

Understanding MCMC Dynamics as Flows on the Wasserstein Space

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- 1 Introduction
- 2 Preliminaries
- 3 MCMC Dynamics as Wasserstein Flows
- 4 Simulation as ParVIs
- 5 Experiments

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Introduction

What is known about dynamics-based MCMC:

- There are many instances, e.g. Langevin dynamics (LD) [30], Hamiltonian Monte Carlo (HMC) [12], stochastic gradient HMC (SGHMC) [8], etc.
- LD is recognized as the gradient flow of the KL divergence on the Wasserstein space [18].
 - Then its asymptotic [30] and non-asymptotic [13, 9] behaviors are clear.
 - Then its relation to existing particle-based variational inference methods (ParVIs) is clear [7, 21].

What remains unknown:

- Whether a general MCMC dynamics can be explained as an interpretable flow.

Introduction

Motivation

Explain a general MCMC dynamics as an interpretable flow.

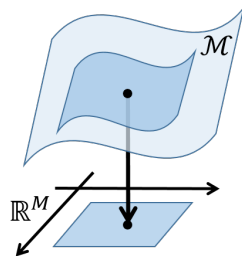
- Then the behavior of general MCMC dynamics is clear.
- Then more MCMC dynamics than LD are connected to the ParVI family: ParVIs with more efficient MCMC dynamics, and MCMCs with more effective ParVI simulation.

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Manifolds

Manifold \mathcal{M} :

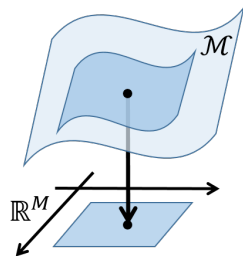
- Locally homeomorphic to an open subset of \mathbb{R}^M .
- We consider manifolds globally homeomorphic to \mathbb{R}^M (global coordinate space).



Manifolds

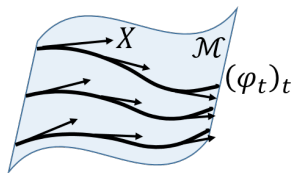
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Flows on \mathcal{M} :

- The set of curves $\{(\varphi_t)_t\}$ s.t. $\frac{d\varphi_t}{dt} = X(\varphi_t)$ given a vector field X .
- We use “vector fields” and “flows” interchangeably.



Manifolds

Riemannian structure on \mathcal{M} :

- An inner product in every tangent space $T_x\mathcal{M}$.
- Coordinate expression:

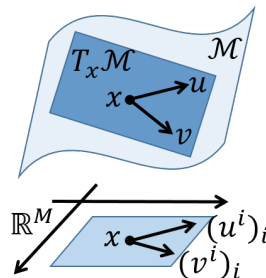
$$\langle u, v \rangle_{T_x\mathcal{M}} = g_{ij}(x)u^i v^j.$$

- Gradient: $\langle \text{grad } f(x), v \rangle_{T_x\mathcal{M}} = v[f] := v^i \partial_i f(x)$,
 \iff steepest ascending direction:

$$\text{grad } f(x) = \max \cdot \operatorname{argmax}_{\|v\|_{T_x\mathcal{M}}=1} \frac{d}{dt} f(\varphi_t).$$

Coordinate expression:

$$(\text{grad } f(x))^i = g^{ij}(x) \partial_j f(x).$$



Manifolds

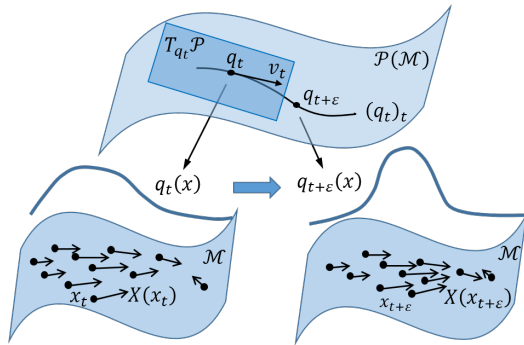
Wasserstein space $\mathcal{P}(\mathcal{M})$:

- Space of distributions on \mathcal{M} (finite variance).
- Tangent vector $v \iff$ vector field X on \mathcal{M} .
- Tangent space at $q \in \mathcal{P}(\mathcal{M})$

$$T_q \mathcal{P}(\mathcal{M}) = \overline{\{\text{grad } f \mid f \in \mathcal{C}_c^\infty(\mathcal{M})\}}^{\mathcal{L}_q^2(\mathcal{M})}$$

is a subspace of the Hilbert space

$$\mathcal{L}_q^2(\mathcal{M}) := \{X \mid \mathbb{E}_{q(x)}[\langle X(x), X(x) \rangle_{T_x \mathcal{M}}] < \infty\}.$$



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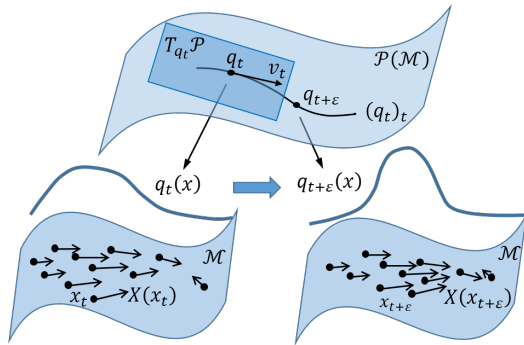
$$\mathcal{L}_q^2(\mathcal{M}) := \{X \mid \mathbb{E}_{q(x)}[\langle X(x), X(x) \rangle_{T_x \mathcal{M}}] < \infty\}.$$

- Riemannian structure:

$T_q \mathcal{P}$ inherits the inner product of \mathcal{L}_q^2 .

- Gradient of $\text{KL}_p(q) := \int_{\mathcal{M}} \log(q/p) \, dq$:

$$\text{grad } \text{KL}_p(q) = \text{grad } \log(q/p), \left(\text{grad } \text{KL}_p(q) \right)^i(x) = g^{ij}(x) \partial_j \log(q(x)/p(x)).$$



LD as Gradient Flow

Equivalent dynamics:

- They produce the same distribution evolution rule.
- X and $\pi_q(X)$ are equivalent, where $\pi_q : \mathcal{L}_q^2 \rightarrow T_q\mathcal{P}$ is the orthogonal projection.

LD as Gradient Flow:

- The Langevin dynamics

$$dx = \nabla \log p(x) dt + \sqrt{2} dB_t(x)$$

is equivalent [7] to the deterministic dynamics:

$$dx = \nabla \log(p(x)/q_t(x)) dt,$$

where q_t is the distribution of x at time t .

It is the gradient flow of KL_p on $\mathcal{P}(\mathcal{M})$ for Euclidean \mathcal{M} !

- The gradient flow interpretation of LD is known earlier from another perspective [18].

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Describe General MCMC Dynamics

The complete recipe [24] (*known knowledge*):

- A general MCMC dynamics on \mathbb{R}^M targeting p can be expressed as the diffusion process:

$$\begin{aligned} dx &= V(x) dt + \sqrt{2D(x)} dB_t(x), \\ V^i(x) &= \frac{1}{p(x)} \partial_j \left(p(x) (D^{ij}(x) + Q^{ij}(x)) \right), \end{aligned} \tag{1}$$

for some positive semi-definite matrix $D_{M \times M}$ (diffusion matrix) and some skew-symmetric matrix $Q_{M \times M}$ (curl matrix).

The First Reformulation

Lemma 1 (Equivalent deterministic MCMC dynamics)

MCMC dynamics Eq. (1) with symmetric D is equivalent to the deterministic dynamics:

$$\begin{aligned} dx &= W_t(x)dt, \\ (W_t)^i(x) &= D^{ij}(x) \partial_j \log(p(x)/q_t(x)) + Q^{ij}(x) \partial_j \log p(x) + \partial_j Q^{ij}(x), \end{aligned} \tag{2}$$

where q_t is the distribution density of x at time t .

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- \implies Barbour's generator [2] $\mathcal{A}f := \frac{d}{dt} \mathbb{E}_{q_t}[f] \Big|_{q_t=\delta_x} = \frac{1}{p} \partial_j [p (D^{ij} + Q^{ij}) (\partial_i f)]$ (c.f. [17]).

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How to interpret $W_t(x)$?

Interpret MCMC Dynamics

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1 $D^{ij}(x) \partial_j \log(p(x)/q_t(x))$ seems like a gradient flow on $\mathcal{P}(\mathcal{M})$.

- Euclidean \mathcal{M} only allows $D = I$.

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 - Hilbert \mathcal{M} only allows constant and non-singular D .
 - Riemannian \mathcal{M} allows position-dependent $D(x)$, but $D(x)$ needs to be non-singular.
 - What kind of \mathcal{M} allows position-dependent and positive *semi*-definite $D(x)$?

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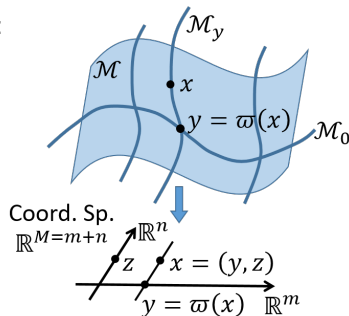
1 $D^{ij}(x) \partial_j \log(p(x)/q_t(x))$ seems like a gradient flow on $\mathcal{P}(\mathcal{M})$.

• Fiber Bundle \mathcal{M} (of dim. $M = m + n$) (*known knowledge*):

- \mathcal{M} is locally $\mathcal{M}_0 \times \mathcal{F}$ (\mathcal{M}_0 of dim. m , \mathcal{F} of dim. n) [27] in terms of a projection ϖ :

$$\varpi : \mathcal{M} \rightarrow \mathcal{M}_0 \overset{\text{locally}}{\iff} \mathcal{M}_0 \times \mathcal{F} \rightarrow \mathcal{M}_0.$$

- The *fiber* through $y \in \mathcal{M}_0$:
 $\mathcal{M}_y := \varpi^{-1}(y)$ (diffeom. to \mathcal{F}).
- Coordinate decomposition: $x = (y, z)$,
 $y \in \mathbb{R}^m$: coord. of \mathcal{M}_0 ; $z \in \mathbb{R}^n$: coord. of \mathcal{M}_y .



Interpret MCMC Dynamics

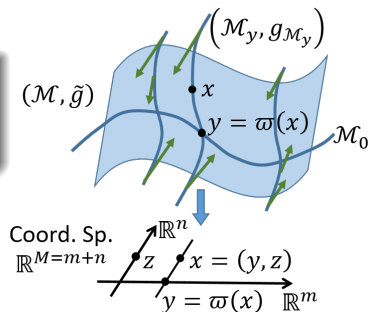
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- Fiber-Riemannian manifold \mathcal{M} :

Definition 3 (Fiber-Riemannian manifold)

\mathcal{M} is a *fiber-Riemannian manifold* if it is a fiber bundle and there is a Riemannian structure $g_{\mathcal{M}_y}$ on each *fiber* \mathcal{M}_y .



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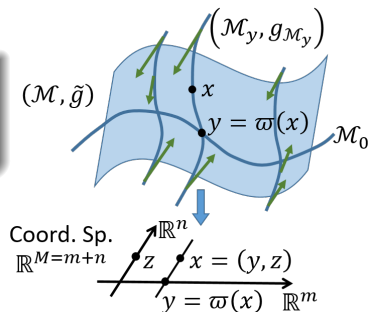
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- **Gradient** on fiber \mathcal{M}_y :

$$(\text{grad}_{\mathcal{M}_y} f(y, z))^a = (g_{\mathcal{M}_y}(z))^{ab} \partial_{z^b} f(y, z),$$

$$1 \leq a, b \leq n.$$
- Define *fiber-gradient* on \mathcal{M} by taking union over y :

$$(\text{grad}_{\text{fib}} f(x))_{\mathcal{M}} := (0_m, (\text{grad}_{\mathcal{M}_{\varpi(x)}} f(\varpi(x), z))_n).$$



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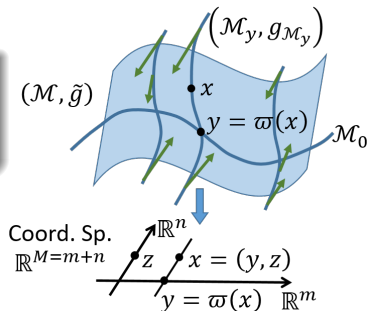
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• Alternatively, the **fiber-gradient** on \mathcal{M} is:

$$\begin{aligned} (\text{grad}_{\text{fb}} f(x))^i &= \tilde{g}^{ij}(x) \partial_j f(x), \quad 1 \leq i, j \leq M, \\ (\tilde{g}^{ij}(x))_{M \times M} &:= \begin{pmatrix} 0_{m \times m} & 0_{m \times n} \\ 0_{n \times m} & ((g_{\mathcal{M}_{\varpi(x)}}(z))^{ab})_{n \times n} \end{pmatrix}. \end{aligned} \quad (3)$$

We use \tilde{g} to denote the fiber-Riemannian structure.



Interpret MCMC Dynamics

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1 $D^{ij}(x) \partial_j \log(p(x)/q_t(x))$ seems like a gradient flow on $\mathcal{P}(\mathcal{M})$.

• Structures on $\mathcal{P}(\mathcal{M})$ with fiber-Riemannian \mathcal{M} .

• Hard to decompose $\mathcal{P}(\mathcal{M})$.

• Consider $\tilde{\mathcal{P}}(\mathcal{M}) := \{q(z|y) \in \mathcal{P}(\mathcal{M}_y) \mid y \in \mathcal{M}_0\} \xLeftrightarrow{\text{locally}} \mathcal{M}_0 \times \mathcal{P}(\mathcal{M}_y)$: fiber-Riemannian!

• On $\mathcal{P}(\mathcal{M}_y)$,

$$\begin{aligned} (\text{grad}_{\text{KL}_{p(\cdot|y)}}(q(\cdot|y))(z))^a &= (g_{\mathcal{M}_y}(z))^{ab} \partial_{z^b} \log \frac{q(z|y)}{p(z|y)} \\ &= (g_{\mathcal{M}_y}(z))^{ab} \partial_{z^b} \log \frac{q(y, z)}{p(y, z)}, 1 \leq a, b \leq n. \end{aligned}$$

• Taking union over $y \in \mathcal{M}_0$, the **fiber-gradient** on $\tilde{\mathcal{P}}(\mathcal{M})$ is:

$$\begin{aligned} (\text{grad}_{\text{fib}} \text{KL}_p(q)(x))_M &= \left(0_m, ((g_{\mathcal{M}_{\varpi(x)}}(z))^{ab} \partial_{z^b} \log (q(x)/p(x)))_n \right) \\ &= (\tilde{g}^{ij}(x) \partial_j \log (q(x)/p(x)))_M. \end{aligned}$$

Project to make a tangent vector on $\mathcal{P}(\mathcal{M})$: $\pi_q(\text{grad}_{\text{fib}} \text{KL}_p(q)) \in T_q \mathcal{P}(\mathcal{M})$.

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Assumption 4 (Regular MCMC dynamics (1/2))

(a) $D = C$ or $D = 0$ or $D = \begin{pmatrix} 0 & 0 \\ 0 & C \end{pmatrix}$, for a symmetric positive definite $C(x)$.

(b) ...

- Satisfied by existing MCMC instances.
- Could be relaxed by coordinate transformation.

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(b) ...

- Satisfied by existing MCMC instances.
- Could be relaxed by coordinate transformation.
- $D^{ij} \partial_j \log(p/q_t)$ is the fiber-gradient with fiber-Riemannian (\mathcal{M}, \tilde{g}) where $(\tilde{g}^{ij}) = D$.

Interpret MCMC Dynamics

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2 $Q^{ij}(x) \partial_j \log p(x) + \partial_j Q^{ij}(x)$ makes a Hamiltonian flow.

- The common Hamiltonian flow: $\mathcal{M} = \mathbb{R}^{2\ell}$, $Q = \begin{pmatrix} 0 & I_\ell \\ -I_\ell & 0 \end{pmatrix}$.

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- Symplectic manifold [10, 25]: \mathcal{M} even-dim., Q non-singular.

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- Symplectic manifold [10, 25]: \mathcal{M} even-dim., Q non-singular.
- What kind of structure can be more general, while being Hamiltonian (conserves a certain function)?

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- Poisson manifold \mathcal{M} [14] (*known knowledge*):

- A Poisson structure on \mathcal{M} can be represented by a *bivector field* β , whose coordinate expression $(\beta^{ij}(x))$ is *skew-symmetric* and satisfies:

$$\beta^{il} \partial_l \beta^{jk} + \beta^{jl} \partial_l \beta^{ki} + \beta^{kl} \partial_l \beta^{ij} = 0, \forall i, j, k. \quad (4)$$

- A Poisson structure defines a *Hamiltonian flow* X_f given a smooth function f :

$$(X_f(x))^i = \beta^{ij}(x) \partial_j f(x).$$

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- Poisson structure on $\mathcal{P}(\mathcal{M})$ [23, 1, 15] (*known knowledge*):
 - The Hamiltonian flow of a function F on $\mathcal{P}(\mathcal{M})$ is

$$\mathcal{X}_F(q) = \pi_q(X_f),$$

where the function f on \mathcal{M} relates to F by $\text{grad}_q \mathbb{E}_q[f] = \text{grad}_q F(q)$.

- The Hamiltonian flow \mathcal{X}_F conserves F : $\frac{d}{dt} F(q_t) = 0$.

Interpret MCMC Dynamics

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- Poisson structure on $\mathcal{P}(\mathcal{M})$ (new):

Lemma 2 (Hamiltonian flow of KL on $\mathcal{P}(\mathcal{M})$)

The Hamiltonian flow of KL_p on $\mathcal{P}(\mathcal{M})$ is

$$\mathcal{X}_{\text{KL}_p}(q) = \pi_q(X_{\log(q/p)}), \text{ where } (X_{\log(q/p)}(x))^i = \beta^{ij}(x) \partial_j \log(q(x)/p(x)).$$

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2 $Q^{ij}(x) \partial_j \log p(x) + \partial_j Q^{ij}(x)$ makes a Hamiltonian flow.

- $-(X_{\log(q/p)}(x))^i = \beta^{ij}(x) \partial_j \log p(x) - \beta^{ij}(x) \partial_j \log q(x).$

Interpret MCMC Dynamics

$$(W_t)^i(x) = D^{ij}(x) \partial_j \log(p(x)/q_t(x)) + Q^{ij}(x) \partial_j \log p(x) + \partial_j Q^{ij}(x).$$

2 $Q^{ij}(x) \partial_j \log p(x) + \partial_j Q^{ij}(x)$ makes a Hamiltonian flow.

- $-(X_{\log(q/p)}(x))^i = \beta^{ij}(x) \partial_j \log p(x) - \beta^{ij}(x) \partial_j \log q(x).$

Assumption 4 (Regular MCMC dynamics (2/2))

(a) $D = C$ or $D = 0$ or $D = \begin{pmatrix} 0 & 0 \\ 0 & C \end{pmatrix}$, for a symmetric positive definite $C(x)$.

(b) $Q(x)$ satisfies Eq. (4): $Q^{il} \partial_l Q^{jk} + Q^{jl} \partial_l Q^{ki} + Q^{kl} \partial_l Q^{ij} = 0, \forall i, j, k.$

- Satisfied by MCMCs except for SGNHT-related methods [11, 34].
- Required to match Poisson structure; unnecessary for conservation of Hamiltonian.

Interpret MCMC Dynamics

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$$Q^{ij} \partial_j \log p + \partial_j Q^{ij} \Leftrightarrow Q^{ij} \partial_j \log p - Q^{ij} \partial_j \log q? \text{ Yes!}$$

Interpret MCMC Dynamics: Main Theorem

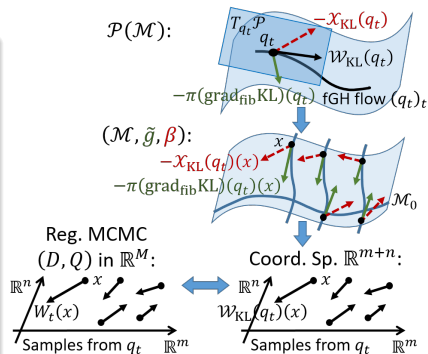
Theorem 5 (Equivalence between regular MCMC dynamics on \mathbb{R}^M and fGH flows on $\mathcal{P}(\mathcal{M})$.)

We call $(\mathcal{M}, \tilde{g}, \beta)$ a fiber-Riemannian Poisson (fRP) manifold, and define the fiber-gradient Hamiltonian (fGH) flow on $\mathcal{P}(\mathcal{M})$ as

$$\begin{aligned} \mathcal{W}_{\text{KL}_p} &:= -\pi(\text{grad}_{\text{fib}} \text{KL}_p) - \mathcal{X}_{\text{KL}_p}, \\ (\mathcal{W}_{\text{KL}_p}(q))^i &= \pi_q((\tilde{g}^{ij} + \beta^{ij}) \partial_j \log(p/q)). \end{aligned} \quad (5)$$

Then:

Regular MCMC dynamics \iff fGH flow with fRP \mathcal{M} ,
 $(D, Q) \iff (\tilde{g}, \beta)$.



Interpret MCMC Dynamics: Case Study

Type 1: D is non-singular ($m = 0$ in Eq. (3)).

- \mathcal{M}_0 degenerates, \mathcal{M} is the unique fiber.
- \mathcal{M} is Riemannian, fiber gradient \implies gradient.
- The fGH flow: $\mathcal{W}_{\text{KL}_p} = -\pi(\text{grad } \text{KL}_p) - \mathcal{X}_{\text{KL}_p}$,
 - $-\pi(\text{grad } \text{KL}_p)$: minimizes KL_p steeply on $\mathcal{P}(\mathcal{M})$.
 - $-\mathcal{X}_{\text{KL}_p}$: conserves KL_p on $\mathcal{P}(\mathcal{M})$ and helps mixing/exploration.
- Converges to p uniquely (c.f. [24]).
- Robust to SG (c.f. [31, 32]).

Instances:

- LD [29] / SGLD [33]: $Q = 0$, \mathcal{M} is Euclidean.
- RLD [16] / SGRLD [28]: $Q = 0$, \mathcal{M} is the manifold under consideration.

Interpret MCMC Dynamics: Case Study

Type 2: $D = 0$ ($n = 0$ in Eq. (3)).

- $\mathcal{M}_0 = \mathcal{M}$, fibers degenerate.
- \mathcal{M} has no (fiber-)Riemannian structures.
- The fGH flow: $\mathcal{W}_{\text{KL}_p} = -\mathcal{X}_{\text{KL}_p}$ conserves KL_p on $\mathcal{P}(\mathcal{M})$ and helps mixing/exploration.
- Fragile against SG: no stabilizing forces (i.e. (fiber-)gradient flows) (c.f. [8, 3]).
- Hard to extend to ParVIs.

Instances (ℓ -dim. sample space \mathcal{S}):

- HMC [12, 26, 4]: $\mathcal{S} = \mathbb{R}^\ell$; \mathcal{M} is $\mathbb{R}^{2\ell}$.
- HMC relies on *geometric ergodicity* for convergence [22, 4].
- RHMC [16] / LagrMC [19] / GMC [5]: manifold \mathcal{S} ; \mathcal{M} is $T^*\mathcal{S}$.

Interpret MCMC Dynamics: Case Study

Type 3: $D \neq 0$ and D is singular ($m, n \geq 1$ in Eq. (3)).

- Non-degenerate \mathcal{M}_0 and \mathcal{M}_y .
- \mathcal{M} is a non-trivial fRP manifold.
- The fGH flow: $\mathcal{W}_{\text{KL}_p} := -\pi(\text{grad}_{\text{fib}} \text{KL}_p) - \mathcal{X}_{\text{KL}_p}$,
 - $-\pi(\text{grad}_{\text{fib}} \text{KL}_p)$: minimizes $\text{KL}_{p(\cdot|y)}(q(\cdot|y))$ steeply on each fiber $\mathcal{P}(\mathcal{M}_y)$.
 - $-\mathcal{X}_{\text{KL}_p}$: conserves KL_p on $\mathcal{P}(\mathcal{M})$ and helps mixing/exploration.
- Robust to SG (SG appears on each fiber) (c.f. [8, 6]).

Instances (ℓ -dim. sample space \mathcal{S}):

- SGHMC [8] ($\mathcal{S} = \mathbb{R}^\ell$) and SGRHMC [24] / SGGMC [20] (manifold \mathcal{S}):
 \mathcal{M}_0 is \mathcal{S} and \mathcal{M}_θ is $T_\theta^* \mathcal{S}$.
- SGNHT [11] ($\mathcal{S} = \mathbb{R}^\ell$) and gSGNHT [20] (manifold \mathcal{S}):
 \mathcal{M}_0 is \mathcal{S} and \mathcal{M}_θ is $\mathbb{R} \times T_\theta^* \mathcal{S}$.

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- 2 Preliminaries
- 3 MCMC Dynamics as Wasserstein Flows
- 4 Simulation as ParVIs**
- 5 Experiments

ParVI Simulation for SGHMC

Simulate the deterministic dynamics of SGHMC:

$$\text{By Lemma 1 (Eq. (2))}: \begin{cases} \frac{d\theta}{dt} = \Sigma^{-1}r, \\ \frac{dr}{dt} = \nabla_{\theta} \log p(\theta) - C\Sigma^{-1}r - C\nabla_r \log q(r). \end{cases}$$

$$\text{By Theorem 5 (Eq. (5))}: \begin{cases} \frac{d\theta}{dt} = \Sigma^{-1}r + \nabla_r \log q(r), \\ \frac{dr}{dt} = \nabla_{\theta} \log p(\theta) - C\Sigma^{-1}r - C\nabla_r \log q(r) - \nabla_{\theta} \log q(\theta). \end{cases}$$

- Problem: estimate $\nabla \log q$ with finite particles.

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- Problem: estimate $\nabla \log q$ with finite particles.
- Solution: use ParVI techniques [21], e.g. Blob [7]:

$$-\nabla_r \log q(r^{(i)}) \approx -\frac{\sum_k \nabla_{r^{(i)}} K_r^{(i,k)}}{\sum_j K_r^{(i,j)}} - \sum_k \frac{\nabla_{r^{(i)}} K_r^{(i,k)}}{\sum_j K_r^{(j,k)}},$$

where $K_r^{(i,j)} := K_r(r^{(i)}, r^{(j)})$.

ParVI Simulation for SGHMC

Simulate the deterministic dynamics of SGHMC:

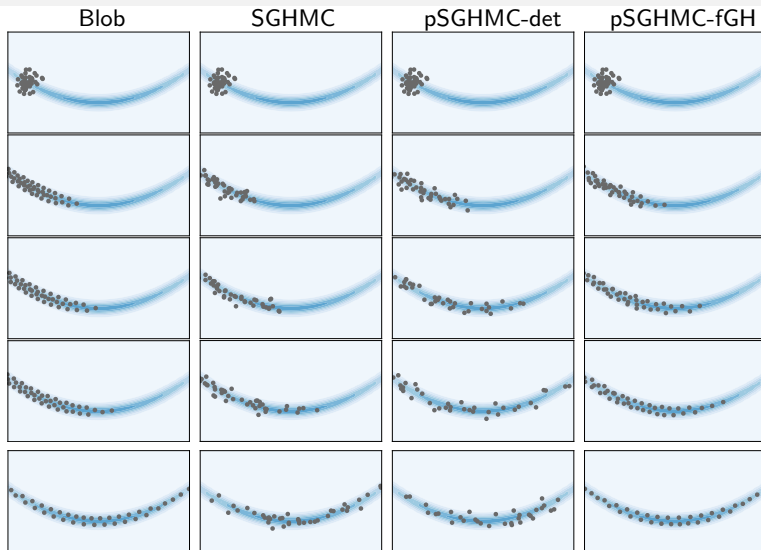
$$\begin{aligned} \text{pSGHMC-det: } & \begin{cases} \frac{\Delta \theta^{(i)}}{\varepsilon} = \Sigma^{-1} r^{(i)}, \\ \frac{\Delta r^{(i)}}{\varepsilon} = \nabla_{\theta} \log p(\theta^{(i)}) - C \Sigma^{-1} r^{(i)} - C \left(\frac{\sum_k \nabla_{r^{(i)}} K_r^{(i,k)}}{\sum_j K_r^{(i,j)}} + \sum_k \frac{\nabla_{r^{(i)}} K_r^{(i,k)}}{\sum_j K_r^{(j,k)}} \right). \end{cases} \\ \text{pSGHMC-fGH: } & \begin{cases} \frac{\Delta \theta^{(i)}}{\varepsilon} = \Sigma^{-1} r^{(i)} + \frac{\sum_k \nabla_{r^{(i)}} K_r^{(i,k)}}{\sum_j K_r^{(i,j)}} + \sum_k \frac{\nabla_{r^{(i)}} K_r^{(i,k)}}{\sum_j K_r^{(j,k)}}, \\ \frac{\Delta r^{(i)}}{\varepsilon} = \nabla_{\theta} \log p(\theta^{(i)}) - \left(\frac{\sum_k \nabla_{\theta^{(i)}} K_{\theta}^{(i,k)}}{\sum_j K_{\theta}^{(i,j)}} + \sum_k \frac{\nabla_{\theta^{(i)}} K_{\theta}^{(i,k)}}{\sum_j K_{\theta}^{(j,k)}} \right) \\ \quad - C \Sigma^{-1} r^{(i)} - C \left(\frac{\sum_k \nabla_{r^{(i)}} K_r^{(i,k)}}{\sum_j K_r^{(i,j)}} + \sum_k \frac{\nabla_{r^{(i)}} K_r^{(i,k)}}{\sum_j K_r^{(j,k)}} \right). \end{cases} \end{aligned}$$

Advantages:

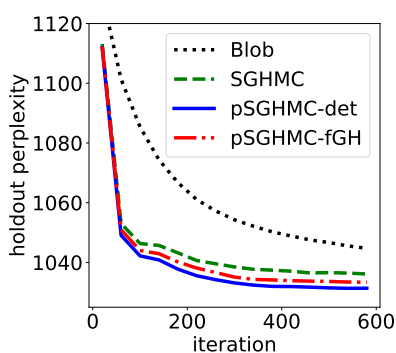
- Over SGHMC: particle-efficiency, ParVI techniques like HE [21].
- Over ParVIs: more efficient dynamics over LD.

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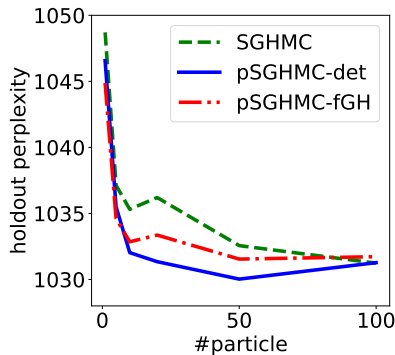
Synthetic Experiment



Latent Dirichlet Allocation (LDA)



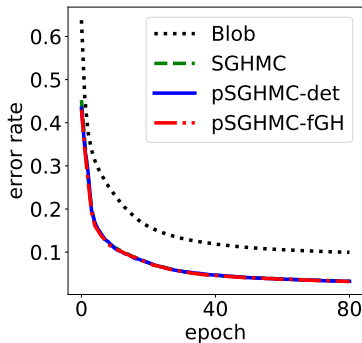
(a) Learning curve (20 ptcls)



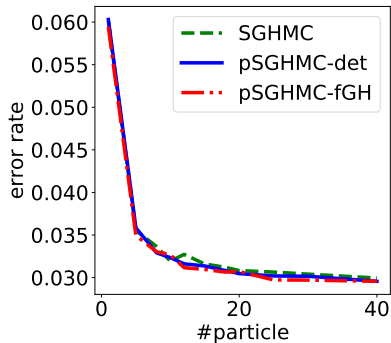
(b) Particle efficiency (iter 600)

Figure: Performance on LDA with the ICML data set.

Bayesian Neural Networks (BNNs)



(a) Learning curve (10 ptcls)



(b) Particle efficiency (epoch 80)

Figure: Performance on BNN with MNIST data set.

Thank you!



Luigi Ambrosio and Wilfrid Gangbo.

Hamiltonian odes in the wasserstein space of probability measures.

Communications on Pure and Applied Mathematics: A Journal Issued by the Courant Institute of Mathematical Sciences, 61(1):18–53, 2008.



Andrew D Barbour.

Stein's method for diffusion approximations.

Probability theory and related fields, 84(3):297–322, 1990.



Michael Betancourt.

The fundamental incompatibility of scalable hamiltonian monte carlo and naive data subsampling.

In *International Conference on Machine Learning*, pages 533–540, 2015.



Michael Betancourt.

A conceptual introduction to hamiltonian monte carlo.

arXiv preprint arXiv:1701.02434, 2017.



Simon Byrne and Mark Girolami.

Geodesic monte carlo on embedded manifolds.

Scandinavian Journal of Statistics, 40(4):825–845, 2013.



Changyou Chen, Nan Ding, and Lawrence Carin.

On the convergence of stochastic gradient mcmc algorithms with high-order integrators.

In Advances in Neural Information Processing Systems, pages 2278–2286, 2015.



Changyou Chen, Ruiyi Zhang, Wenlin Wang, Bai Li, and Liqun Chen.

A unified particle-optimization framework for scalable bayesian sampling.

arXiv preprint arXiv:1805.11659, 2018.



Tianqi Chen, Emily Fox, and Carlos Guestrin.

Stochastic gradient hamiltonian monte carlo.

In Proceedings of the 31st International Conference on Machine Learning (ICML-14), pages 1683–1691, 2014.



Xiang Cheng and Peter Bartlett.

Convergence of langevin mcmc in kl-divergence.

arXiv preprint arXiv:1705.09048, 2017.



Ana Cannas Da Silva.

Lectures on symplectic geometry, volume 3575.

Springer, 2001.

-  Nan Ding, Youhan Fang, Ryan Babbush, Changyou Chen, Robert D Skeel, and Hartmut Neven.
Bayesian sampling using stochastic gradient thermostats.
In Advances in neural information processing systems, pages 3203–3211, 2014.
-  Simon Duane, Anthony D Kennedy, Brian J Pendleton, and Duncan Roweth.
Hybrid monte carlo.
Physics Letters B, 195(2):216–222, 1987.
-  Alain Durmus and Eric Moulines.
High-dimensional bayesian inference via the unadjusted langevin algorithm.
arXiv preprint arXiv:1605.01559, 2016.
-  Rui Loja Fernandes and Ioan Marcut.
Lectures on Poisson Geometry.
Springer, 2014.
-  Wilfrid Gangbo, Hwa Kil Kim, and Tommaso Pacini.
Differential forms on Wasserstein space and infinite-dimensional Hamiltonian systems.
American Mathematical Soc., 2010.
-  Mark Girolami and Ben Calderhead.

Riemann manifold langevin and hamiltonian monte carlo methods.

Journal of the Royal Statistical Society: Series B (Statistical Methodology), 73(2):123–214, 2011.



Jackson Gorham, Andrew B Duncan, Sebastian J Vollmer, and Lester Mackey.

Measuring sample quality with diffusions.

arXiv preprint arXiv:1611.06972, 2016.



Richard Jordan, David Kinderlehrer, and Felix Otto.

The variational formulation of the fokker–planck equation.

SIAM journal on mathematical analysis, 29(1):1–17, 1998.



Shiwei Lan, Vasileios Stathopoulos, Babak Shahbaba, and Mark Girolami.

Markov chain monte carlo from lagrangian dynamics.

Journal of Computational and Graphical Statistics, 24(2):357–378, 2015.



Chang Liu, Jun Zhu, and Yang Song.

Stochastic gradient geodesic mcmc methods.

In *Advances In Neural Information Processing Systems*, pages 3009–3017, 2016.



Chang Liu, Jingwei Zhuo, Pengyu Cheng, Ruiyi Zhang, Jun Zhu, and Lawrence Carin.

Accelerated first-order methods on the wasserstein space for bayesian inference.

arXiv preprint arXiv:1807.01750, 2018.



Samuel Livingstone, Michael Betancourt, Simon Byrne, and Mark Girolami.

On the geometric ergodicity of hamiltonian monte carlo.

arXiv preprint arXiv:1601.08057, 2016.



John Lott.

Some geometric calculations on wasserstein space.

Communications in Mathematical Physics, 277(2):423–437, 2008.



Yi-An Ma, Tianqi Chen, and Emily Fox.

A complete recipe for stochastic gradient mcmc.

In *Advances in Neural Information Processing Systems*, pages 2917–2925, 2015.



Jerrold E Marsden and Tudor S Ratiu.

Introduction to mechanics and symmetry: a basic exposition of classical mechanical systems, volume 17.

Springer Science & Business Media, 2013.



Radford M Neal et al.

Mcmc using hamiltonian dynamics.

Handbook of Markov Chain Monte Carlo, 2(11), 2011.



Liviu I Nicolaescu.

Lectures on the Geometry of Manifolds.

World Scientific, 2007.



Sam Patterson and Yee Whye Teh.

Stochastic gradient riemannian langevin dynamics on the probability simplex.

In Advances in Neural Information Processing Systems, pages 3102–3110, 2013.



Gareth O Roberts and Osnat Stramer.

Langevin diffusions and metropolis-hastings algorithms.

Methodology and computing in applied probability, 4(4):337–357, 2002.



Gareth O Roberts, Richard L Tweedie, et al.

Exponential convergence of langevin distributions and their discrete approximations.

Bernoulli, 2(4):341–363, 1996.



Issei Sato and Hiroshi Nakagawa.

Approximation analysis of stochastic gradient langevin dynamics by using fokker-planck equation and ito process.

In International Conference on Machine Learning, pages 982–990, 2014.



Yee Whye Teh, Alexandre H Thiery, and Sebastian J Vollmer.

Consistency and fluctuations for stochastic gradient langevin dynamics.

The Journal of Machine Learning Research, 17(1):193–225, 2016.



Max Welling and Yee W Teh.

Bayesian learning via stochastic gradient langevin dynamics.

In *Proceedings of the 28th International Conference on Machine Learning (ICML-11)*, pages 681–688, 2011.



Yizhe Zhang, Changyou Chen, Zhe Gan, Ricardo Henao, and Lawrence Carin.

Stochastic gradient monomial gamma sampler.

arXiv preprint arXiv:1706.01498, 2017.