Sampling Methods: From MCMC to Generative Modeling
Part II: Gradient flows and Langevin Monte Carlo

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Outline

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About this part

We view the Sampling problem as an Optimization problem over the space of probability distributions.

Objective

- Leverage the powerful geometry of optimal transport on the space of probability distributions and in particular Wasserstein gradient flows
- Exploit the analogy between Euclidean gradient flows and Wasserstein gradient flows to design and analyze sampling algorithms

Structure of this tutorial

1. Motivation for Sampling, Sampling as Optimization and high-level presentation of the ideas
2. Review of Euclidean Gradient Flows (GF) on $\mathbb{R}^d$ and their properties, rates of convergence for discretized GF (=optimization algorithms)
3. Introduction of Wasserstein Gradient Flows and analogies with $\mathbb{R}^d$
4. Illustrations with sampling algorithms as discretizations of Wasserstein GF: rates on Langevin Monte Carlo and Stein Variational Gradient Descent, quick tour of closely related algorithms.

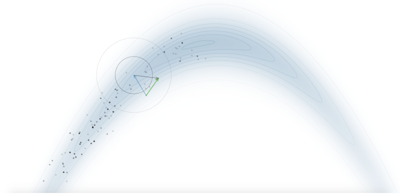
Outline

(Some, Non parametric) Sampling methods

(1) Markov Chain Monte Carlo (MCMC) methods: generate a Markov chain in $\mathbb{R}^d$ whose law converges to $\pi \propto \exp(-V)$

Example: Langevin Monte Carlo (LMC) [Roberts and Tweedie, 1996]

$$x_{m+1} = x_m - \gamma \nabla V(x_m) + \sqrt{2\gamma}\eta_m, \quad \eta_m \sim \mathcal{N}(0, \mathrm{Id}).$$

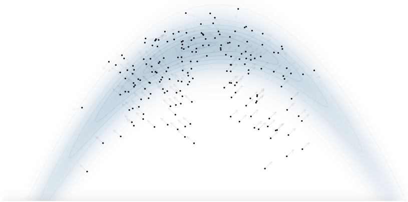


Picture from `https://chi-feng.github.io/mcmc-demo/app.html`.

(2) Interacting particle systems, whose empirical measure at stationarity approximates $\pi \propto \exp(-V)$

Example: Stein Variational Gradient Descent (SVGD) [Liu and Wang, 2016]

$$x_{m+1}^i = x_m^i - \frac{\gamma}{N}\sum_{j=1}^{N} \nabla V(x_m^j) k(x_m^i, x_m^j) - \nabla_2 k(x_m^i, x_m^j), \quad i = 1, \dots, N.$$



Picture from `https://chi-feng.github.io/mcmc-demo/app.html`.

Sampling as minimization of the KL

The Kullback-Leibler (KL) divergence between $\mu, \pi \in \mathcal{P}(\mathbb{R}^d)$ is:

$$\mathrm{KL}(\mu|\pi) = \begin{cases} \int_{\mathbb{R}^d} \log\left(\frac{\mu}{\pi}(x)\right) d\mu(x) & \text{if } \mu \ll \pi \\ +\infty & \text{else.} \end{cases}$$

Note that

$$\pi = \operatorname*{arg\,min}_{\mu \in \mathcal{P}(\mathbb{R}^d)} \mathrm{KL}(\mu|\pi).$$

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Note that

$$\pi = \arg\min_{\mu \in \mathcal{P}(\mathbb{R}^d)} \mathrm{KL}(\mu|\pi).$$

The KL as an objective is convenient since it **does not depend on the normalization constant Z!**

Recall that writing $\pi(x) = e^{-V(x)}/Z$ we have:

$$\mathrm{KL}(\mu|\pi) = \int_{\mathbb{R}^d} \log\left(\frac{\mu}{e^{-V}}(x)\right) d\mu(x) + \log(Z).$$

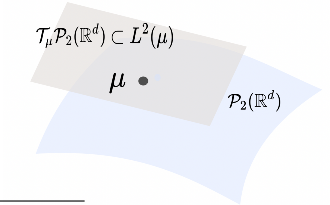
Sampling as optimization over $\mathcal{P}_2(\mathbb{R}^d)$

Assume $\pi \in \mathcal{P}_2(\mathbb{R}^d) = \{\mu \in \mathcal{P}(\mathbb{R}^d), \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) < \infty\}$.

Sampling can be recast as optimization over $\mathcal{P}_2(\mathbb{R}^d)$:

$$\min_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \mathcal{F}(\mu), \quad \mathcal{F}(\mu) := \mathrm{KL}(\mu|\pi).$$

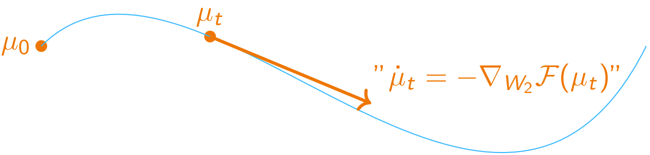
Equipped with the Wasserstein-2 (W_2) distance from optimal transport[1], the metric space $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ has a convenient **Riemannian structure** [Otto and Villani, 2000].



[1] $W_2^2(\mu, \nu) = \inf_{s \text{ coupling of } \mu,\nu} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 ds(x, y)$.

Starting from some μ_0, one can then consider the **Wasserstein gradient flow** of $\mathcal{F} = \mathrm{KL}(\cdot|\pi)$ over $\mathcal{P}_2(\mathbb{R}^d)$, **i.e. path of distributions** $(\mu_t)_{t\geq 0}$ **decreasing** $\mathcal{F}$, to transport μ_0 to π.

We will see that these paths $(\mu_t)_{t\geq 0}$ obey PDE (Partial Differential Equations)



which themselves rule the dynamics of particles $(x_t)_{t\geq 0}$ in $\mathbb{R}^d$

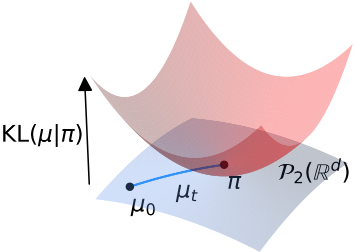
$$dx_t = v(x_t, \mu_t)dt + \sigma(x_t, \mu_t)db_t, \quad x_t \sim \mu_t, \ (b_t)_{t\geq 0} \text{ Brownian motion.}$$

Discretizing these dynamics $(x_t)_{t\geq 0}$ **yields sampling algorithms.**

Recall that $\pi(x) \propto \exp(-V(x)), \quad V(x) = \underbrace{\sum_{i=1}^{p} \|y_i - g(w_i, x)\|^2}_{\text{loss of the model } g(\cdot, x)} + \frac{\|x\|^2}{2}.$

We will see that in the Wasserstein geometry, the $\mathrm{KL}(\cdot|\pi)$ objective inherits convexity properties of V, i.e.:

- if V is convex (e.g. $g(w,x) = \langle w, x\rangle$ linear), π is "log-concave" and "sampling is easy"



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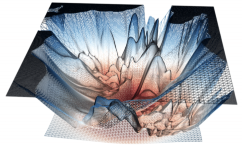
We will see that in the Wasserstein geometry, the $\mathrm{KL}(\cdot|\pi)$ objective inherits convexity properties of V, i.e.:

- if V is nonconvex (e.g. $g(w,x)$ is a neural network), π is "non log-concave" and "sampling is hard"



A highly nonconvex loss surface, as is common in deep neural nets. From https://www.telesens.co/2019/01/16/neural-network-loss-visualization.

Sampling as optimization: how it started

Since the seminal paper of [Jordan et al., 1998], it is known that the distributions $(\mu_t)_{t\geq 0}$ of Langevin dynamics in $\mathbb{R}^d$

$$dx_t = -\nabla V(x_t)dt + \sqrt{2}db_t,$$

where $(b_t)_{t\geq 0}$ is the Brownian motion in $\mathbb{R}^d$, follow a Wasserstein gradient flow of the Kullback-Leibler divergence.

Recently, this optimization point of view has been used to derive rates of convergence for variants of the Langevin Monte Carlo algorithm [Wibisono, 2018][Durmus et al., 2019][Bernton, 2018]

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Gradient

Let $V : \mathbb{R}^d \to \mathbb{R}$ differentiable. What is the gradient of V?

Definition: If a Taylor expansion of V yields:

$$V(x + \varepsilon h) = V(x) + \varepsilon \langle g_x, h \rangle + o(\varepsilon),$$

where $\langle \cdot, \cdot \rangle$ is some inner product, then g_x is the gradient of V at x under the inner product $\langle \cdot, \cdot \rangle$.

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- If $\langle\cdot,\cdot\rangle_{\mathbb{R}^d}$ is the Euclidean inner product then $g_x = \nabla V(x)$.
- If $\langle\cdot,\cdot\rangle_P$ is the inner product induced by a positive definite matrix P (i.e. $\langle x, y\rangle_P = \langle Px, y\rangle_{\mathbb{R}^d}$) then $g_x = P^{-1}\nabla V(x)$.

Euclidean Gradient Flow

Problem:

$$\min_{x \in \mathbb{R}^d} V(x),$$

where $V : \mathbb{R}^d \to \mathbb{R}$ s.t. ∇V is L-Lipschitz (V is L-smooth).

Using Cauchy-Lipschitz, consider

$$\boxed{\dot{x}_t = -\nabla V(x_t), \quad t \geq 0,}$$

where we denote $x_t = x(t)$, $\dot{x}_t = \frac{dx_t}{dt}$.

Gradient flow of V = the solution of this Ordinary Differential Equation (ODE) for any initial data $x(0)$.

Descent property of gradient flows

Using (1) the chain rule and (2) $\dot{x}_t = -\nabla V(x_t)$,

$$\frac{dV(x_t)}{dt} \overset{(1)}{=} \langle \dot{x}_t, \nabla V(x_t) \rangle \overset{(2)}{=} -\|\nabla V(x_t)\|^2 \leq 0.$$

The gradient flow decreases the objective function.

This is a fundamental property of the gradient flow [De Giorgi et al., 1980, De Giorgi, 1993].

Particular case: V convex

Let $\lambda \geq 0$. V is λ-strongly convex if $\forall x, y \in \mathbb{R}^d, t \in [0,1]$,

$$V((1-t)x + ty) \leq (1-t)V(x) + tV(y) - \frac{\lambda t(1-t)}{2}\|x-y\|^2.$$

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0-strong convexity is simply convexity.
Since V smooth, this is equivalent to

$$\forall y \in \mathbb{R}^d, V(x) + \langle \nabla V(x), y - x \rangle + \frac{\lambda}{2}\|y-x\|^2 \leq V(y).$$

Outline

Time discretizations of the gradient flow

Let $\gamma > 0$ a step-size.

- Gradient descent algorithm:

$$x_{m+1} = x_m - \gamma \nabla V(x_m),$$

  i.e. Forward Euler (explicit):

$$\frac{x_{m+1} - x_m}{\gamma} = -\nabla V(x_m).$$

- Proximal point algorithm (V convex):

$$x_{m+1} = \mathrm{prox}_{\gamma V}(x_m) := \operatorname*{arg\,min}_{y \in \mathbb{R}^d} \gamma V(y) + \frac{1}{2}\|x_m - y\|^2$$

  i.e. Backward Euler (implicit):

$$\frac{x_{m+1} - x_m}{\gamma} = -\nabla V(x_{m+1}).$$

Other time discretizations: splitting schemes

- Proximal gradient algorithm ($V = F + G$, G convex):

$$x_{m+\frac{1}{2}} = x_m - \gamma \nabla F(x_m)$$
$$x_{m+1} = \mathrm{prox}_{\gamma G}(x_{m+\frac{1}{2}})$$

i.e. Forward Backward Euler (explicit implicit):

$$\frac{x_{m+1} - x_m}{\gamma} = -\nabla F(x_m) - \nabla G(x_{m+1}).$$

These time discretizations are unbiased (i.e. they preserve $x_\star \in \arg\min V$ as a fixed point).

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Time discretization of a flow ⇒ Optimization algorithm

Descent lemma

The time discretizations of the gradient flow decrease the objective function:

$$\frac{V(x_{m+1}) - V(x_m)}{\gamma} \leq -\frac{1}{2}\|\nabla V(\hat{x}_m)\|^2.$$

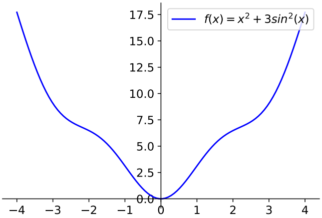
- For Forward Euler (i.e. gradient descent), $\hat{x}_m = x_m$ and $\gamma \leq 1/L$ (we need smoothness of V),
- For Backward Euler $\hat{x}_m = x_{m+1}$ (we don't need smoothness of V)

It is known that gradient descent converges at $1/M$ rate when V is convex, and faster if V is λ-strongly convex. But we can actually ask a bit less than convexity (see next slide).

Gradient dominance is more general than convexity

$$\forall x \in \mathbb{R}^d, \quad V(x) - V_\star \leq \frac{1}{2\lambda}\|\nabla V(x)\|^2.$$

- λ-Strong convexity $\Rightarrow$ gradient dominance with the same constant $\lambda > 0$
- Gradient dominance $\Rightarrow$ invexity[1]
- Gradient dominance $\not\Rightarrow$ convexity



[1] any local minimum of V is a global minimum.

Outline

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Definition of the Wasserstein space

Let $\mathcal{P}_2(\mathbb{R}^d)$ the space of probability measures on $\mathbb{R}^d$ with finite second moments, i.e.

$$\mathcal{P}_2(\mathbb{R}^d) = \{\mu \in \mathcal{P}(\mathbb{R}^d), \int \|x\|^2 d\mu(x) < \infty\}$$

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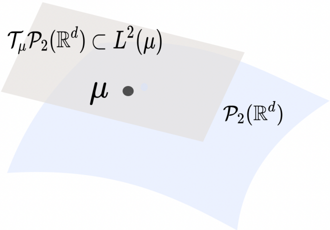
$\mathcal{P}_2(\mathbb{R}^d)$ is endowed with the Wasserstein-2 distance from Optimal transport: $\forall \mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$,

$$W_2^2(\mu, \nu) = \inf_{s \in \Gamma(\mu,\nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 \, ds(x, y),$$

where $\Gamma(\mu, \nu)$ is the set of possible couplings between μ and ν.

The metric space $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ is called **the Wasserstein space**.

Riemannian structure of $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ and L^2 spaces



Denote by

$$L^2(\mu) = \{f : \mathbb{R}^d \to \mathbb{R}^d, \int_{\mathbb{R}^d} \|f(x)\|^2 d\mu(x) < \infty\}$$

the space of vector-valued, square-integrable functions w.r.t μ.

It is a Hilbert space of functions equipped with the inner product

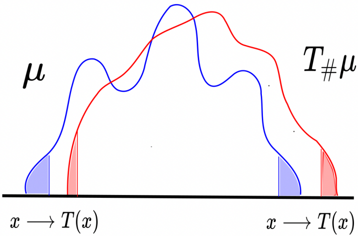
$$\langle f, g\rangle_\mu = \int_{\mathbb{R}^d} \langle f(x), g(x)\rangle_{\mathbb{R}^d} d\mu(x).$$

Pushforward measure

Let $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, $T : \mathbb{R}^d \to \mathbb{R}^d$ a measurable map.

The pushforward measure $T_{\#}\mu$ is characterized by:

$$X \sim \mu \implies T(X) \sim T_{\#}\mu.$$



Remark: $\mathrm{Id}_{\#}\,\mu = \mu$ where Id denotes the identity map.

Moving on $\mathcal{P}_2(\mathbb{R}^d)$ through L^2 maps

Note that if $T \in L^2(\mu)$ and $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, then $T_\# \mu \in \mathcal{P}_2(\mathbb{R}^d)$:

$$\int \|y\|^2 d(T_\# \mu)(y) = \int \|T(x)\|^2 d\mu(x) < \infty,$$

since $T \in L^2(\mu)$.

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Brenier's theorem [Brenier, 1991] : Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ s.t. $\mu \ll$ Leb. Then, there exists a unique $T_\mu^\nu : \mathbb{R}^d \to \mathbb{R}^d$ such that

1. $T_{\mu\#}^\nu \mu = \nu$
2. $W_2^2(\mu, \nu) = \|\mathrm{Id} - T_\mu^\nu\|_\mu^2 \stackrel{\textbf{def.}}{=} \int \|x - T_\mu^\nu(x)\|^2 d\mu(x)$.

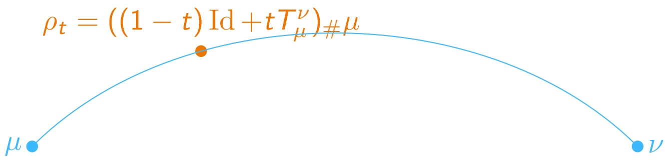
and T_μ^ν is called the Optimal Transport map between μ and ν.

Wasserstein geodesics between μ, ν?

The path

$$\rho_t = ((1-t)\,\mathrm{Id} + tT_\mu^\nu)_\# \mu, \quad t \in [0,1]$$

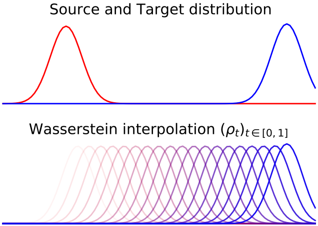
is the Wasserstein geodesic between $\rho_0 = \mu$ and $\rho_1 = \nu$.



It differs completely from the (mixture) path

$$\tilde{\rho}_t = (1-t)\mu + t\nu$$

which also interpolates between $\tilde{\rho}_0 = \rho_0 = \mu, \tilde{\rho}_1 = \rho_1 = \nu$.



If μ is supported on a set of particles $x^1, \ldots, x^N$,
these particles would be **pushed continuously through** ρ_t,
while they would be **teleported to other locations through** $\tilde{\rho}_t$.

Figure made with `https://pythonot.github.io/`.

Convexity along Wasserstein geodesics

Let $\mathcal{F} : \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$.

$\mathcal{F}$ λ-strongly geo. convex with $\lambda \geq 0$, if for any $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$:

$$\mathcal{F}(\rho_t) \leq (1-t)\mathcal{F}(\mu) + t\mathcal{F}(\nu) - \frac{\lambda t(1-t)}{2} W_2^2(\mu, \nu),$$

where $(\rho_t)_{t \in [0,1]}$ is a Wasserstein-2 geodesic between μ and ν.

Examples of geo. convex functionals

1. Potential energy $\mathcal{F}(\mu) = \int V(x)d\mu(x)$ with $V : \mathbb{R}^d \to \mathbb{R}$ convex.

Proof: write $\mathcal{F}(\rho_t)$ along a geodesic $\rho_t = ((1-t)\,\mathrm{Id} + tT_\mu^\nu)_\# \mu$ and use V convex.

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2. Negative entropy **(non trivial)** $\mathcal{F}(\mu) = \int \log(\mu(x))d\mu(x)$.

3. KL w.r.t. log concave distribution $\mathcal{F}(\mu) = \mathrm{KL}(\mu|\pi)$, where $\pi \propto \exp(-V)$, V convex.

Proof:

$$\begin{aligned}\mathrm{KL}(\mu|\pi) &= \int \log\left(\frac{\mu}{\pi}(x)\right) d\mu(x)\\ &= \underbrace{\int V(x)d\mu(x)}_{\text{Potential}} + \underbrace{\int \log(\mu(x))d\mu(x)}_{\text{(Neg.) Entropy}} + C.\end{aligned}$$

Outline

Gradient flows on probability distributions?

Recall that we want to approximate a distribution π by solving

$$\min_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \mathcal{F}(\mu), \quad \mathcal{F}(\mu) = \mathrm{KL}(\mu|\pi).$$

We have reviewed Euclidean GF of $V : \mathbb{R}^d \to \mathbb{R}$:

$$\dot{x}_t = -\nabla V(x_t), \quad x_t \in \mathbb{R}^d.$$

In an analog manner, what is the gradient flow of $\mathcal{F} : \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$? i.e. something of the form

$$\boxed{\text{"}\,\dot{\mu}_t = -\nabla_{W_2}\mathcal{F}(\mu_t)\text{"}, \quad \mu_t \in \mathcal{P}_2(\mathbb{R}^d).}$$

We need to define both sides of the equality.

LHS: Velocity field

Let $(\mu_t)_{t\geq 0} \in (\mathcal{P}_2(\mathbb{R}^d))^{\mathbb{R}^+}$. What is the time derivative of $(\mu_t)_{t\geq 0}$?

Definition: If there exists $(v_t)_{t\geq 0} \in (L^2(\mu_t))_{t\geq 0}$ such that,

$$\boxed{\frac{d}{dt}\int \varphi d\mu_t = \langle \nabla\varphi, v_t\rangle_{\mu_t}}$$

for every test function $\varphi : \mathbb{R}^d \to \mathbb{R}$ (e.g., $C^\infty(\mathbb{R}^d)$ with compact support), then $(v_t)_{t\geq 0}$ is a velocity field of $(\mu_t)_{t\geq 0}$.

The velocity field rules the dynamics of $(\mu_t)_{t\geq 0}$.

Continuity Equation

Equivalently, a velocity field $(v_t)_{t\geq 0}$ of $(\mu_t)_{t\geq 0}$ satisfies the PDE:

$$\boxed{\frac{\partial \mu_t}{\partial t} + \boldsymbol{\nabla} \cdot (\mu_t v_t) = 0, \quad t \geq 0.}$$

where $\boldsymbol{\nabla} \cdot A(x) = \sum_{i=1}^{d} \frac{\partial A_i(x)}{\partial x_i}$ for $A(x) = (A_1(x), \ldots, A_d(x))$, $A : \mathbb{R}^d \to \mathbb{R}^d$.

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Proof: If $\mu_t(\cdot)$ density of μ_t, for every test function $\varphi : \mathbb{R}^d \to \mathbb{R}$,

$$(1): \ \frac{d}{dt} \int \varphi(x)\mu_t(x)dx = \int \varphi(x)\frac{\partial \mu_t}{\partial t}(x)dx$$

$$(2): \ \frac{d}{dt} \int \varphi(x)\mu_t(x)dx \overset{\text{def.}}{=} \int \langle \nabla \varphi(x), v_t(x)\rangle_{\mathbb{R}^d} \mu_t(x)dx$$

$$\overset{\text{i.b.p.}}{=} -\int \varphi(x)\boldsymbol{\nabla} \cdot (v_t(x)\mu_t(x))dx.$$

This equation describes the dynamics of $(\mu_t)_{t\geq 0}$.

RHS: Wasserstein gradient

Let $\mathcal{F} : \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$. What is the "gradient" of $\mathcal{F}$ at μ?

Definition: Let $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. Consider a perturbation on the Wasserstein space $(\mathrm{Id} + \varepsilon h)_{\#}\mu$ for $h \in L^2(\mu)$.

If a Taylor expansion of $\mathcal{F}$ yields:

$$\mathcal{F}((\mathrm{Id} + \varepsilon h)_{\#}\mu) = \mathcal{F}(\mu) + \varepsilon \langle \nabla_{W_2}\mathcal{F}(\mu), h \rangle_{\mu} + o(\varepsilon),$$

then $\nabla_{W_2}\mathcal{F}(\mu) \in L^2(\mu)$ is the Wasserstein gradient of $\mathcal{F}$ at μ.

First Variation

In comparison, what is the First Variation of $\mathcal{F}$ at μ?

Definition: Let $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. Consider a linear perturbation $\mu + \varepsilon\xi \in \mathcal{P}_2(\mathbb{R}^d)$ for a perturbation ξ.

If a Taylor expansion of $\mathcal{F}$ yields:

$$\mathcal{F}(\mu + \varepsilon\xi) = \mathcal{F}(\mu) + \varepsilon \int \mathcal{F}'(\mu)(x) d\xi(x) + o(\varepsilon),$$

then $\mathcal{F}'(\mu) : \mathbb{R}^d \to \mathbb{R}$ is the First Variation of $\mathcal{F}$ at μ.

Wasserstein gradient = Gradient of First Variation

Typically[1],

$$\boxed{\nabla_{W_2}\mathcal{F}(\mu) = \nabla\mathcal{F}'(\mu).}$$

$\nabla_{W_2}\mathcal{F}(\mu) : \mathbb{R}^d \to \mathbb{R}^d$, $\mathcal{F}'(\mu) : \mathbb{R}^d \to \mathbb{R}$.

[1] see [Ambrosio et al., 2008, Th. 10.4.13] for precise statement.

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Proof: Let $\mu_t = (\mathrm{Id} + th)_{\#}\mu$.
First, expand μ_ε around μ using the continuity equation of $(\mu_t)_{t\geq 0}$:

$$\mu_\varepsilon = \mu + \varepsilon(\underbrace{-\nabla \cdot (\mu h)}_{=\xi}) + o(\varepsilon).$$

Then, expand $\mathcal{F}(\mu + \varepsilon\xi)$ using the definition of First Variation, and use an i.b.p. to identify the Wasserstein gradient.

[1] see [Ambrosio et al., 2008, Th. 10.4.13] for precise statement.

Examples of Wasserstein gradients

Below: $\mathcal{F}(\mu) \longrightarrow \mathcal{F}'(\mu) \longrightarrow \nabla\mathcal{F}'(\mu)$

1. Potential energy (linear function of μ)

$$\mathcal{F}(\mu) = \int V(x)d\mu(x) \longrightarrow V \longrightarrow \nabla V$$

2. Negative entropy

$$\mathcal{F}(\mu) = \int \log(\mu(x))d\mu(x)^1 \longrightarrow \log(\mu) + 1^2 \longrightarrow \nabla \log \mu.$$

[1] The Negative entropy $\mathcal{F}(\mu) = +\infty$ if μ does not have a density.
[2] $(y \log y)' = \log y + 1$

Wasserstein gradient of KL

More generally, let

$$\mathcal{F}(\mu) = \underbrace{\int V(x) d\mu(x)}_{\textit{Potential}} + \underbrace{\int \log(\mu(x)) d\mu(x)}_{\text{(Neg.) Entropy}} .$$

Then, for $\pi \propto \exp(-V)$,

$$\mathrm{KL}(\mu|\pi) = \mathcal{F}(\mu) - \underbrace{\mathcal{F}(\pi)}_{\textit{Constant}} .$$

By additivity, the Wasserstein gradient of KL is given by[1]

$$\boxed{\nabla_{W_2}\mathcal{F}(\mu) = \nabla\mathcal{F}'(\mu) = \nabla V + \nabla \log(\mu) = \nabla \log\left(\frac{\mu}{\pi}\right) .}$$

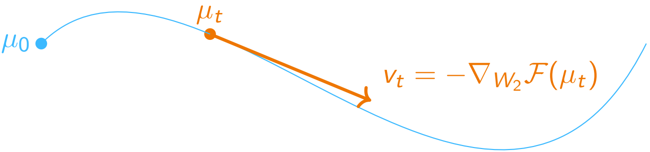
[1] See [Ambrosio et al., 2008, Th. 10.4.13] for precise statement.

Velocity field = negative Wasserstein gradient

Recall that we wanted to define the equation

$$"\dot{\mu}_t = -\nabla_{W_2}\mathcal{F}(\mu_t)".$$

We consider the direction $v_t = -\nabla_{W_2}\mathcal{F}(\mu_t)$ at each time to decrease $\mathcal{F}$:



since for this choice of velocity field,

$$\frac{d\mathcal{F}(\mu_t)}{dt} = -\left\|\nabla_{W_2}\mathcal{F}(\mu_t)\right\|^2_{\mu_t} \leq 0.$$

Wasserstein gradient flows (WGF) [Ambrosio et al., 2008]

The Wasserstein GF of $\mathcal{F}$ is ruled by:

$$\boxed{v_t = -\nabla_{W_2}\mathcal{F}(\mu_t)} \tag{1}$$

Equivalently:

$$\boxed{\frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot \left(\mu_t \nabla_{W_2}\mathcal{F}(\mu_t)\right),} \tag{2}$$

Problem: How to construct such a flow on $\mathcal{P}_2(\mathbb{R}^d)$?

In the following, we will see some examples of dynamics $(x_t)_{t\geq 0} \in \mathbb{R}^d$ whose law $(\mu_t)_{t\geq 0}$ obeys (2). We will call such dynamics over $\mathbb{R}^d$ **realizations** of the WGF of $\mathcal{F}$.

Example I - Constant vector field

Let $x_0 \sim \mu_0$ and $V : \mathbb{R}^d \to \mathbb{R}$. Consider the dynamics:

$$\dot{x}_t = -\nabla V(x_t), \quad x_t \in \mathbb{R}^d. \tag{3}$$

Let μ_t be the law of x_t at each time $t \geq 0$. **Then, $v_t = -\nabla V$ is a velocity field of $(\mu_t)_{t\geq 0}$.**

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Let μ_t be the law of x_t at each time $t \geq 0$. **Then, $v_t = -\nabla V$ is a velocity field of $(\mu_t)_{t \geq 0}$.**

Proof: Let $t \geq 0$. Using the chain rule and (3),

$$\frac{d}{dt}\varphi(x_t) = \langle \nabla\varphi(x_t), \dot{x}_t\rangle_{\mathbb{R}^d} = \langle \nabla\varphi(x_t), -\nabla V(x_t)\rangle_{\mathbb{R}^d}.$$

$$\frac{d}{dt}\int \varphi d\mu_t = \frac{d}{dt}\mathbb{E}\left[\varphi(x_t)\right] = \mathbb{E}\left[\frac{d}{dt}\varphi(x_t)\right]$$
$$= \mathbb{E}\left[\langle \nabla\varphi(x_t), -\nabla V(x_t)\rangle_{\mathbb{R}^d}\right] = \langle \nabla\varphi, -\nabla V\rangle_{\mu_t}.$$

Therefore we can identify $v_t = -\nabla V$.

Example I : WGF of Potential energy

- We have just seen that:

$$\dot{x}_t = -\nabla V(x_t), \quad x_t \in \mathbb{R}^d, \quad x_t \sim \mu_t, \tag{4}$$

$$\Downarrow$$

$$\frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot \left(\mu_t \nabla V\right). \tag{5}$$

- In other words, $v_t = -\nabla V = -\nabla_{W_2}\mathcal{F}(\mu_t)$ where $\mathcal{F}(\mu) = \int V d\mu$ is a Potential energy.

Hence (4) **realizes the WGF of the Potential energy** $\mathcal{F}$ (5).

Example II : WGF of generic $\mathcal{F}$

More generally, let $x_0 \sim \mu_0$ and consider the dynamics:

$$\dot{x}_t = v_t(x_t).$$

Let μ_t be the law of x_t at each time $t \geq 0$. **Then, $(v_t)_{t\geq 0}$ is a velocity field of $(\mu_t)_{t\geq 0}$.**

[1]The randomness only comes from $x_0 \sim \mu_0$.

Example II : WGF of generic $\mathcal{F}$

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Let μ_t be the law of x_t at each time $t \geq 0$. **Then, $(v_t)_{t\geq 0}$ is a velocity field of $(\mu_t)_{t\geq 0}$.**

In particular, let $\mathcal{F} : \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$. The dynamics

$$\dot{x}_t = -\nabla_{W_2}\mathcal{F}(\mu_t)(x_t), \quad x_t \in \mathbb{R}^d, \quad x_t \sim \mu_t, \tag{6}$$

realizes the Wasserstein GF of $\mathcal{F}$.

Note that $(x_t)_{t\geq 0}$ follows a deterministic dynamics[1]. There may be other realizations of the Wasserstein GF!

[1] The randomness only comes from $x_0 \sim \mu_0$.

Example III : Brownian motion

Let $x_0 \sim \mu_0$ independent of $b_t \sim \mathcal{N}(0, t\,\mathrm{Id})$ the Brownian motion, and consider the dynamics

$$x_t = x_0 + \sqrt{2} b_t.$$

Let μ_t be the law of x_t at each time $t \geq 0$. **Then,** $v_t = -\nabla \log(\mu_t)$ **is a velocity field of** $(\mu_t)_{t \geq 0}$.

[1] Using $\Delta = \boldsymbol{\nabla} \cdot \nabla$ (Divergence of Gradient = Laplacian).

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Let μ_t be the law of x_t at each time $t \geq 0$. **Then,** $v_t = -\nabla \log(\mu_t)$ **is a velocity field of** $(\mu_t)_{t\geq 0}$.

Proof: Differentiate $\varphi(x_t)$ using Itô formula, take the expectation and identify the velocity field from its definition.

In this case, the Continuity Equation is the Heat equation[1]

$$\frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot \left(\underbrace{\mu_t \nabla \log(\mu_t)}_{=\mu_t . \nabla \mu_t / \mu_t} \right) = \Delta \mu_t.$$

[1] Using $\Delta = \boldsymbol{\nabla} \cdot \nabla$ (Divergence of Gradient = Laplacian).

Example III $\Longrightarrow$ WGF of (Neg.) Entropy

- We have just seen that:

$$x_t = x_0 + \sqrt{2} b_t, \quad b_t \sim \mathcal{N}(0, t\,\mathrm{Id}), \quad x_t \in \mathbb{R}^d, \quad x_t \sim \mu_t, \quad (7)$$

$$\Downarrow$$

$$\frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot (\mu_t \nabla \log(\mu_t)) = \Delta \mu_t. \quad (8)$$

- In other words, $v_t = -\nabla \log(\mu_t) = -\nabla_{W_2} \mathcal{F}(\mu_t)$ where $\mathcal{F}(\mu) = \int \log(\mu(x)) d\mu(x)$ is the Negative entropy.

Hence (7) realizes the WGF of the Negative entropy $\mathcal{F}$ (8).

Other realizations of WGF of (Neg.) Entropy

Remark: While we have just seen that

$$x_t = x_0 + \sqrt{2} b_t, \quad b_t \sim \mathcal{N}(0, t\,\mathrm{Id})$$

realizes the WGF of the Negative entropy, it is also the case of

$$x_t = x_0 + \sqrt{2t}\eta, \quad \eta \sim \mathcal{N}(0, \mathrm{Id}). \tag{9}$$

Indeed, the latter satisfies

$$\dot{x}_t = -\nabla \log(\mu_t)(x_t),$$

which has the same velocity field $v_t = -\nabla \log(\mu_t)$.

All these processes have the same distribution μ_t realizing the WGF of the Negative entropy.

Example IV - Langevin diffusion

More generally, let $x_0 \sim \mu_0$, and consider the dynamics (Langevin diffusion)

$$dx_t = -\nabla V(x_t)dt + \sqrt{2}db_t,$$

where $(b_t)_{t\geq 0}$ is the Brownian motion. Let μ_t be the law of x_t at each time $t \geq 0$. **Then,** $v_t = -\nabla V + \nabla \log(\mu_t) = -\nabla \log\left(\frac{\mu_t}{\pi}\right)$ **where** $\pi \propto \exp(-V)$**, is a velocity field of** μ_t.

Proof: Combine Example I and III.

In this case, the Continuity Equation is the Fokker-Planck equation.

$$\frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot \left(\mu_t \nabla \log\left(\frac{\mu_t}{\pi}\right)\right) = \Delta \mu_t + \boldsymbol{\nabla} \cdot (\mu_t \nabla V).$$

Example IV $\Longrightarrow$ WGF of the KL

- We have just seen that:

$$x_t = -\nabla V(x_t) + \sqrt{2}db_t, \quad x_t \in \mathbb{R}^d, \quad x_t \sim \mu_t, \tag{10}$$

$$\Downarrow$$

$$\frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot \left(\mu_t \nabla \log\left(\frac{\mu_t}{\pi}\right)\right) = \Delta \mu_t + \boldsymbol{\nabla} \cdot (\mu_t \nabla V). \tag{11}$$

- In other words, $v_t = -\nabla \log\left(\frac{\mu_t}{\pi}\right) = -\nabla_{W_2}\mathcal{F}(\mu_t)$ where $\mathcal{F}(\mu) = \mathrm{KL}(\mu|\pi)$ and $\pi \propto \exp(-V)$.

Hence (10) realizes the WGF of the KL divergence $\mathcal{F}$ (11).

Example IV $\Longrightarrow$ WGF of the KL

- We have just seen that:

$$x_t = -\nabla V(x_t) + \sqrt{2} db_t, \quad x_t \in \mathbb{R}^d, \quad x_t \sim \mu_t, \tag{10}$$
$$\Downarrow$$
$$\frac{\partial \mu_t}{\partial t} = \boldsymbol{\nabla} \cdot \left(\mu_t \nabla \log\left(\frac{\mu_t}{\pi}\right)\right) = \Delta \mu_t + \boldsymbol{\nabla} \cdot (\mu_t \nabla V). \tag{11}$$

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Hence (10) **realizes the WGF of the KL divergence** $\mathcal{F}$ (11).

Remark: Another realization is given by

$$\dot{x}_t = -\nabla \log\left(\frac{\mu_t}{\pi}\right)(x_t), \; x_t \sim \mu_t.$$

Design of (Some) Sampling algorithms

A take home message.

As in Optimization, time discretizations of the Wasserstein GF can be seen as Sampling algorithms (= optimization algorithms in $\mathcal{P}_2(\mathbb{R}^d)$).

This point of view allows to **design** Sampling algorithms by discretizing Wasserstein GF.

Outline

Outline

Sampling as Optimization

$$\pi(x) \propto \exp(-V(x)),$$

$$\pi = \operatorname*{arg\,min}_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \mathrm{KL}(\mu|\pi) = \operatorname*{arg\,min}_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \mathcal{F}(\mu),$$

Sampling as Optimization

$$\boxed{\pi(x) \propto \exp(-V(x)),}$$

$$\boxed{\pi = \underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\min}\ \mathrm{KL}(\mu|\pi) = \underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\min}\ \mathcal{F}(\mu),}$$

where

$$\mathcal{F}(\mu) := \underbrace{\int V(x) d\mu(x)}_{Potential} + \underbrace{\int \log(\mu(x)) d\mu(x)}_{(Neg.) Entropy}$$

satisfies

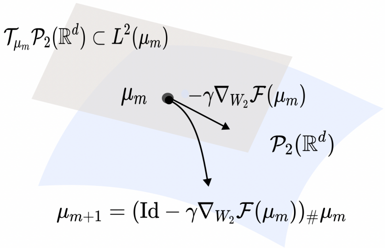
$$\mathcal{F}(\mu) - \underbrace{\mathcal{F}(\pi)}_{Constant} = \mathrm{KL}(\mu|\pi).$$

Time discretizations of the Wasserstein GF

Let $\gamma > 0$ a step-size.

- Wasserstein gradient descent or Forward Euler (explicit):

$$\mu_{m+1} = (\mathrm{Id} - \gamma \nabla_{W_2} \mathcal{F}(\mu_m))_{\#} \mu_m$$



Problem: If $\mathcal{F}(\mu) = \mathrm{KL}(\mu|\pi)$, $\nabla_{W_2}\mathcal{F}(\mu_m) = \nabla \log \left(\frac{\mu_m}{\pi}\right)$ requires the knowledge of the density μ_m.

- JKO scheme [Jordan et al., 1998] ($\mathcal{F}$ geo. convex):

$$\mu_{m+1} \in \mathrm{JKO}_{\gamma\mathcal{F}}(\mu_m) := \operatorname*{arg\,min}_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \left\{ \gamma\mathcal{F}(\mu) + \frac{1}{2} W_2^2(\mu, \mu_m) \right\}.$$

i.e. Backward Euler (implicit) [SKL20].

- JKO scheme [Jordan et al., 1998] ($\mathcal{F}$ geo. convex):

$$\mu_{m+1} \in \mathrm{JKO}_{\gamma\mathcal{F}}(\mu_m) := \underset{\mu\in\mathcal{P}_2(\mathbb{R}^d)}{\arg\min} \left\{ \gamma\mathcal{F}(\mu) + \frac{1}{2} W_2^2(\mu, \mu_m) \right\}.$$

  i.e. Backward Euler (implicit) [SKL20].

- Splitting scheme [SKL20] ($\mathcal{F} = \mathcal{F}_1 + \mathcal{F}_2$, $\mathcal{F}_2$ geo. convex):

$$\mu_{m+\frac{1}{2}} = (\mathrm{Id} - \gamma\, \nabla_{W_2}\mathcal{F}_1(\mu_m))_{\#}\mu_m$$
$$\mu_{m+1} = \mathrm{JKO}_{\gamma\,\mathcal{F}_2}\left(\mu_{m+\frac{1}{2}}\right)$$

Problem: these (unbiased) schemes are also hard to implement (global optimization subroutine).

Outline

Langevin Monte Carlo

Langevin Monte Carlo (LMC) to sample from $\pi \propto \exp(-V)$:

$$\boxed{x_{m+1} = x_m - \gamma \nabla V(x_m) + \sqrt{2\gamma}\eta_m,}$$

where $\gamma > 0$ and $(\eta_m)_{m \geq 0}$ i.i.d. standard Gaussian.

Intuition: Discretization of Langevin diffusion

$$dx_t = -\nabla V(x_t)dt + \sqrt{2}db_t.$$

Can be used for analysis of Langevin
[Durmus and Moulines, 2017, Dalalyan, 2017].

Gradient dominance

Log Sobolev inequality is a gradient dominance condition for KL. [Otto and Villani, 2000, Blanchet and Bolte, 2018].

$$\forall \mu \in \mathcal{P}_2(\mathbb{R}^d), \quad \mathrm{KL}(\mu|\pi) \leq \frac{1}{2\lambda} \|\nabla \log(\mu|\pi)\|^2_{L^2(\mu)}.$$

- V is λ-strongly convex $\Rightarrow \pi \propto \exp(-V)$ satisfies Log Sobolev with λ (Bakry–Emery theorem)
- Log Sobolev $\not\Rightarrow$ V convex.

Non log concave π satisfying Log Sobolev

Example: Consider a standard Gaussian distribution

$$\pi(x) \propto \exp\left(-\frac{\|x\|^2}{2}\right),$$

i.e. $\pi \propto \exp(-V)$ with V 1-strongly convex, i.e. π is (1-)strongly log-concave.

A small (bounded) perturbation of π is not necessarily log-concave, but still verifies a Log Sobolev inequality (Holley–Stroock perturbation theorem).

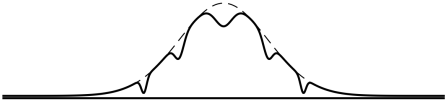


Figure from [?].

Outline

Stein Variational Gradient Descent (SVGD)

SVGD [Liu and Wang, 2016] to sample from $\pi \propto \exp(-V)$.

SVGD updates the positions of a set of N particles $x^1, \ldots, x^N$, i.e. for any $i = 1, \ldots, N$, at each time $m \geq 0$:

$$x^i_{m+1} = x^i_m - \frac{\gamma}{N} \sum_{j=1}^{N} \nabla V(x^j_m) k(x^i_m, x^j_m) - \nabla_2 k(x^i_m, x^j_m),$$

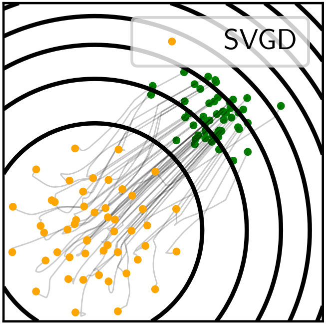
where k is a kernel associated to a **Reproducing Kernel Hilbert Space** H_k.

Reproducing kernel Hilbert Space

- Hilbert space of functions H_k (here, $\mathrm{H}_k \subset L^2(\mu)$ for every μ)
- For every x, $k(x,\cdot) \in \mathrm{H}_k$ ($k(x,\cdot) : \mathbb{R}^d \to \mathbb{R}$)
- Reproducing property: for every $f \in \mathrm{H}_k$, $f(x) = \langle f, k(x,\cdot)\rangle_{\mathrm{H}_k}$.

Example: $k(x,y) = \exp\big(-\|x-y\|^2\big)$.

Two dimensional example



Simulation from [KAFMA21]. Pytorch code available at `https://github.com/pierreablin/ksddescent`.

What's happening over the Wasserstein space

Let $\mu_m = \frac{1}{N}\sum_{j=1}^{N} \delta_{x_m^j}$. Then,

$$\boxed{\mu_{m+1} = (\mathrm{Id} - \gamma h_{\mu_m})_{\#}\, \mu_m,}$$

where $h_\mu := \int \nabla V(x) k(x,\cdot) - \nabla_1 k(x,\cdot) d\mu(x)$.

Actually,

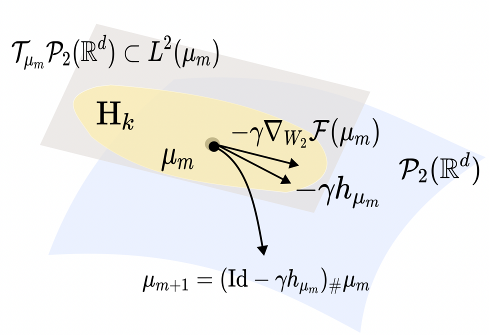
$$h_\mu = P_\mu \nabla \log\left(\frac{\mu}{\pi}\right), \text{ where } P_\mu : L^2(\mu) \to \mathrm{H}_k, f \mapsto \int f(x)k(x,\cdot)d\mu(x).$$

Gradient descent interpretation

A Taylor expansion around μ for $h \in \mathrm{H}_k$, if μ has a density yields [Liu, 2017]:

$$\mathrm{KL}((\mathrm{Id} + \varepsilon h)_{\#}\mu|\pi) = \mathrm{KL}(\mu|\pi) + \varepsilon \langle h_\mu, h \rangle_{\mathrm{H}_k} + o(\varepsilon).$$

Therefore, h_μ plays the role of the Wasserstein gradient in H_k.



Outline

Extensions to other optimization techniques

- Accelerated methods: accelerated LMC [Ma et al., 2019, Dalalyan and Riou-Durand, 2020, Shen and Lee, 2019], accelerated particle methods [Liu et al., 2019]
- "Mirror-descent" like sampling algorithms to sample from a distribution with compact support: Mirror Langevin [Hsieh et al., 2018, Zhang et al., 2020, Ahn and Chewi, 2021, Li et al., 2022], Mirror SVGD [Shi et al., 2021]
- "Proximal" algorithms for non-smooth potentials V (i.e. no gradients of V) [Durmus et al., 2019, Wibisono, 2019], [SKR19, SR20]
- Variance reduction for potentials V written as finite sums [Ding and Li, 2021, Zou et al., 2018, Zou et al., 2019, Dubey et al., 2016], [BCE$^+$22].

Outline

Conclusion

- Sampling can be seen as an optimization problem on a "Wasserstein manifold", and we can consider Wasserstein gradient flows, that decrease a loss (e.g. here the KL)
- Their discretizations (space/time) lead to different algorithms: LMC is a splitting (forward-flow) scheme, SVGD is a gradient descent
- One can design Sampling algorithms by discretizing Wasserstein GF

Some limitations of the framework

- The presented framework does not cover all sampling algorithms, e.g. involving dynamics such as accept/reject steps, birth and death of particles...
- It does not cover neither the analysis for finite number of particles (last iterates of Langevin Monte Carlo, SVGD stationary particles...)
- We did not talk about practical considerations, e.g. improving convergence (for π multimodal, high-dimensional)

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