi = \phi' F + \frac{\sigma^2}{2}\sum_{a=1}^{d}\phi''(D_a, D_a) = F\cdot\nabla\phi + \frac{\sigma^2}{2}Tr((\nabla^2\phi)DD^T).$$

1.1 Weak order of an integrator

An integrator $X_1 = \Phi_h(X_0)$ with the weak Taylor expansion

$$\mathbb{E}[\phi(X_1)] = \phi(X_0) + h\mathcal{A}_1\phi(X_0) + \dots + h^k\mathcal{A}_k\phi(X_0) + \cdots, \quad (1.1)$$

has weak order p if $\mathcal{A}_k = \frac{1}{k!}\mathcal{L}^{\circ k}$ for $k = 1,\dots,p$. [9]

1.2 Order w.r.t. the invariant measure sampling

For an ergodic model (e.g. overdamped Langevin dynamics where $F = -\nabla V$ and mild assumptions) with invariant measure μ, the solution $X(t)$ satisfies

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

An ergodic integrator $X_n \mapsto X_{n+1}$ has order q with respect to invariant measure sampling if

$$\left|\lim_{N\to\infty}\frac{1}{N+1}\sum_{k=0}^{N}\phi(X_k) - \int_{\mathbb{R}^d}\phi(x)d\mu(x)\right| \le Ch^q, \quad (1.2)$$

Given the differential operators $\mathcal{A}_k$ from the weak Taylor expansion (1.1) of $\mathbb{E}[\phi(X_1)]$, the condition (1.2) is satisfied if,

$$\int_{\mathbb{R}^d}\mathcal{A}_k\phi(x)d\mu(x) = 0, \quad k = 1,\dots,q. \quad (1.3)$$

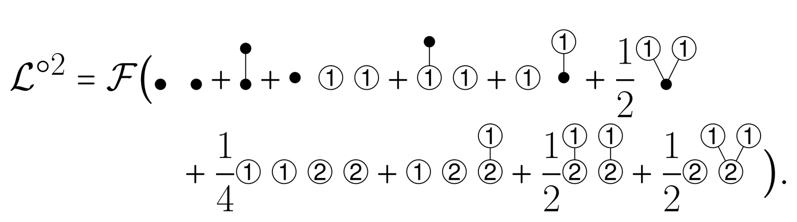
If the integrator has weak order p, then $q \ge p$. [1, 9]

1.3 Taylor expansions are tedious to manipulate!

Third term of the weak Taylor expansion of $X(h)$:

$$\begin{aligned}\mathcal{L}^{\circ 2} &= F^iF^j\partial_{ij} + F^i\partial_iF^j\partial_j + \sigma^2F^iD^j_aD^k_a\partial_{ijk} + \sigma^2F^i\partial_iD^j_aD^k_a\partial_{jk}\\ &+ \sigma^2D^j_aD^k_a\partial_kF^i\partial_{ij} + \frac{1}{2}\sigma^2D^j_aD^k_a\partial_{jk}F^i\partial_i\\ &+ \frac{1}{4}\sigma^4D^i_{a_1}D^j_{a_1}D^k_{a_2}D^l_{a_2}\partial_{ijkl} + \sigma^4D^i_{a_1}D^k_{a_2}D^j_{a_1}\partial_jD^l_{a_2}\partial_{ikl}\\ &+ \frac{1}{2}\sigma^4D^i_{a_1}\partial_iD^k_{a_2}D^j_{a_1}\partial_jD^l_{a_2}\partial_{kl} + \frac{1}{2}\sigma^4D^k_{a_2}D^i_{a_1}D^j_{a_1}\partial_{ij}D^l_{a_2}\partial_{kl}.\end{aligned}$$

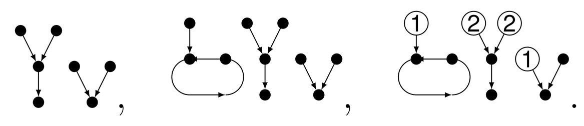
and using exotic aromatic forests:



Example taken from [5].

2. Exotic aromatic forests

An *exotic aromatic forest* is a forest with edges oriented from top to bottom. This forest can contain cycles with edges oriented counterclockwise, and some of its vertices may be paired. For example:



In these forests, vertices represent vector fields, and edges represent directional derivatives. Cycles allow us to represent divergences, while paired vertices correspond to Laplacians. [2, 6]

2.1 Using forests to check weak order

We write $\mathcal{A}_k = \mathcal{F}(\sum_{\pi\in F_k}\frac{a(\pi)}{\sigma(\pi)}\pi)$ and obtain the following order conditions for weak order p:

$$a(\pi) = \frac{\alpha(\pi)}{|\pi|!}, \quad \text{for all } \pi \in EAF, |\pi| \le p,$$

where $a(\pi) : EAF \to \mathbb{R}$ is a functional coming from the integrator, $\sigma(\pi)$ is the symmetry of π, $|\pi|$ is the number of vertices, and $\alpha(\pi)$ is a number of ordered labelings.

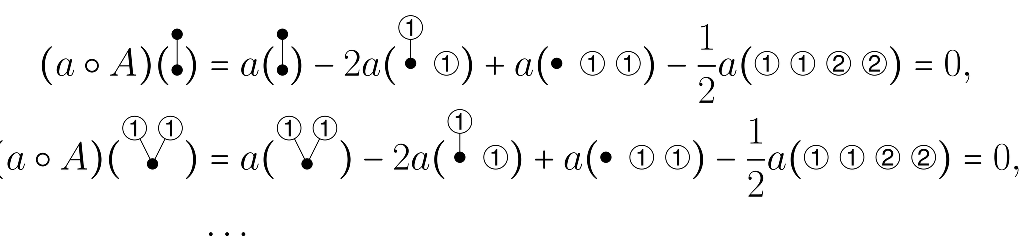
2.2 Using forests to check inv. measure sampling order

Theorem 1 ([2, 5]). *We can use integration by parts denoted by ~ to modify $\mathcal{A}_k$ without changing the value of the integral in (1.3). The order conditions become*

$$(a \circ A)(\tau) = 0, \quad \textit{for all } \tau \in EAT, |\tau| \le q,$$

where A is an adjoint operation of the integration by parts.

For example, we obtain among the order two conditions:



3. New order two scheme w.r.t. the inv. measure

Consider the Langevin dynamics, $V : \mathbb{R}^d \to \mathbb{R}, D \in \mathbb{R}^{d\times d}$,

$$dX = -D^2\nabla V(X)dt + \sigma D dW, \quad X(t) \in \mathbb{R}^d,$$

and Leimkuhler-Matthews scheme [7], $\xi_n \sim \mathcal{N}(0, I_d)$,

$$X_{n+1} = X_n - hD^2\nabla V(X_n) + \sqrt{h}\sigma D\frac{\xi_n + \xi_{n+1}}{2},$$

which can be rewritten in Markovian form as

$$\begin{aligned}X_{n+1} &= X_n - hD^2\nabla V(\overline{X}_n) + \sqrt{h}\sigma D\xi_n,\\ \overline{X}_n &= X_n + \frac{1}{2}\sqrt{h}\sigma D\xi_n.\end{aligned}$$

Then, $\overline{X}_n \to \overline{X}_{n+1}$ is second-order w.r.t the invariant measure sampling and has only one evaluation of ∇V per step.

3.1 New generalization

We consider Langevin equation with variable diffusion matrix $D : \mathbb{R}^d \to \mathbb{R}^{d\times d}$, with D uniformly s.p.d.

$$dX = -D^2(X)\nabla V(X)dt + \frac{\sigma^2}{2}\mathrm{div}(D^2)(X)dt + \sigma D(X)dW,$$

where $D(X)$ is symmetric. The new scheme has the form

$$\begin{aligned}X_{n+1} &= X_n + hF(\overline{X}_n) + \hat{\Phi}^D_h(X_n + \frac{1}{4}hF(\overline{X}_{n-1})),\\ \overline{X}_n &= X_n + \frac{1}{2}\sigma\sqrt{h}D(X_n)\xi_n,\end{aligned} \quad (3.1)$$

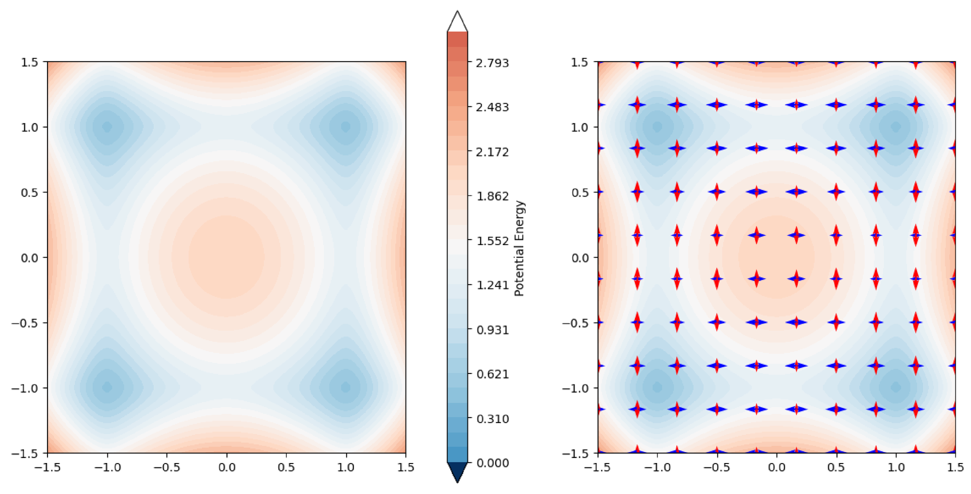
where $I + \hat{\Phi}^D_h$ is a weak order 2 integrator of

$$dX = \sigma D(X)dW.$$

Theorem 2 ([5]). *The scheme $\overline{X}_n \to \overline{X}_{n+1}$ is second-order w.r.t the invariant measure sampling and has only one evaluation of ∇V per step.*

3.2 Example model

Diffusion matrix D can be selected to aid in sampling the invariant measure ([8] for details). An example of a potential (a) and eigenvectors of a diffusion matrix (b) are shown.



(a) Four-well potential (b) Diffusion matrix

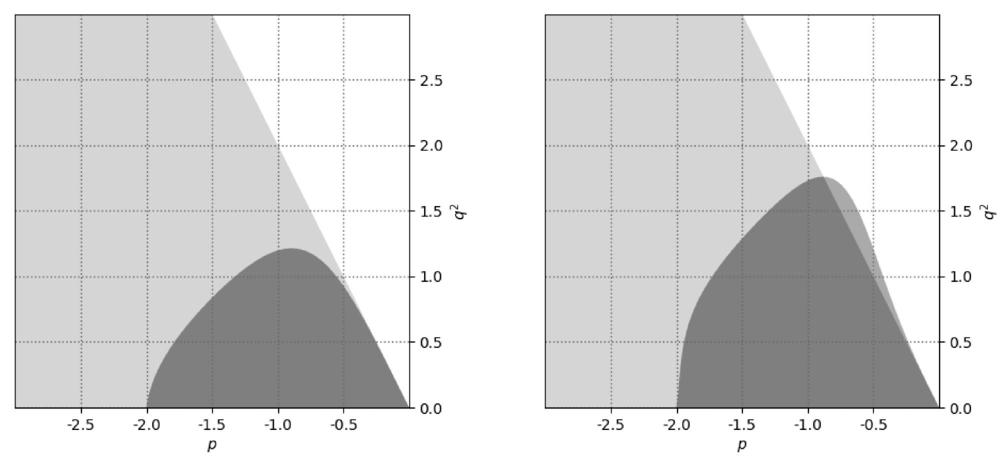
Figure 1: *Example model in 2D*

3.3 Stability analysis of the new scheme

We consider the following Saito-Mitsui (1996) test model:

$$dX(t) = \lambda X(t)dt + \mu X(t)dW(t), \quad X(0) = 1.$$

We take $\lambda, \mu \in \mathbb{R}$ and let $p = h\lambda$ and $q = \sqrt{h}\mu$ and obtain the following mean-square stability domains (i.e. where $\mathbb{E}(X_n^2)$ is bounded). Light gray denotes the mean-square stability domain of the exact solution:



(a) new method (3.1) (b) stabilized (3.1)

Figure 2: *Mean-square stability domains*

Figure (b) shows the stability region of the new method with a modified noise integrator $I + \Phi^D_h$ for better stabilization.

4. Related ongoing work

In a joint work [4] with Adrien Laurent (INRIA Rennes), we uncover the following algebraic structures of exotic aromatic forests:

- a free tracial pre-Lie-Rinehart algebra,
- a free D-algebra, pre-Hopf algebroid,
- a multi-pre-Lie algebra,
- a comodule-bialgebra structure,

which are essential in the description of the backward error analysis in the context of ergodic stochastic differential equations.

In a joint work [3] with Jean-Luc Falcone (University of Geneva), we develop a Haskell package to automate computations involving exotic aromatic forests. GitLab: https://gitlab.unige.ch/Eugen.Bronasco/graphalgebra.hs.

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