An Introduction to Optimization over the Space of Probability Measures: From Sampling to Wasserstein Gradient Flow

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Outline

Introduction

- **Optimization over the space of probability measures** $\mathcal{P}(\mathbb{R}^d)$:

$$\min_{\mu \in \mathcal{P}(\mathbb{R}^d)} \mathcal{F}(\mu).$$

- **Applications:**
  - **Sampling with target distribution** π [Wibisono, 2018]:

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

  - **Variational inference (VI)** [Jordan et al., 1999]:

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

  - **Other examples:** distributed robust optimization [Xu and Zhu, 2025], deep learning [Chizat, 2022]; single-cell analysis in mathematical biology [Lavenant et al., 2023], etc.

Outline

Sampling

Goal: Sample from a distribution π on $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$.
Two main settings of sampling:

- **Setting 1: π is given in explicit form up to a normalization constant:**

$$\pi(x) = \frac{e^{-f(x)}}{\int_{\mathbb{R}^d} e^{-f(x)} dx}, \quad x \in \mathbb{R}^d,$$

  Applications: Bayesian inference, numerical integration in high dimensions, differential privacy, simulation in physics, finance, and machine learning.

- **Setting 2: π is given with a collection if i.i.d. samples:**

$$\text{only have } \{x_i\}_{i=1}^N \overset{\text{i.i.d.}}{\sim} \pi$$

  Applications: generative models (diffusion models, GANs, etc).

Markov Chain Monte Carlo

- Markov Chain Monte Carlo (MCMC): generate a Markov chain $\{X_n\}$ such that

$$\mu_n = \mathrm{Law}(X_n) \xrightarrow{\text{in some sense}} \pi$$

- Algorithms: **Unadjusted Langevin Algorithm (ULA)** (also called Langevin Monte Carlo (LMC)), **Metropolis-Adjusted Langevin Algorithm (MALA)**, etc.

Unadjusted Langevin Algorithm

The Unadjusted Langevin Algorithm for sampling from target distribution $\pi \propto e^{-f(x)}$ is given by

$$X_{k+1,h} = X_{k,h} - h\nabla f(X_{k,h}) + \sqrt{2h}\,\xi_{k+1}, \tag{ULA}$$

where $h > 0$ is the step size, $\xi_1, \cdots, \xi_k, \cdots$ are i.i.d. $N(0, I_d)$ random variables.

probabilistic perspective $\Longrightarrow$ geometric perspective

Unadjusted Langevin Algorithm

Unadjusted Langevin Algorithm: $X_{k+1,h} = X_{k,h} - h\nabla f(X_{k,h}) + \sqrt{2h}\,\xi_{k+1}$

- **Probabilistic perspective:** ULA is the Euler-Maruyama discretization of the Langevin dynamics
$$dX_t = -\nabla f(X_t)dt + \sqrt{2}dB_t, \tag{LD}$$
By Fokker-Planck equation
$$\frac{\partial \mu_t}{\partial t} = \nabla \cdot \left(\mu_t \nabla \log \frac{\mu_t}{\pi}\right), \quad \mu_t \text{ denotes the density of } X_t \text{ for all } t \geq 0,$$
the target distribution π is the unique invariant measure of LD.

- **Geometric perspective:** $(\mathcal{P}_{2,ac}(\mathbb{R}^d), \mathrm{W}_2)$ can be viewed as a Riemannian manifold and the Langevin dynamics can be viewed as the Wasserstein gradient flow of KL divergence functional $\mathrm{KL}(\cdot\|\pi)$ [Otto, 2001].

Outline

Wasserstein Space

- The **Wasserstein space** $(\mathcal{P}_2(\mathbb{R}^d), \mathrm{W}_2)$ is a metric space, where

$$\mathcal{P}_2(\mathbb{R}^d) := \{\mu \in \mathcal{P}(\mathbb{R}^d) \mid \int_{\mathbb{R}^d} \|x\|_2^2 \, \mu(dx) < +\infty\},$$

$$\mathrm{W}_2(\mu, \nu) = \inf_{\gamma \in \Pi(\mu,\nu)} \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 \, \gamma(\mathrm{d}x, \mathrm{d}y) \right)^{1/2}, \quad \text{for all } \mu, \nu \in \mathcal{P}_2(\mathbb{R}^d),$$

$$\Pi(\mu, \nu) = \{\gamma \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d) | \gamma(A \times \mathbb{R}^d) = \mu(A), \ \gamma(\mathbb{R}^d \times A) = \nu(A), \ \text{ for all } A \in \mathcal{B}(\mathbb{R}^d)\}$$

- **(Isometric embedding property)** The mapping $x \mapsto \delta_x$ is an isometric embedding from $(\mathbb{R}^d, \|\cdot\|)$ to $(\mathcal{P}_2(\mathbb{R}^d), \mathrm{W}_2)$:

$$\mathrm{W}_2(\delta_x, \delta_y) = \|x - y\|, \ \text{for all } x, y \in \mathbb{R}^d.$$

- We will work on

$$\mathcal{P}_{2,ac}(\mathbb{R}^d) = \{\mu \in \mathcal{P}(\mathbb{R}^d) \mid \mu \ll m \text{ and } \int_{\mathbb{R}^d} \|x\|_2^2 \, \mu(dx) < +\infty\}$$

Tangent Space of $\mathcal{P}_{2,ac}(\mathbb{R}^d)$

For evolution $t \mapsto \mu_t$ in $\mathcal{P}_{2,ac}(\mathbb{R}^d)$, there are two main perspectives:

Lagrangian viewpoint

Let X_t be random variable representing the particle trajectory, evolving according to

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{dt}} X_t = v_t(X_t), \quad a.s. \\ X_0 \sim \mu_0, \end{cases}$$

and let $\mu_t = \mathrm{Law}(X_t)$.

Eulerian viewpoint

Let μ_t be probability density representing the mass density and $v_t : \mathbb{R}^d \to \mathbb{R}^d$ be the velocity field and they satisfies the **continuity equation**

$$\frac{\partial \mu_t}{\partial t} + \nabla \cdot (\mu_t v_t) = 0.$$

Under some regularity conditions, the two view points above are equivalent.

Tangent Space of $\mathcal{P}_{2,ac}(\mathbb{R}^d)$: Continuity Equation

From continuity equation

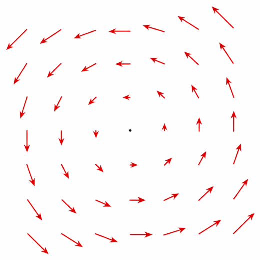
$$\begin{cases} \frac{\partial \mu_t}{\partial t} + \nabla \cdot (\mu_t v_t) = 0 \\ \int_{\mathbb{R}^d} \mu_t(x)\,\mathrm{d}x = 1, \quad \forall t \geq 0 \end{cases}$$

- if $(v_t)_{t\geq 0}$ is given, then under some regularity conditions, $(\mu_t)_{t\geq 0}$ is unique;
- but if the curve $t \mapsto \mu_t$ is given, the velocity field $(v_t)_{t\geq 0}$ is often **not unique**.

- example: let $\mu_t \equiv N(0, I_d)$, and $v_t^{(1)} \equiv 0$ and $v_t^{(2)}$ be the rotation vector field, then they both satisfy the continuity equation.
- if vector field $(w_t)_{t\geq 0}$ satisfies

$$\nabla \cdot (\mu_t w_t) \equiv 0,$$

then the vector field $(v_t + w_t)_{t\geq 0}$ also satisfies the continuity equation.



Rotation vector field

Tangent Space of $\mathcal{P}_{2,ac}(\mathbb{R}^d)$

Idea: minimize the kinetic energy

$$\min_{v_t:\mathbb{R}^d\to\mathbb{R}^d} \quad \frac{1}{2}\|v_t\|_{\mu_t}^2 := \frac{1}{2}\int_{\mathbb{R}^d} \|v_t\|^2 \,\mathrm{d}\,\mu_t$$
$$\text{s. t.} \quad \frac{\partial \mu_t}{\partial t} + \nabla\cdot(\mu_t v_t) = 0$$

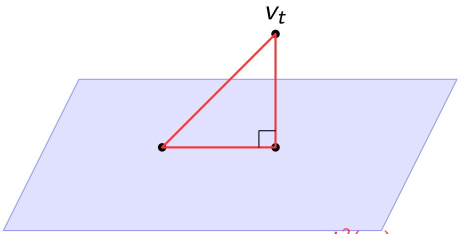
Weak form of continuity equation: for all $\varphi \in C_c^\infty(\mathbb{R}^d, \mathbb{R})$,

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^d} \varphi(x)\mu_t(\mathrm{d}x) = \int_{\mathbb{R}^d} \langle \nabla\varphi(x), v_t(x)\rangle\, \mu_t(\mathrm{d}x).$$

Theorem 1 ([Chewi et al., 2024])

For "nice enough" curve $t \mapsto \mu_t$, there is a unique vector field $t \mapsto v_t$ minimizing the kinetic energy such that the continuity equation holds. Furthermore, v_t is the minimizer if and only if it belongs to the set

$$\overline{\{\nabla\varphi \mid \varphi \in C_c^\infty(\mathbb{R}^d,\mathbb{R})\}}^{L^2(\mu_t)}.$$



$$\overline{\{\nabla\varphi \mid \varphi \in C_c^\infty(\mathbb{R}^d,\mathbb{R})\}}^{L^2(\mu_t)}$$

A Riemannian Manifold View of $(\mathcal{P}_{2,ac}(\mathbb{R}^d), \mathrm{W}_2)$

- **Tangent space**: $\mathrm{T}_\mu \mathcal{P}_{2,ac}(\mathbb{R}^d) := \overline{\{\nabla\varphi \mid \varphi \in C_c^\infty(\mathbb{R}^d, \mathbb{R})\}}^{L^2(\mu)}$;
- We say vector field (v_t) **is tangent to** (μ_t) if and only if $v_t \in \mathrm{T}_{\mu_t} \mathcal{P}_{2,ac}(\mathbb{R}^d)$ for all $t \geq 0$ and the continuity holds;
- **Riemannian distance**:

$$d(\mu_0, \mu_1) := \inf \left\{ \int_0^1 \|v_t\|_{\mu_t} \,\mathrm{d}t \;\middle|\; (v_t)_{t\in[0,1]} \text{ is tangent to } (\mu_t)_{t\in[0,1]} \right\} = \mathrm{W}_2(\mu_0, \mu_1);$$

- **Geodesics:** let $X_0 \sim \mu_0$, $X_1 \sim \mu_1$ be optimally coupled, and

$$X_t = (1-t)X_0 + tX_1, \;\; t \in [0,1],$$

then $\mu_t = \mathrm{Law}(X_t), \;\; t \in [0,1]$ gives the geodesic from μ_0 to μ_1.

Convexity of KL Divergence Functional

Definition 2 (Strongly convex of a functional)

We say a functional $\mathcal{F} : \mathcal{P}_{2,ac}(\mathbb{R}^d) \to \mathbb{R} \cup \{\infty\}$ is $m-$strongly convex along Wasserstein geodesics if for geodesic $(\mu_t)_{t\in[0,1]}$ and all $t \in [0,1]$,

$$\mathcal{F}(\mu_t) \leq (1-t)\,\mathcal{F}(\mu_0) + t\,\mathcal{F}(\mu_1) - \frac{mt(1-t)}{2} \mathrm{W}_2(\mu_0, \mu_1)^2$$

Theorem 3 (Convexity of the KL divergence functional)

If $\pi \propto e^{-f(x)}$, where f is $m-$strongly convex, then $\mathrm{KL}(\cdot\|\pi)$ is also $m-$strongly convex along Wasserstein geodesics.

Wasserstein Gradient

Definition 4 (Wasserstein gradient)

Let $\mathcal{F} : \mathcal{P}_{2,ac}(\mathbb{R}^d) \to \mathbb{R} \cup \{\infty\}$ be a functional. The Wasserstein gradient of $\mathcal{F}$ at μ, denoted by $\nabla_{\mathrm{W}_2} \mathcal{F}(\mu)$, is the unique element of $\mathrm{T}_\mu \mathcal{P}_{2,ac}(\mathbb{R}^d)$ such that for all curves $t \mapsto \mu_t$ with $\mu_0 = \mu$ with tangent vector v_0,

$$\frac{\mathrm{d}}{\mathrm{dt}}\Big|_{t=0} \mathcal{F}(\mu_t) = \langle \nabla_{\mathrm{W}_2} \mathcal{F}(\mu), v_0 \rangle_\mu$$

Definition 5 (First variational derivative of a functional)

Let $\mathcal{F} : \mathcal{P}_{2,ac}(\mathbb{R}^d) \to \mathbb{R} \cup \{\infty\}$ be a functional. The first variational derivative of $\mathcal{F}$ at μ is a function, denoted by $\frac{\delta \mathcal{F}}{\delta \mu}[\mu]$, such that for any perturbation in measure ν such that $\mu + \varepsilon \nu \in \mathcal{P}_{2,ac}(\mathbb{R}^d)$,

$$\frac{\mathrm{d}}{\mathrm{d}\,\varepsilon}\Big|_{\varepsilon=0} \mathcal{F}(\mu + \varepsilon \nu) = \int_{\mathbb{R}^d} \frac{\delta \mathcal{F}}{\delta \mu}[\mu](x) \,\mathrm{d}\, \nu(x).$$

Wasserstein Gradient

Theorem 6

Let $\mathcal{F} : \mathcal{P}_{2,ac}(\mathbb{R}^d) \to \mathbb{R} \cup \{\infty\}$ be a functional. Then the Wasserstein gradient of $\mathcal{F}$ at μ is just the gradient of first variational derivative of $\mathcal{F}$ at μ, namely

$$\nabla_{\mathrm{W}_2} \mathcal{F}(\mu) = \nabla \frac{\delta \mathcal{F}}{\delta \mu}[\mu].$$

Example 7

Let $\mathcal{F}(\mu) := \mathrm{KL}(\mu \| \pi)$, then

$$\nabla_{\mathrm{W}_2} \mathcal{F}(\mu) = \nabla \frac{\delta \mathcal{F}}{\delta \mu}[\mu] = \nabla \log \frac{\mu}{\pi}.$$

Wasserstein Gradient Flow

Definition 8 (Wasserstein gradient flow)

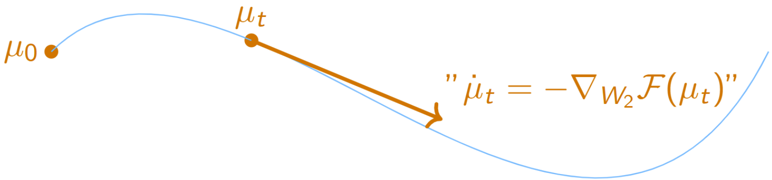
The Wasserstein gradient flow of $\mathcal{F}$ is the curve $t \mapsto \mu_t$ with tangent vector $-\nabla_{W_2} \mathcal{F}(\mu_t)$ at time t, which means

$$\frac{\partial \mu_t}{\partial t} = \nabla \cdot (\mu_t \nabla_{W_2} \mathcal{F}(\mu_t))$$

Theorem 9

The functional value decreases along the Wasserstein gradient flow trajectory

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



Geometric Perspective of ULA: Wasserstein Gradient Flow

Recall the Langevin dynamics

$$dX_t = -\nabla f(X_t)\,\mathrm{dt} + \sqrt{2}\,\mathrm{d}\,B_t$$

with our target distribution $\pi \propto e^{-f(x)}$. Now we consider the functional $\mathcal{F}$ as KL divergence

$$\mathcal{F}(\mu) = \mathrm{KL}(\mu\|\pi), \quad \nabla_{\mathrm{W}_2}\mathcal{F}(\mu) = \nabla\frac{\delta\,\mathcal{F}}{\delta\mu}[\mu] = \nabla\log\frac{\mu}{\pi}.$$

Wasserstein gradient flow

$$\frac{\partial\mu_t}{\partial t} = \nabla\cdot(\mu_t\nabla\log\frac{\mu_t}{\pi})$$

Fokker-Planck equation

$$\frac{\partial\mu_t}{\partial t} = \nabla\cdot(\mu_t\nabla\log\frac{\mu_t}{\pi})$$

Theorem 10 ([Jordan et al., 1998])

The Langevin dynamics can be viewed as the Wasserstein gradient flow of $\mathrm{KL}(\cdot\|\pi)$.

Wasserstein Gradient Flow Framework for Algorithm Design

Techniques from gradient flow

Wasserstein gradient flow
Functional $\mathcal{F}$

Continuity equation
$\frac{\partial \mu_t}{\partial t} = \nabla \cdot (\mu_t \nabla_{W_2} \mathcal{F}(\mu_t))$

Fokker-Planck equation
$\frac{\partial \mu_t}{\partial t} = -\nabla \cdot (a \mu_t) + \frac{1}{2} \nabla \cdot (b_t b_t^\top \nabla \mu_t)$

Stochastic differential equation (SDE)
$dX_t = a(t, X_t)\, dt + b_t \,\mathrm{d} B_t$

Numerical scheme for SDE
e.g. Euler-Maruyama Method

Outline

Metropolis-Hastings Adjusted Method

- Proposal kernel $Q : \mathbb{R}^d \times \mathcal{B}(\mathbb{R}^d) \to [0,1]$, with $Q(x, dy) = q(x,y)\,\mathrm{dy}$;
- Accept each move with probability

$$\alpha(x,y) = \min\left[1, \frac{\pi(y)\ q(y,x)}{\pi(x)\ q(x,y)}\right],$$

  otherwise don't move;
- New kernel

$$P(x, \mathrm{dy}) = \alpha(x,y)Q(x,\mathrm{dy}) + \left(1 - \int_{\mathbb{R}^d} \alpha(x,z)Q(x,\mathrm{dz})\right)\delta_x(dy);$$

- Ensure the Markov chain is reversible with respect to probability measure π

$$\pi(\mathrm{dx})P(x,\mathrm{dy}) = \pi(\mathrm{dy})P(y,\mathrm{dx}), \quad \text{for all } x, y \in \mathbb{R}^d,$$

  which implies it has the desired invariant measure π.

Metropolis-Adjusted Langevin Algorithm (MALA)

Input: Initial point x_0 from a starting distribution μ_0, step size h, number of steps n.

Output: Sequence of samples $x_1, x_2, \ldots, x_n$

for $k = 0, 1, \ldots, n-1$ **do**

  Draw from the proposal distribution $y_k \sim \mathcal{N}(x_k - h\nabla f(x_k), 2h\mathbf{I}_d)$;

  Compute the acceptance rate

$$\alpha_k \leftarrow \min\left\{ \frac{\exp\left(-f(y_k) - \|x_k - y_k + h\nabla f(y_k)\|_2^2 / 4h\right)}{\exp\left(-f(x_k) - \|y_k - x_k + h\nabla f(x_k)\|_2^2 / 4h\right)}, 1 \right\};$$

  Draw $u \sim \mathrm{Unif}[0,1]$;

  if $u < \alpha_k$ **then**

    Accept the proposal: $x_{k+1} \leftarrow y_k$;

  else

    Reject the proposal: $x_{k+1} \leftarrow x_k$;

  end

end

Metropolis-Hastings Algorithms Are Fast

Definition 11 ($\varepsilon-$mixing time)

Suppose a MCMC algorithm with target distribution π starts from initial distribution μ_0 and the distribution at step k denoted by μ_k, then the $\varepsilon-$mixing time is defined by

$$t_{\mathrm{mix}}(\varepsilon, \mu_0) := \min\{k \in \mathbb{N} \mid \mathrm{TV}(\mu_k, \pi) \leq \varepsilon\}.$$

Algorithm	Strongly log-concave	Weakly log-concave
ULA [Dalalyan, 2017]	$\mathcal{O}\left(\frac{d\kappa^2 \log^2(\beta/\varepsilon)}{\varepsilon^2}\right)$	$\widetilde{\mathcal{O}}\left(\frac{d^3 L^2}{\varepsilon^4}\right)$
MALA [Dwivedi et al., 2019]	$\mathcal{O}\left(\max\left\{d\kappa,\, d^{0.5}\kappa^{1.5}\right\}\log\left(\frac{\beta}{\varepsilon}\right)\right)$	$\widetilde{\mathcal{O}}\left(\frac{d^2 L^{1.5}}{\varepsilon^{1.5}}\right)$

Table: Scalings of upper bounds on ε-mixing time for ULA and MALA in $\mathbb{R}^d$ with target $\pi \propto e^{-f}$.

Geometric Interpretation of the MH Adjustment

- Proposal kernel Q and $P(Q)$ be the Metropolis-Hastings kernel obtained from Q;
- $\mathcal{R}(\pi)$ be the space of kernels K which are reversible with respect to π and such that for each $x \in \mathbb{R}^d$, $K(x, dy) = k(x, y)\,\mathrm{dy}$, for $y \neq x$;
- Distance on the space of kernels $K(x, dy) = k(x, y)\,\mathrm{dy}$, for $y \neq x$,

$$d(K, K') := \int_{(\mathbb{R}^d \times \mathbb{R}^d)\setminus\Delta} \left|k(x, y) - k'(x, y)\right| \pi(\mathrm{dx})\, \mathrm{dy}$$

where $\Delta := \{(x, x) \mid x \in \mathbb{R}^d\}$ is the diagonal in $\mathbb{R}^d \times \mathbb{R}^d$;

Theorem 12 ([Billera and Diaconis, 2001])

The mapping $Q \mapsto P(Q)$ is a projection of the proposal kernel Q onto the space of reversible Markov chains with stationary distribution π with respect to distance d,

$$P(Q) \in \operatorname*{arg\,min}_{K \in \mathcal{R}(\pi)} d(Q, K).$$

MH Adjustment Based Sampling Algorithms

Optimization algorithms

e.g. Newton method

$$x_{k+1} = x_k - \alpha_k \left(\nabla^2 f(x_k)\right)^{-1} \nabla f(x_k)$$

↓

Add some noise at each iteration

$$x_{k+1} = x_k - \alpha_k \left(\nabla^2 f(x_k)\right)^{-1} \nabla f(x_k) + \beta_k \xi_k,$$

where $\xi_k \sim N(0, I_d)$

↓

Do Metropolis-Hastings adjustment at each iteration

Goal: Sampling from target distribution

$$\pi(x) \propto e^{-f(x)}$$

Need to analysis:

- What is the optimal noise level β_k?
- What is the optimal step size α_k?
- Bound the mixing time.

Outline

Generative Modeling: Density Estimation

- **Setting 2:** We only have a collection of i.i.d. samples $x_1, x_2, \cdots, x_N$;
- **Density estimation:** Setting 2 $\Longrightarrow$ Setting 1;
- But density estimation can NOT avoid the curse of dimensionality.

Theorem 13 ([Tsybakov, 2009])

Given N i.i.d. samples $x_1, \ldots, x_N$ from a bounded pdf $f \in C^{m,\alpha}(\mathbb{R}^d)$ and let $\beta = m + \alpha$, then the minimax risk of an estimation $\hat{f}$ of f under the quadratic loss function $\ell(\hat{f}, f) := \|\hat{f} - f\|_2^2 = \int_{[0,1]^n} (f(x) - \hat{f}(x))^2 \, dx$ satisfies

$$\inf_{\hat{f}} \sup_{f \in P_\beta} \|\hat{f} - f\|_2^2 \gtrsim N^{-\frac{2\beta}{d+\beta}}.$$

The infimum is taken over all estimators $\hat{f}$ built on the data $x_1, \ldots, x_N$.

Likelihood-based Models

- Parameterization: $\pi(x) \approx p_\theta(x)$;
- MLE: learn θ by maximizing the log-likelihood of the data

$$\max_\theta \sum_{i=1}^{N} \log p_\theta(x_i).$$

- Examples: autoregressive models, normalizing flow models, energy-based models, variational auto-encoders (VAEs), etc.
- Disadvantage: The normalization constant becomes difficult to compute when the dimension is high.

MLE as Optimization in the Space of Probability Measures

Consider the space of probability measures $\{P_\theta \; ; \; \theta \in \Theta, P_\theta \ll m, \; p_\theta = \frac{\mathrm{d}\, P_\theta}{\mathrm{d}\, m}\}$, then

$$\mathrm{KL}(\pi \| P_\theta) = \int_{\mathbb{R}^d} \log \frac{\mathrm{d}\,\pi}{\mathrm{d}\,P_\theta} \,\mathrm{d}\,\pi = \underbrace{\int_{\mathbb{R}^d} \log \pi(x) \,\mathrm{d}\,\pi}_{\text{independent of } \theta} - \underbrace{\int_{\mathbb{R}^d} \log p_\theta(x) \,\mathrm{d}\,\pi}_{= \mathbb{E}_{X\sim\pi}[\log p_\theta(X)]} .$$

Hence,

$$\theta^* \in \arg\min_{\theta\in\Theta} \mathrm{KL}(\pi \| P_\theta) \iff \theta^* \in \arg\max_{\theta\in\Theta} \mathbb{E}_{X\sim\pi}[\log p_\theta(X)].$$

By the Law of Large Numbers (LLN),

$$\mathbb{E}_{X\sim\pi}[\log p_\theta(X)] \approx \frac{1}{N}\sum_{i=1}^{N} \log p_\theta(x_i) \longleftarrow \textbf{log-likelihood}.$$

$$\boxed{\textbf{MLE} \iff \textbf{minimizing } \mathrm{KL}(\pi \| \cdot) + \textbf{LLN}}$$

Score-based Generative Models

- ULA with target $\pi(x) \propto e^{-f(x)}$ needs the information of $-\nabla f(x) = \nabla \log \pi(x)$, which is the definition of **score of** π;

- **Score matching:**

$$\min_{\theta \in \Theta} \ \mathbb{E}_{X \sim \pi} \left\| \nabla \log \pi(X) - s_\theta(X) \right\|_2^2 \iff \min_{Q \in \mathcal{M}} \mathcal{J}(\pi \| Q), \tag{SM}$$

where $\mathcal{J}(\pi \| Q)$ is the Fisher divergence of π w.r.t. Q defined by

$$\mathcal{J}(\pi \| Q) := \mathbb{E}_{X \sim \pi}[\|\nabla \log \pi(X) - \nabla \log q(X)\|^2]$$

and $\mathcal{M} = \{Q \in \mathcal{P}(\mathbb{R}^d) \ ; \ \text{the score of } Q \text{ belongs to } \{s_\theta \ ; \ \theta \in \Theta\}\}$.

Denoising Score Matching

- Denoising score matching problem

$$\min_{\theta \in \Theta} \; DSM(s_\theta) := \mathbb{E} \left\| \nabla \log \mu_Y(Y) - s_\theta(Y) \right\|_2^2, \tag{DSM}$$

  where $Y = aX + \sigma Z$, $a \in \mathbb{R}, \sigma > 0$,$X \sim \pi$, $Z \sim N(0, I_d)$, Z is independent of X and μ_Y is the density of Y w.r.t. Lebesgue measure.
- Equivalent optimization problem:

$$\arg\min_{Q \in \mathcal{M}} \mathcal{J}(\mu_Y \| Q) = \arg\min_{\theta} DSM(s_\theta) = \arg\min_{\theta} \mathbb{E} \left[\left\| s_\theta(Y) + \frac{1}{\sigma} Z \right\|_2^2 \right],$$

- By LLN, the objective can be replaced with

$$\min_{\theta} \; \frac{1}{N} \sum_{i=1}^{N} \left\| s_\theta(ax_i + \sigma z_i) + \frac{1}{\sigma} z_i \right\|_2^2,$$

  where $\{x_i\}_{i=1}^N$ are i.i.d. given samples drawing from π and $\{z_i\}_{i=1}^N \overset{i.i.d.}{\sim} N(0, I_d)$.

Score-based Diffusion Model: DDPM

Forward process:

$$dX_t = -X_t dt + \sqrt{2}\, dB_t, \quad X_0 \sim q_0 := \pi,\ X_t \sim q_t,\ t \in [0, T],$$

by Ito's lemma, whose solution can be written as

$$X_t = e^{-t} X_0 + \left(1 - e^{-2t}\right)^{1/2} Z_t, \quad Z_t \sim N(0, I_d).$$

Reverse process:

$$dX_t^{\leftarrow} = \left[X_t^{\leftarrow} + 2\nabla \log q_{T-t}(X_t^{\leftarrow})\right] dt + \sqrt{2}\, dB_t, \quad X_0^{\leftarrow} \sim q_T \approx \gamma^d := \text{law of } N(0, I_d),$$

which is designed by Fokker-Planck equation to ensure $\text{Law}(X_t^{\leftarrow}) = \text{Law}(X_{T-t})$.

DDPM: Score Matching

For all given t, the score matching problem for X_t

$$\min_{\theta_t \in \Theta_t} \mathbb{E} \left\| \nabla \log q_t(X_t) - s_t^{(\theta_t)}(X_t) \right\|_2^2 \iff \min_{\theta_t \in \Theta_t} \mathbb{E} \left[\left\| s_t^{(\theta_t)}(X_t) + \frac{1}{\sqrt{1 - e^{-2t}}} Z_t \right\|_2^2 \right],$$

By LLN,

$$\min_{\theta_t \in \Theta_t} \frac{1}{N} \sum_{i=1}^{N} \left\| s_t^{(\theta_t)}\left(x_t^{(i)}\right) + \frac{1}{\sqrt{1 - \exp(-2t)}} z_t^{(i)} \right\|^2, \qquad \text{(DDPM-SM)}$$

where $(z_t^{(i)})_{i \in [N]}$ are i.i.d. standard Gaussian samples independent of the data $(x_0^{(i)})_{i \in [N]}$.

DDPM: Error Analysis

Forward process:

$$dX_t = -X_t dt + \sqrt{2}\, dB_t, \quad X_0 \sim q_0 := \pi,\ X_t \sim q_t,\ t \in [0, T].$$

Reverse process:

$$dX_t^{\leftarrow} = \left[X_t^{\leftarrow} + 2\nabla \log q_{T-t}(X_t^{\leftarrow})\right] dt + \sqrt{2}\, dB_t, \quad X_0^{\leftarrow} \sim q_T \approx \gamma^d := \text{law of } N(0, I_d),$$

Partition : Partition the interval $[0, T]$ to $[kh, (k+1)h]$, $k = 0, 1, \cdots, K-1$ with $h > 0,\ K = T/h$. Integrate the reverse process from $[kh, t],\ t \in [kh, (k+1)h]$,

$$X_t^{\leftarrow} = X_{kh}^{\leftarrow} + \int_{kh}^{t} X_s^{\leftarrow} ds + \int_{kh}^{t} 2 \underbrace{\nabla \log q_{T-s}(X_s^{\leftarrow})}_{\approx s_{T-s}^{(\theta_{T-s})}(X_s^{\leftarrow}) \approx s_{T-kh}^{(\theta_{T-kh})}(X_{kh}^{\leftarrow})} ds + \sqrt{2}(B_t - B_{kh}).$$

Score matching and integral approximation:

$$dX_t^{\leftarrow} = \left\{ X_t^{\leftarrow} + 2\, s_{T-kh}^{(\theta_{T-kh})}(X_{kh}^{\leftarrow}) \right\} dt + \sqrt{2}\, dB_t, \qquad t \in [kh, (k+1)h],$$

which is a linear SDE and can be integrated in closed form.

Diffusion Model: Convergence Analysis

Let $p_t := \mathrm{Law}(X_t^{\leftarrow})$, DDPM has mainly three types of errors.

1. The error made at initialization of reverse process, γ^d used instead of q_T.
2. The score matching error, which depends on sample size N and neural network.
3. The discretization of the reverse process, which depends on the step-size h.

Assumption 1 (Lipschitz score)

For any $t \geq 0$, the score $\nabla \log q_t$ is L-Lipschitz.

Assumption 2 (Second moment bound)

Assume that $M_2^2 := \mathbb{E}_{X \sim q_0} \|X\|_2^2 < \infty$.

Assumption 3 (Score estimation error bound)

For $k = 1, \ldots, K$,

$$\mathbb{E}\left[\left\| s_{kh}^{(\theta_{kh})}(X_{kh}) - \nabla \log q_{kh}(X_{kh}) \right\|_2^2\right] \leq \varepsilon_{\text{score}}^2.$$

Diffusion Model: Convergence Analysis

Theorem 14 ([Chen et al., 2023])

Under the three previous assumptions. Let p_T be the output of the DDPM algorithm at time $T > 0$, with $h = T/K$ and K the number of steps, suppose $h \lesssim 1/L$, then

$$\mathrm{TV}(p_T, q_0) \lesssim \underbrace{\sqrt{\mathrm{KL}(q_0 \,\|\, \gamma^d)}\, e^{-T}}_{\text{convergence of forward process}} + \underbrace{(L\sqrt{d\,h} + LM_2 h)\sqrt{T}}_{\text{discretization error}} + \underbrace{\epsilon_{\text{score}}\sqrt{T}}_{\text{score estimation error}} .$$

DDPM can efficiently sample from multi-modal target measures as long as the score estimation is good.

Outline

Summary

- Many applications can be viewed as optimization problems over the space of probability measures;
- From the idea of sampling: **probability perspective** $\Longleftrightarrow$ **geometric perspective**;

  The merit of the right gradient flow formulation of a dissipative evolution equation is that it separates energetics and kinetics: The energetics endow the state space with a functional, the kinetics endow the state space with a (Riemannian) geometry via the metric tensor.

  [Otto, 2001].
- **Functional:** exclusive KL divergence $\mathrm{KL}(\pi\|\cdot)$, inclusive KL divergence $\mathrm{KL}(\mu\|\cdot)$, Fisher divergence $\mathcal{J}(\pi\|\cdot)$, etc.
- **Geometry:** Wasserstein geometry, maximum mean discrepancy (MMD) geometry, Fisher-Rao geometry, etc.

Future Works

- What role does the **Metropolis–Hastings adjustment** play in Wasserstein gradient flows, and how can this approach be applied to other applications?

- From the perspective of optimization over spaces of probability measures, what are many **learning-based methods in generative modeling** actually doing? How can we transfer these methods to other applications?

- Many optimization problems over spaces of probability measures come with **constraints** (e.g., variational inference, sampling for generative models with hard constraints, etc.). Can we systematically summarize and further develop the algorithms and theory for **constrained optimization problems over spaces of probability measures**?

Thanks!

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