Order conditions for sampling the invariant measure of ergodic SDEs in $\mathbb{R}^d$ or on manifolds

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Abstract

We derive a new methodology for the construction of high order integrators for sampling the invariant measure of ergodic stochastic differential equations subjected to a scalar constraint. For a class of Runge-Kutta type methods, we derive the conditions for the order two of accuracy. Numerical experiments in dimension 3 on the sphere and the torus confirm the theoretical findings. We also discuss a possible extension of the exotic aromatic B-series formalism.

1. Long time approximation of constrained ergodic SDEs

We consider (Stratonovich) stochastic differential equations in $\mathbb{R}^d$, subjected to a smooth scalar constraint $\zeta = 0$, that have the form

$$dX = \Pi_{\mathcal{M}}(X)f(X)dt + \Pi_{\mathcal{M}}(X)\Sigma(X)\circ dW, \qquad (1.1)$$

where $X(0) = X_0 \in \mathcal{M}$, $\zeta\colon \mathbb{R}^d \to \mathbb{R}$, $\mathcal{M} = \{x \in \mathbb{R}^d, \zeta(x) = 0\}$ is a compact smooth manifold or $\mathcal{M} = \mathbb{R}^d$, $\Pi_{\mathcal{M}}\colon \mathbb{R}^d \to \mathbb{R}^{d\times d}$ is the orthogonal projection on the tangent bundle of $\mathcal{M}$, $f\colon \mathbb{R}^d \to \mathbb{R}^d$ and $\Sigma\colon \mathbb{R}^d \to \mathbb{R}^{d\times d}$ are smooth and W is a standard d-dimensional Brownian motion.

Equations of the form (1.1) appear naturally when studying conservative SDEs, that is, SDEs possessing an invariant H. The solution of conservative SDEs are subjected to the constraint $\zeta = 0$ with $\zeta = H - H(X_0)$. The major motivation of this work appears in computational problems in molecular dynamics with the constrained overdamped Langevin equation (obtained in the particular case where $\Sigma = \sigma I_d$)

$$dX = \Pi_{\mathcal{M}}(X)f(X)dt + \sigma\Pi_{\mathcal{M}}(X)\circ dW, \qquad (1.2)$$

with $\sigma \in \mathbb{R}$, $f = -\nabla V$ and $V\colon \mathbb{R}^d \to \mathbb{R}$ is smooth. The overdamped Langevin equation is widely used to model the motion of a set of particles subjected to a potential V in a high friction regime. The possible constraints can be induced for example by strong covalent bonds between atoms, or fixed angles in molecules. We refer to [5] for further details on applications and numerical methods for sampling constrained SDEs.

Weak error: A numerical scheme $(X_n)_n$ is said to have local weak order p if for every test function ϕ,

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

The backward Kolmogorov equation yields

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

where $\mathcal{L}$ is the generator of (1.1) and is given by

$$\mathcal{L}\phi = \phi' f - G^{-1}(g,f)\phi' g - \frac{\sigma^2}{2}G^{-1}\operatorname{div}(g)\phi'(g) \qquad (1.3)$$
$$+ \frac{\sigma^2}{2}G^{-2}(g,g'g)\phi'(g) + \frac{\sigma^2}{2}\Delta\phi - \frac{\sigma^2}{2}G^{-1}\phi''(g,g),$$

where $g = \nabla\zeta$ and $G = g^T g$. We compare with the Talay-Tubaro expansion of the integrator

$$\mathbb{E}[\phi(X_1)|X_0 = x] = \phi(x) + h\mathcal{A}_0\phi(x) + h^2\mathcal{A}_1\phi(x) + \dots$$

Then the scheme has weak order p if $\forall j \leq p$, $\mathcal{L}^j/j! = \mathcal{A}_{j-1}$.

Ergodicity property: there exists a probability density ρ_∞ such that

$$\lim_{T\to+\infty}\frac{1}{T}\int_0^T \phi(X(s))ds = \int_{\mathcal{M}} \phi(y)\rho_\infty(y)d\sigma_{\mathcal{M}}(y) \quad a.s.$$

where $d\sigma_{\mathcal{M}}$ is the canonical measure on $\mathcal{M}$ induced by the euclidean metric of $\mathbb{R}^d$.
We call error of the invariant measure the quantity

$$e(\phi,h) = \left|\lim_{N\to+\infty}\frac{1}{N+1}\sum_{n=0}^{N}\phi(X_n) - \int_{\mathcal{M}}\phi\rho_\infty d\sigma_{\mathcal{M}}\right|.$$

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

Theorem 1. [3] (related work in $\mathbb{R}^d$: [2, 1])

Under technical assumptions, if $\mathcal{A}_j^*\rho_\infty = 0$ (in $L^2(d\sigma_{\mathcal{M}})$) for $j = 1,\dots p-1$, i.e. for every test function ϕ,

$$\int_{\mathcal{M}}(\mathcal{A}_j\phi)\rho_\infty d\sigma_{\mathcal{M}} = 0, \qquad j = 1,\dots p-1,$$

then the scheme has order p for the invariant measure.

2. High order Runge-Kutta methods for overdamped Langevin in $\mathbb{R}^d$

We consider Runge-Kutta methods of the form

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

Theorem 2. [3] (Order conditions in $\mathbb{R}^d$)

A Runge-Kutta method has weak order 1 if $c_s = 1$. In addition, it has order 2 for the invariant measure if the following 2 conditions are satisfied:

$$\sum_{j=1}^{s} a_{sj}c_j = \sum_{j=1}^{s} a_{sj}d_j^2 = 2\sum_{j=1}^{s} a_{sj}d_j - \frac{1}{2}.$$

Remark. *We find 3 order conditions for weak order 2. There are 11 conditions for the weak order 3 and 6 conditions for the invariant measure.*

Example.
The θ-method for solving (1.2) is

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

It has order 2 for the invariant measure if $\theta = \frac{1}{2}$ and order 1 else.

3. High order Runge-Kutta methods for constrained overdamped Langevin

We consider the following class of Runge-Kutta integrators

$$Y_i = X_n + h\sum_{j=1}^{s} a_{ij}f(Y_j) + \sigma\sqrt{h}d_i\xi_n + \lambda_i\sum_{j=1}^{s}\widehat{a}_{ij}g(Y_j),$$
$$\zeta(Y_i) = 0 \quad \text{if} \quad \delta_i = 1, \qquad (3.1)$$
$$X_{n+1} = Y_s,$$

where $\delta_i = \sum_{j=1}^{s}\widehat{a}_{ij} \in \{0,1\}$ and $\delta_s = 1$.

Proposition. *If $c_s = d_s = 1$ and $\sum\widehat{a}_{sj}d_j = \sum\widehat{a}_{sj}\delta_j d_j$, the method is consistent, that is, $\mathcal{A}_0 = \mathcal{L}$.*

Example.
The simplest numerical scheme for approximating ergodic integrals on manifolds is the Euler method

$$X_{n+1} = X_n + hf(X_n) + \sigma\sqrt{h}\xi_n + \lambda g(X_{n+1}), \qquad (3.2)$$
$$\zeta(X_{n+1}) = 0.$$

It is a Runge-Kutta method of weak order 1 with the coefficients given by the following Butcher tableau.

$$c\,\Big|\,A\,\Big\|\,\delta\,\Big|\,\widehat{A}\,\Big\|\,d = \begin{array}{c|cc||c|cc||c} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 1 \end{array}$$

Theorem 3. [4] (Order conditions on the manifold $\mathcal{M}$)

We consider a consistent ergodic Runge-Kutta method of the form (3.1) applied to solve (1.2), then the integrator has order 2 for the invariant measure if the coefficients of the method satisfy 23 order conditions:

$$\sum_{j=1}^{s}\widehat{a}_{sj}d_j = \sum_{j=1}^{s}a_{sj}d_j, \quad \sum_{j=1}^{s}a_{sj}c_j = 2\sum_{j=1}^{s}a_{sj}d_j - \frac{1}{2}, \quad \dots$$

Remark. *We find 25 Runge-Kutta order conditions for weak order 2. These conditions are detailed in [4].*

4. Exotic aromatic B-series for the computation of order conditions

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 [3]).
We rewrite our differentials with partitioned aromatic forests (see Chartier, Murua, 2007 and Bogfjellmo, 2015). We denote $F(\gamma)(\phi)$ the elementary differential of a tree γ.

$$F(\bullet)(\phi) = \phi' f$$
$$F(\circlearrowright\circ)(\phi) = \sigma^2 G^{-1}\operatorname{div}(g)\phi' g$$
$$F(\circ\!\smile\!\circ)(\phi) = \sigma^2 G^{-1}\phi''(g, g'f)$$

We also introduce lianas and non-oriented edges in our forests and call these exotic aromatic forests.

$$F(\tau)(\phi) = \sum_i \phi''(e_i, e_i) = \Delta\phi$$
$$F(\tau)(\phi) = \sigma^4 G^{-2}(g, g'g)\sum_i \phi''(g'(e_i), e_i)$$
$$F(\tau)(\phi) = \sigma^2 G^{-1}(g, f)(\Delta\phi)' g$$

Example.
The operator $\mathcal{L}$ in (1.3) can be rewritten with exotic aromatic forests as

$$\mathcal{L}\phi = F\Big(\bullet - \circ\!-\!\bullet\,\circ - \frac{1}{2}\,\tau + \frac{1}{2}\,\tau + \frac{1}{2}\,\tau - \frac{1}{2}\,\tau\Big)(\phi).$$

In $\mathbb{R}^d$, we have $g = 0$, so that the trees with white nodes vanish and $\mathcal{L}$ is given by

$$\mathcal{L}\phi = F\Big(\bullet + \frac{1}{2}\,\tau\Big)(\phi) = \phi' f + \frac{\sigma^2}{2}\Delta\phi.$$

The operator $\mathcal{A}_1$ can be expressed with exotic aromatic forests.

$$\mathcal{A}_1\phi = F\Big(\frac{1}{2}\,\tau - \frac{1}{4}\,\tau + \frac{1}{2}\sum\widehat{a}_{sj}d_j\,\tau - \frac{1}{2}\,\tau + \dots\Big)(\phi).$$

For the θ-method (2.1) in $\mathbb{R}^d$, we find

$$\mathcal{A}_1 = F\Big(\theta\,\tau + \frac{1}{2}\,\tau + \frac{\theta}{2}\,\tau + \theta\,\tau + \frac{1}{2}\,\tau + \frac{1}{8}\,\tau\Big).$$

To compute the order conditions for the invariant measure, we apply multiple integrations by parts to get

$$\int_{\mathcal{M}}(\mathcal{A}_j\phi)\rho_\infty d\sigma_{\mathcal{M}} = \int_{\mathcal{M}}(\mathcal{A}_j^0\phi)\rho_\infty d\sigma_{\mathcal{M}},$$

where $\mathcal{A}_j^0\phi$ is a differential operator of order 1 on ϕ.

Lemma 4. *The process of integration by parts can be rewritten with exotic aromatic forests as a straightforward procedure on graphs. Moreover $\mathcal{A}_j^0\phi$ can be expressed with exotic aromatic forests.*

For the θ-method (2.1) in $\mathbb{R}^d$, we find

$$\mathcal{A}_1^0 = \Big(\frac{1}{2} - \theta\Big)F\Big(\tau + \frac{1}{2}\,\tau\Big).$$

5. Numerical experiments

By solving numerically the order conditions of Theorem 3, we find a new Runge-Kutta method that has order 2 for the invariant measure. In addition, the method is explicit in f and uses only 3 evaluations of f per step.
To check the numerical order 2 for the invariant measure of this integrator, we apply it on the sphere (with $\zeta(x) = (x_1^2+x_2^2+x_3^2-1)/2$) and the torus (with $\zeta(x) = (x_1^2+x_2^2+x_3^2+R^2-r^2)^2 - 4R^2(x_1^2+x_2^2)$, $R = 3$ and $r = 1$) in dimension $d = 3$ and compare it with the Euler scheme (3.2). We plot the error for the invariant measure versus different timesteps h. In both cases, we observe order 1 for the Euler scheme (3.2) and order 2 for the new Runge-Kutta scheme.

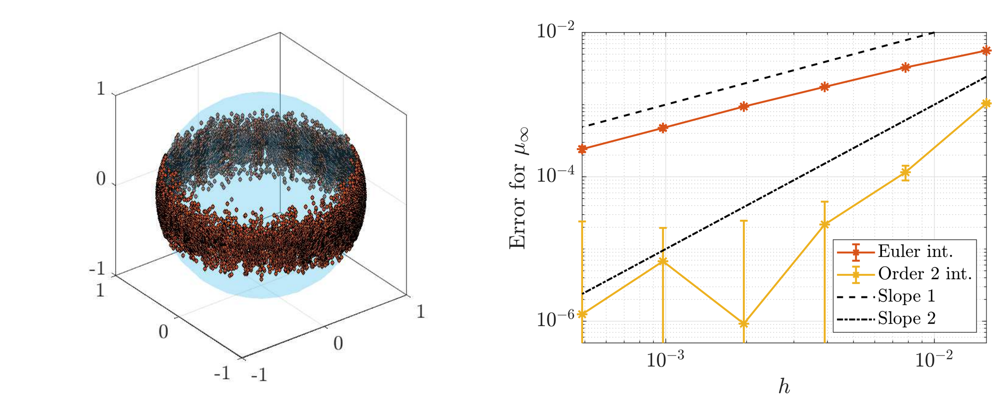

Figure 1: *A trajectory of the order 2 method (left) and the convergence curve for the sphere for the invariant measure (right) with $V(x) = 25(1 - x_1^2 - x_2^2)$, $\phi(x) = x_3^2$ and $M = 10^7$ trajectories*

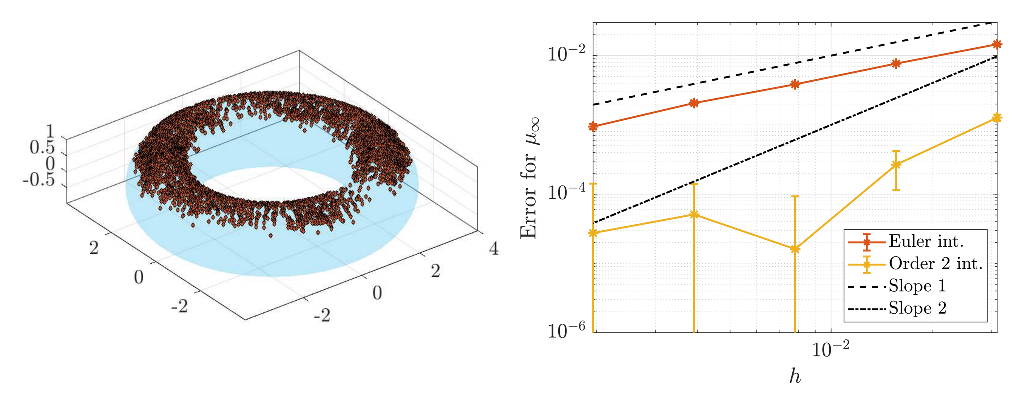

Figure 2: *A trajectory of the order 2 method (left) and the convergence curve for the torus for the invariant measure (right) with $V(x) = 25(x_3 - r)^2$, $\phi(x) = x_3^2$ and $M = 10^7$ trajectories*

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