Séminaire de Mathématiques Appliquées du CERMICS

École des Ponts
ParisTech

A numerical sampling scheme for the conditional probability measure on submanifold

Wei Zhang (Zuse Institute Berlin)

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Outline

- Motivations
- Numerical schemes
- Error analysis of Θ-scheme
- Numerical examples

Overdamped Langevin dynamics

SDE

$$dx_s = J\,ds - a\nabla U\,ds + \frac{1}{\beta}(\nabla \cdot a)\,ds + \sqrt{2\beta^{-1}}\sigma\,dw_s\,,\ \ s \geq 0\,.$$

$\beta > 0$, smooth $U : \mathbb{R}^d \to \mathbb{R}$, matrix $a = \sigma\sigma^T$ is uniformly positive definite.

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Non-reversible part $J : \mathbb{R}^d \to \mathbb{R}^d$, s.t. $\mathrm{div}(Je^{-\beta U}) \equiv 0$.
Special cases: (1) $J = A\nabla U$, with const. matrix $A^T = -A$.
(2) $J \equiv 0 \iff x_s$ is reversible.

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Infinitesimal generator

$$\mathcal{L}f = J\cdot\nabla f + \frac{e^{\beta U}}{\beta}\sum_{1\leq i,j\leq d}\frac{\partial}{\partial x_i}\Big(a_{ij}e^{-\beta U}\frac{\partial f}{\partial x_j}\Big), \quad f : \text{test function}$$

Invariant measure $\frac{d\mu}{dx} = \frac{1}{Z}e^{-\beta U}$.

Reaction coordinate

In MD applications, **reaction coordinate** is often used to understand the essential behavior of high dimensional molecular systems.

Mathematically, we consider the map

$$\xi : \mathbb{R}^d \to \mathbb{R}^k, \quad C^3 - \text{smooth}, \quad 1 \leq k < d.$$

Effective dynamics

Aim: understand the dynamics of reaction coordinate on $\mathbb{R}^k$.

Ito's formula $\Longrightarrow$ (non-closed dynamics)

$$d\xi(x_s) = (\mathcal{L}\xi)(x_s)\, ds + \sqrt{2\beta^{-1}}(\nabla\xi^T\sigma)(x_s)\, dw_s\,.$$

Idea of "closure": averaging the coefficients on level sets $\Sigma_z = \left\{x \in \mathbb{R}^d \mid \xi(x) = z\right\}, z \in \mathbb{R}^k$, using **conditional prob. measure**

$$d\mu_z = \frac{1}{Q(z)Z} e^{-\beta U}\left[\det(\nabla\xi^T\nabla\xi)\right]^{-\frac{1}{2}} d\nu_z\,, \quad \text{on } \Sigma_z\,.$$

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Effective dynamics (Legoll and Lelièvre, 2010) :

$$dz_s = \widetilde{b}(z_s)\, ds + \sqrt{2\beta^{-1}}\widetilde{\sigma}(z_s)\, d\widetilde{w}_s\,,$$

$$\widetilde{b}(z) = \int_{\Sigma_z} (\mathcal{L}\xi)(x)\, d\mu_z(x)\,, \quad \widetilde{\sigma}(z) = \Big[\int_{\Sigma_z} (\nabla\xi^T a\nabla\xi)(x)\, d\mu_z(x)\Big]^{\frac{1}{2}}\,.$$

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Motivation 1: numerical simulation of effective dynamics.

Effective dynamics and free energy

Co-area formula

$$\int_{\mathbb{R}^d} f(x)\, d\mu(x) = \int_{\mathbb{R}^k} \Big(\int_{\Sigma_z} f(x) d\mu_z \Big) Q(z)\, dz\,, \quad \forall f\,,$$

and $\quad Q(z) = \frac{1}{Z} \int_{\mathbb{R}^d} \delta(\xi(x) - z)\, e^{-\beta U(x)}\, dx\,.$

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and $$Q(z) = \frac{1}{Z} \int_{\mathbb{R}^d} \delta(\xi(x) - z)\, e^{-\beta U(x)}\, dx\,.$$

Effective dynamics can be written as

$$dz_s = \widetilde{J}\, ds - \widetilde{a} \nabla_z F\, ds + \nabla_z \cdot \widetilde{a}\, ds + \sqrt{2\beta^{-1}} \widetilde{\sigma}\, d\widetilde{w}_s\,.$$

1. $\widetilde{J} = \int_{\Sigma_z} (J \cdot \nabla \xi) d\mu_z$, $\mathrm{div}_z(\widetilde{J} Q) \equiv 0$.
2. $F(z) = -\beta^{-1} \ln Q(z)$ is free energy. (Different definitions exist)
3. invariant measure: $d\widetilde{\mu} = Q(z) dz = e^{-\beta F(z)} dz$.

(Zhang, Hartmann, and Schütte, 2016)

Free energy calculation

$z(\cdot)$: a curve in $\mathbb{R}^k$ connecting $z(0)$ and $z(T)$.
$\Psi = \nabla\xi^T a \nabla\xi \in \mathbb{R}^{k\times k}$. $\quad F(z) = -\beta^{-1}\ln Q(z)$.

Thermodynamic Integration (TI):

$$\begin{aligned}
& F(z(T)) - F(z(0)) \\
=& -\beta^{-1}\ln\frac{Q(z(T))}{Q(z(0))} \\
=& -\beta^{-1}\int_0^T \frac{d}{ds}\Big(\ln\frac{Q(z(s))}{Q(z(0))}\Big)\,ds \\
=& \int_0^T \mathbf{E}_{\mu_{z(s)}}\Big[(a\nabla\xi_{\gamma'})_i(\Psi^{-1})_{\gamma'\gamma}\frac{\partial U}{\partial x_i} - \frac{1}{\beta}\frac{\partial}{\partial x_i}\Big((a\nabla\xi_{\gamma'})_i(\Psi^{-1})_{\gamma\gamma'}\Big)\Big]\,\dot{z}_\gamma(s)\,ds\,.
\end{aligned}$$

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\end{aligned}
$$

Motivation 2: free energy calculation using TI.

Approximate Bayesian computation (ABC)

Motivation 3: Bayesian statistics.

Reaction coordinate $\hookrightarrow$ **summary statistics** $S : \mathbb{R}^d \to \mathbb{R}^k$.

- inequality constraints: $\rho(S(\hat{D}), S(D)) \leq \epsilon$.
- k can be large ($10 - 100$).

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Sampling on level set

- Reaction coordinate $\xi : \mathbb{R}^d \to \mathbb{R}^k, \quad C^3$ – smooth.
- Potential $U : \mathbb{R}^d \to \mathbb{R}$.
- Level set $\Sigma = \left\{x \in \mathbb{R}^d \mid \xi(x) = \mathbf{0} \in \mathbb{R}^k\right\}, \quad \mathrm{dim}\Sigma = d - k$.
- Surface measure ν.
- $f : \Sigma \to \mathbb{R}$.
- Conditional prob. measure

$$d\mu_1 = \frac{1}{Z} e^{-\beta U} \left[\det(\nabla\xi^T \nabla\xi)\right]^{-\frac{1}{2}} d\nu \, .$$

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Goal: numerical scheme for

$$\overline{f} = \mathbf{E}_{\mu_1}(f) = \int_\Sigma f(x)\, d\mu_1\,.$$

Remark: $d\mu_2 = \frac{1}{Z} e^{-\beta U} d\nu\,.$

Θ-scheme on level set

$f : \Sigma \to \mathbb{R}$. $\widehat{f}_n = \frac{1}{n} \sum_{l=0}^{n-1} f(x^{(l)})$. $a = \sigma\sigma^T$. $h > 0$, $x^{(0)} \in \Sigma$.

$$\begin{aligned} x_i^{(l+\frac{1}{2})} =& x_i^{(l)} + \Big(- a_{ij} \frac{\partial U}{\partial x_j} + \frac{1}{\beta} \frac{\partial a_{ij}}{\partial x_j} \Big)(x^{(l)})\, h + \sqrt{2\beta^{-1} h}\, \sigma_{ij}(x^{(l)})\, \eta_j^{(l)}\,, \ 1 \le i \le d\,, \\ x^{(l+1)} =& \Theta\big(x^{(l+\frac{1}{2})}\big)\,. \end{aligned}$$

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$\Theta(x) = \lim_{s\to+\infty} \varphi(x,s)$ is the limit of the flow map

$$
\frac{d\varphi(x,s)}{ds} = -\,(a\nabla F)\big(\varphi(x,s)\big)\,, \quad \varphi(x,0) = x\,,
$$

with $F(x) = \frac{1}{2}|\xi(x)|^2 = \frac{1}{2}\sum_{\alpha=1}^{k} \xi_\alpha^2(x)$.

Special case $a = \mathrm{id}$

When $a \equiv \mathrm{id}$, the scheme becomes

$$\begin{aligned} x^{(l+\frac{1}{2})} &= x^{(l)} - \nabla U(x^{(l)})\, h + \sqrt{2\beta^{-1} h}\, \boldsymbol{\eta}^{(l)}\,, \\ x^{(l+1)} &= \Theta(x^{(l+\frac{1}{2})})\,. \end{aligned}$$

$\Longrightarrow$ Update by Euler-Maruyama, then project by Θ.

Projection map

$F(x) = \frac{1}{2}|\xi(x)|^2$. Projection: $\Theta(x) = \lim_{s \to +\infty} \varphi(x, s)$.

$$\frac{d\varphi(x,s)}{ds} = -\nabla F\big(\varphi(x,s)\big), \quad \varphi(x,0) = x. \tag{1}$$

Remarks:

1. only use first order derivatives of ξ.
2. (1) is a gradient flow, and Θ is often globally defined.
3. integrate ODE (1) by Runge-Kutta (RK) methods.
   complexity: $\mathcal{O}(n \cdot k \cdot d \cdot n_{ode})$. n_{ode} is no. of RK steps.
4. $0 \le \kappa < 1$. Instead of (1), one can use

$$\frac{d\bar{\varphi}(x,s)}{ds} = -(\nabla|\xi|^{2-\kappa})\big(\bar{\varphi}(x,s)\big), \quad \bar{\varphi}(x,0) = x.$$

$\bar{\varphi}$ is a **reparametrization** of φ, because $\nabla|\xi|^{2-\kappa} = (2-\kappa)|\xi|^{-\kappa}\nabla F$.

Comparison with other projections

- Orthogonal projection

$$\Pi(x) = \operatorname*{argmin}_{y\in\Sigma} \|x-y\|^2 , \quad x \in \mathbb{R}^d .$$

  1. sample $d\mu_2 = \frac{1}{Z} e^{-\beta U} d\nu$, not μ_1.
  2. need to solve optimization problem.

- Constraint by Lagrange multiplier. (Ciccotti, Lelièvre, and Vanden-Eijnden, 2008; Lelièvre, Rousset, and Stoltz, 2012)

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Example: $\xi(x) = \frac{1}{2}\left(\frac{x_1^2}{c^2} + x_2^2 - 1\right)$, $x \in \mathbb{R}^2$. $\Sigma = \left\{(x_1, x_2)^T \mid \frac{x_1^2}{c^2} + x_2^2 = 1\right\}$.

$c = 3$. $U = 0$. We have $d\mu_1 = \frac{1}{Z}\left(\frac{x_1^2}{c^4} + x_2^2\right)^{-\frac{1}{2}} d\nu\,, \quad d\mu_2 = \frac{1}{Z}\, d\nu\,.$

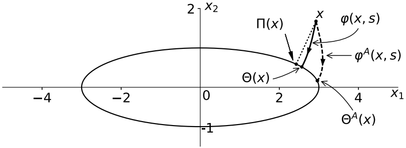

Figure: $\Theta(x)$ and $\Pi(x)$.

Comparison with Metropolis-adjusted methods

Metropolis-adjusted methods (Zappa, Holmes-Cerfon, and Goodman, 2018; Lelievre, Rousset, and Stoltz, 2018) based on

(1) Newton's method. (2) reversibility check.

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(1) Newton's method. (2) reversibility check.

Remarks:

1. either sample ν, or $d\mu_2 = \frac{1}{Z} e^{-\beta U} d\nu$.
2. unbiased, also for large step-sizes.
3. Newton convergence is fast, but local.
4. choice of proposal distributions.
5. need to tune step-sizes.
6. cost of Newton's method: $\mathcal{O}(n \cdot k^2 \cdot d \cdot N_{iter})$.
   N_{iter} is no. of Newton steps, usually $N_{iter} \leq 10$.

Idea behind Θ-scheme: soft constraint

Recall the scheme

$$
\begin{aligned}
x_i^{(l+\frac{1}{2})} &= x_i^{(l)} + \Big(- a_{ij}\frac{\partial U}{\partial x_j} + \frac{1}{\beta}\frac{\partial a_{ij}}{\partial x_j}\Big)(x^{(l)})\, h + \sqrt{2\beta^{-1} h}\, \sigma_{ij}(x^{(l)})\, \eta_j^{(l)}\,, \ 1 \le i \le d\,, \\
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with $F(x) = \frac{1}{2}|\xi(x)|^2 = \frac{1}{2}\sum\limits_{\alpha=1}^{k}\xi_\alpha^2(x)$.

Idea behind Θ-scheme: soft constraint

Softly constrained SDE (under stiff potential)

$$dX_s^{\epsilon,i} = \Big[- a_{ij}\frac{\partial U}{\partial x_j} - \frac{1}{\epsilon} a_{ij}\frac{\partial}{\partial x_j}\Big(\frac{1}{2}\sum_{\alpha=1}^{k} \xi_\alpha^2\Big) + \frac{1}{\beta}\frac{\partial a_{ij}}{\partial x_j}\Big] ds + \sqrt{2\beta^{-1}}\sigma_{ij}\, dW_s^j\,, \qquad (2)$$

where $0 < \epsilon \ll 1$. Invariant measure is

$$d\mu^\epsilon(x) = \frac{1}{Z^\epsilon} \exp\Big[- \beta\Big(U(x) + \frac{1}{2\epsilon}\sum_{\alpha=1}^{k} \xi_\alpha^2(x)\Big)\Big]\, dx\,.$$

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Proposition 1

$$\lim_{\epsilon\to 0}\int_{\mathbb{R}^d} f(x)\, d\mu^\epsilon(x) = \int_\Sigma f(x)\, d\mu_1(x)\,, \quad \forall\, f : \mathbb{R}^d \to \mathbb{R} \quad \textit{bounded, smooth.}$$

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Observation: Θ-scheme on Σ is a **multiscale method** for the stiff SDE in (2). (Katzenberger, 1991)

Possible extension: Θ^A-scheme

Constant matrix $A^T = -A$. Softly constrained **Non-reversible** dynamics

$$dX_s^{\epsilon,A,i} = \left[(A_{ij} - a_{ij})\frac{\partial}{\partial x_j}\Big(U + \frac{1}{2\epsilon}\sum_{\alpha=1}^{k}\xi_\alpha^2\Big) + \frac{1}{\beta}\frac{\partial a_{ij}}{\partial x_j}\right](X_s^{\epsilon,A})\,ds + \sqrt{2\beta^{-1}}\sigma_{ij}(X_s^{\epsilon,A})\,dW_s^j\,.$$

Scheme:

$$\begin{aligned} x_i^{(l+\frac{1}{2})} =& x_i^{(l)} + \Big(A_{ij}\frac{\partial U}{\partial x_j} - a_{ij}\frac{\partial U}{\partial x_j} + \frac{1}{\beta}\frac{\partial a_{ij}}{\partial x_j}\Big)(x^{(l)})\,h + \sqrt{2\beta^{-1}h}\,\sigma_{ij}(x^{(l)})\,\eta_j^{(l)}\,,\\ x^{(l+1)} =& \Theta^A\big(x^{(l+\frac{1}{2})}\big)\,, \end{aligned}$$

where $\Theta^A(x) = \lim\limits_{s\to+\infty}\varphi^A(x,s)$ and the (non-gradient) flow map

$$\frac{d\varphi^A(x,s)}{ds} = -\,((a - A)\nabla F)\big(\varphi^A(x,s)\big)\,,\quad \varphi^A(x,0) = x,\quad \forall\, x\in\mathbb{R}^d\,,$$

with $F(x) = \frac{1}{2}|\xi(x)|^2 = \frac{1}{2}\sum\limits_{\alpha=1}^{k}\xi_\alpha^2(x)$.

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Main result for Θ-scheme

Theorem 1

Suppose that h and n are fixed. $f : \Sigma \to \mathbb{R}$ *is smooth on* Σ *and* $\bar{f} = \int_\Sigma f \, d\mu_1$*. The running average* $\widehat{f}_n = \frac{1}{n}\sum_{l=0}^{n-1} f(x^{(l)})$ *is computed by simulating the* Θ*-scheme. Let* $T = nh$ *and* C *denote a generic positive constant that is independent of h, n. We have*

1. $\left|\mathbf{E}\widehat{f}_n - \bar{f}\right| \leq C(h + \frac{1}{T})$.
2. $\mathbf{E}\left|\widehat{f}_n - \bar{f}\right|^2 \leq C(h^2 + \frac{1}{T})$.
3. *For any* $0 < \epsilon < \frac{1}{2}$*, there is an a.s. bounded positive random variable* $\zeta(\omega)$*, such that* $|\widehat{f}_n - \bar{f}| \leq Ch + \frac{\zeta(\omega)}{T^{1/2-\epsilon}}$ *, almost surely.*

Analysis via Poisson equation: sampling on $\mathbb{T}^d$

(Mattingly, Stuart, and Tretyakov, 2010)

Recall the numerical task

$$\bar{f} = \mathbf{E}_\mu(f) = \frac{1}{Z}\int_{\mathbb{T}^d} f(x)\, e^{-\beta U(x)} dx.$$

Analysis via Poisson equation: sampling on $\mathbb{T}^d$

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Recall the numerical task

$$\bar{f} = \mathbf{E}_\mu(f) = \frac{1}{Z}\int_{\mathbb{T}^d} f(x)\, e^{-\beta U(x)} dx.$$

SDE (on torus)

$$dx_s = -\nabla U\, ds + \sqrt{2\beta^{-1}} dw_s$$

has a unique invariant measure μ, under proper assumptions.

Numerical scheme:

$$\widehat{f}_n = \frac{1}{n}\sum_{l=0}^{n-1} f(x^{(l)}),$$

$$\text{where} \quad x^{(l+1)} = x^{(l)} - \nabla U(x^{(l)})\, h + \sqrt{2\beta^{-1} h}\, \boldsymbol{\eta}^{(l)},$$

and $\boldsymbol{\eta}^{(l)}$ are independent d-dim. std. Gaussians.

Analysis via Poisson equation: sampling on $\mathbb{T}^d$

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Generator $\mathcal{L} = -\nabla U \cdot \nabla + \frac{1}{\beta}\Delta$.

Poisson equation $\mathcal{L}\psi = f - \bar{f}\,,$ period b.c.

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Let $\boldsymbol{\delta}^{(l)} := x^{(l+1)} - x^{(l)} = -\nabla U(x^{(l)})\, h + \sqrt{2\beta^{-1} h}\, \boldsymbol{\eta}^{(l)} \Longrightarrow$

$$\begin{aligned} &\psi^{(l+1)} := \psi\big(x^{(l)} + \boldsymbol{\delta}^{(l)}\big) \\ =&\psi^{(l)} + \nabla\psi^{(l)} \cdot \boldsymbol{\delta}^{(l)} + \frac{1}{2} D^2\psi^{(l)}[\boldsymbol{\delta}^{(l)}, \boldsymbol{\delta}^{(l)}] + \frac{1}{6} D^3\psi^{(l)}[\boldsymbol{\delta}^{(l)}, \boldsymbol{\delta}^{(l)}, \boldsymbol{\delta}^{(l)}] + R^{(l)} \\ =&\psi^{(l)} + (\mathcal{L}\psi)^{(l)} h + \sqrt{2\beta^{-1} h}\, \nabla\psi^{(l)} \cdot \boldsymbol{\eta}^{(l)} + \frac{h}{\beta}\Big(D^2\psi^{(l)}[\boldsymbol{\eta}^{(l)}, \boldsymbol{\eta}^{(l)}] - \Delta\psi^{(l)}\Big) + o(h)\,. \end{aligned}$$

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(Mattingly, Stuart, and Tretyakov, 2010)

Generator $\mathcal{L} = -\nabla U \cdot \nabla + \frac{1}{\beta}\Delta$.

Poisson equation $\mathcal{L}\psi = f - \bar{f}$, period b.c.

Let $\boldsymbol{\delta}^{(l)} := x^{(l+1)} - x^{(l)} = -\nabla U(x^{(l)})\, h + \sqrt{2\beta^{-1} h}\,\boldsymbol{\eta}^{(l)} \Longrightarrow$

$$
\begin{aligned}
\psi^{(l+1)} &:= \psi\big(x^{(l)} + \boldsymbol{\delta}^{(l)}\big) \\
&= \psi^{(l)} + \nabla\psi^{(l)} \cdot \boldsymbol{\delta}^{(l)} + \frac{1}{2} D^2\psi^{(l)}[\boldsymbol{\delta}^{(l)}, \boldsymbol{\delta}^{(l)}] + \frac{1}{6} D^3\psi^{(l)}[\boldsymbol{\delta}^{(l)}, \boldsymbol{\delta}^{(l)}, \boldsymbol{\delta}^{(l)}] + R^{(l)} \\
&= \psi^{(l)} + (\mathcal{L}\psi)^{(l)} h + \sqrt{2\beta^{-1} h}\, \nabla\psi^{(l)} \cdot \boldsymbol{\eta}^{(l)} + \frac{h}{\beta}\Big(D^2\psi^{(l)}[\boldsymbol{\eta}^{(l)}, \boldsymbol{\eta}^{(l)}] - \Delta\psi^{(l)}\Big) + o(h)\,.
\end{aligned}
$$

Therefore, for $T = nh$,

$$
\begin{aligned}
\widehat{f}_n - \bar{f} &= \frac{1}{n}\sum_{l=0}^{n-1} f(x^{(l)}) - \bar{f} \\
&= \frac{\psi^{(n)} - \psi^{(0)}}{T} - \frac{\sqrt{2\beta^{-1} h}}{T}\sum_{l=0}^{n-1} \nabla\psi^{(l)} \cdot \boldsymbol{\eta}^{(l)} - \frac{h}{\beta T}\sum_{l=0}^{n-1}\Big(D^2\psi^{(l)}[\boldsymbol{\eta}^{(l)}, \boldsymbol{\eta}^{(l)}] - \Delta\psi^{(l)}\Big) + \frac{o(h)}{T}\,.
\end{aligned}
$$

Analysis of Θ-scheme on Σ: new difficulties

$\bar{f} = \int_\Sigma f \, d\mu_1$. Poisson equation $\mathcal{L}\psi = f - \bar{f}$ on Σ.

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   $\hookrightarrow \int_\Sigma \mathcal{L} f \, d\mu_1 = 0$, for test functions $f : \Sigma \to \mathbb{R}$.

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   Equivalently, can we construct a diffusion process (SDE) on Σ, whose invariant measure is μ_1?

2. 1st and 2nd derivatives of Θ are needed

in order to continue the calculation

$$\begin{aligned} &\psi^{(l+1)} \\ =&\psi(x^{(l+1)}) \\ =&(\psi \circ \Theta)\big(x^{(l)} + \boldsymbol{\delta}^{(l)}\big) \\ =&\psi^{(l)} + D(\psi \circ \Theta)^{(l)}[\boldsymbol{\delta}^{(l)}] + \frac{1}{2} D^2(\psi \circ \Theta)^{(l)}[\boldsymbol{\delta}^{(l)}, \boldsymbol{\delta}^{(l)}] + \frac{1}{6} D^3(\psi \circ \Theta)^{(l)}[\boldsymbol{\delta}^{(l)}, \boldsymbol{\delta}^{(l)}, \boldsymbol{\delta}^{(l)}] + R^{(l)} \\ =&\cdots \end{aligned}$$

Analysis of Θ-scheme on Σ: new ingredient 1

Recall $\Psi = \nabla\xi^T a \nabla\xi \in \mathbb{R}^{k\times k}$. Define $P = \mathrm{id} - a\nabla\xi\Psi^{-1}\nabla\xi^T$

$\Longrightarrow aP^T = Pa, \quad P^2 = P\,, \quad P^T\nabla\xi = 0\,.$

Theorem 2

Consider the SDE on $\mathbb{R}^d$

$$dX_s^i = -\,(Pa)_{ij}\frac{\partial U}{\partial x_j}\,ds + \frac{1}{\beta}\frac{\partial (Pa)_{ij}}{\partial x_j}\,ds + \sqrt{2\beta^{-1}}\,P_{j,i}\,dW_s^j\,, \tag{3}$$

for $1 \le i \le d$. *Suppose* $X_0 \in \Sigma$, *then* $X_s \in \Sigma$ *a.s. for* $s \ge 0$. *Furthermore, the unique invariant measure of* X_s *is* μ_1.

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Remark: infinitesimal generator of (3)

$$\mathcal{L} = \frac{e^{\beta U}}{\beta}\frac{\partial}{\partial x_i}\Big(e^{-\beta U}(Pa)_{ij}\frac{\partial}{\partial x_j}\Big)$$

satisfies $\int_\Sigma \mathcal{L}f\,d\mu_1 = 0$, for test functions $f:\Sigma\to\mathbb{R}$.

Analysis of Θ-scheme on Σ: new ingredient 2

Recall $\Theta(x) = \lim_{s\to+\infty} \varphi(x,s)$ is the limit of the flow map

$$\frac{d\varphi(x,s)}{ds} = -\,(a\nabla F)\big(\varphi(x,s)\big)\,, \quad \varphi(x,0) = x, \quad \forall\, x \in \mathbb{R}^d\,,$$

with $F(x) = \frac{1}{2}|\xi(x)|^2 = \frac{1}{2}\sum_{\alpha=1}^{k} \xi_\alpha^2(x)$.

Proposition 2

Let $x \in \Sigma$. For $1 \le i, j \le d$, we have

$$\frac{\partial \Theta_i}{\partial x_j} = P_{ij}\,,$$

$$a_{lr}\frac{\partial^2 \Theta_i}{\partial x_l \partial x_r} = \frac{\partial (Pa)_{il}}{\partial x_l} - P_{il}\frac{\partial a_{lr}}{\partial x_r}\,.$$

Analysis of Θ-scheme on Σ: sketch of proof

Define $\mathcal{L} = \frac{e^{\beta U}}{\beta}\frac{\partial}{\partial x_i}\Big(e^{-\beta U}(Pa)_{ij}\frac{\partial}{\partial x_j}\Big)$. Poisson equation $\mathcal{L}\psi = f - \overline{f}$.

Let $\boldsymbol{\delta}^{(l)} = x^{(l+\frac{1}{2})} - x^{(l)}$, i.e., E-M update,

Θ-scheme $\Longrightarrow \quad x^{(l+1)} = \Theta\big(x^{(l+\frac{1}{2})}\big) = \Theta\big(x^{(l)} + \boldsymbol{\delta}^{(l)}\big)$.

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We can compute

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=&\,\psi^{(l)} + (\mathcal{L}\psi)^{(l)}h + \sqrt{2\beta^{-1}h}\,D\psi^{(l)}[(P\sigma)^{(l)}\boldsymbol{\eta}^{(l)}] \\
&+ \frac{hD\psi^{(l)}}{\beta}\big[D^2\Theta^{(l)}[\sigma^{(l)}\boldsymbol{\eta}^{(l)},\sigma^{(l)}\boldsymbol{\eta}^{(l)}] - a^{(l)} : \nabla^2\Theta^{(l)}\big] \\
&+ \frac{h}{\beta}\Big(D^2\psi^{(l)}[(P\sigma)^{(l)}\boldsymbol{\eta}^{(l)},(P\sigma)^{(l)}\boldsymbol{\eta}^{(l)}] - (Pa)^{(l)} : D^2\psi^{(l)}\Big) + o(h)
\end{aligned}
$$

The proof can be worked out smoothly!

Poincaré inequality

Poincaré inequality

$$\mathrm{Var}_{\mu_1}(f) := \int_\Sigma (f-\bar{f})^2\, d\mu_1 \leq -\frac{1}{K}\int_\Sigma (\mathcal{L}f) f\, d\mu_1 = \frac{1}{K\beta}\int_\Sigma (Pa\nabla f)\cdot \nabla f\, d\mu_1\,, \tag{4}$$

for $\forall\, f:\Sigma\to\mathbb{R}$ s.t. the r.h.s. of (4) is finite. $K>0$ is Poincaré constant. $\mathcal{L} = \frac{e^{\beta U}}{\beta}\frac{\partial}{\partial x_i}\Big(e^{-\beta U}(Pa)_{ij}\frac{\partial}{\partial x_j}\Big)$.

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Corollary 1

Under the same assumptions and further assuming (4) is satisfied, we have

$$\mathbf{E}\big|\widehat{f}_n - \bar{f}\big|^2 \le \frac{2C_1\mathrm{Var}_{\mu_1}(f)}{KT} + C_2\Big(h^2 + \frac{h}{T} + \frac{1}{T^2}\Big)\,,$$

where C_1 is any constant larger than 1, C_2 depends on C_1 but is independent of both h and n.

Outline

- Motivations
- Numerical schemes
- Error analysis of Θ-scheme
- Numerical examples

Example 1

$\xi(x) = \frac{1}{2}\left(\frac{x_1^2}{c^2} + x_2^2 - 1\right), \ x \in \mathbb{R}^2. \quad \Sigma = \left\{(x_1, x_2)^T \mid \frac{x_1^2}{c^2} + x_2^2 = 1\right\}.$
$a = \mathrm{id}$, $c = 3$. $U = 0$. Let $x_1 = c\cos\theta, x_2 = \sin\theta$, where $\theta \in [0, 2\pi]$.
$\Longrightarrow \ d\mu_1 = \frac{1}{Z}d\theta, \quad d\mu_2 = \frac{1}{Z}\left(c^2\sin^2\theta + \cos^2\theta\right)^{\frac{1}{2}} d\theta.$

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Three schemes:

1. Θ-Scheme: $x^{(l+1)} = \Theta(x^{(l)} + \sqrt{2\beta^{-1}h}\,\boldsymbol{\eta}^{(l)})$. $\Theta(x)$ is the limit of the map φ, given by

$$\dot{y}_1(s) = -\frac{1}{c^2}\xi(y(s))\,y_1(s)\,, \quad \dot{y}_2(s) = -\xi(y(s))\,y_2(s)\,, \quad s \geq 0\,.$$

2. Θ^A-scheme: $x^{(l+1)} = \Theta^A(x^{(l)} + \sqrt{2\beta^{-1}h}\,\boldsymbol{\eta}^{(l)})$. The skew-symmetric matrix

$$A = \begin{pmatrix} 0 & 1/2 \\ -1/2 & 0 \end{pmatrix}.$$

$\Theta^A(x)$ is the limit of φ^A, given by

$$\dot{y}_1(s) = -\xi(y(s))\left(\frac{y_1(s)}{c^2} - \frac{y_2(s)}{2}\right), \quad \dot{y}_2(s) = -\xi(y(s))\left(\frac{y_1(s)}{2c^2} + y_2(s)\right), \quad s \geq 0\,.$$

3. Π-scheme: $x^{(l+1)} = \Pi(x^{(l)} + \sqrt{2\beta^{-1}h}\,\boldsymbol{\eta}^{(l)})$.

Example 1

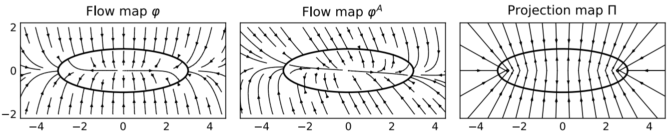

Figure: Streamlines of flow maps φ, φ^A, and the projection Π.

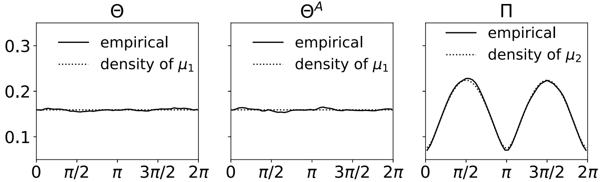

Figure: Probability densities of θ, computed using projections Θ, Θ^A, and Π.

Example 2

Choose $\xi : \mathbb{R}^{11\times 11} \to \mathbb{R}^{66}$, such that the level set Σ is

$$SO(11) = \left\{ M \in \mathbb{R}^{11\times 11} \mid M^T M = \mathrm{id},\ \det(M) = 1 \right\}.$$

$\implies \mu_1 = \mu_2$, and $k = 66$. Choose $f(x) = \mathrm{Tr}(x)$, $n = 10^6$.

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- Θ-scheme:

  $h = 0.022$. $a = \mathrm{id}$. ODE (with $\kappa = 0.5$) is solved until $|\xi(\varphi(x, s))| < 10^{-9}$. Initial ODE step-size $\Delta s = 0.2$. On average 37 Runge-Kutta steps.

  Total time: 2676.9 seconds.

- Metropolis-adjusted method:

  Maximal Newton steps: 10. Proposal length scale: 0.257. Convergence criteria is $|\xi(x)| < 10^{-9}$. Success rate of Newton's method: 67.2%. On average, 5–6 Newton iterations.

  Total time: 7315.9 seconds.

Example 2

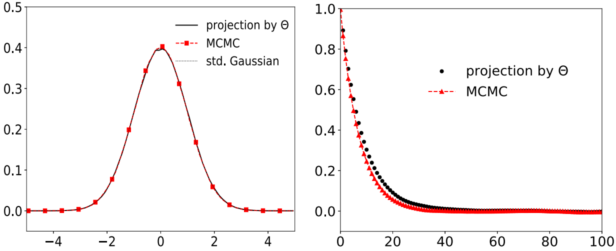

Figure: Left: empirical density plots of Tr(x). Right: autocorrelation functions.

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Thank you !

Preprint:

Ergodic SDEs on submanifolds and related numerical sampling schemes, W.Z., 2018.

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