Discretization Issues in Sampling

Wasserstein Gradient Flow : Applications

September 17, 2025

Outline

1. Discretization in Optimization
2. Handling Non-Smoothness: Proximal Methods
3. Discretization in Sampling: Langevin Dynamics
4. Correcting Discretization Bias: MALA
5. Analysis of Metropolized Methods
6. Improving Conditioning: Proximal Sampling

Optimization Example: Finite Dimensions

Problem Setup

Minimize a smooth convex loss $\mathcal{L}(\theta)$ over $\theta \in \mathbb{R}^d$:

$$\min_{\theta \in \mathbb{R}^d} \mathcal{L}(\theta)$$

Example: Linear regression loss $\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \|y_i - \theta^T x_i\|^2$.

Continuous Ideal: Gradient Flow

The path of steepest descent is given by the differential equation:

$$\dot{\theta}_t = -\nabla \mathcal{L}(\theta_t)$$

This continuous flow converges to the minimum under convexity.

Optimization Example: Finite Dimensions

Discrete Approximation: Gradient Descent

We approximate the flow using discrete steps (Euler discretization):

$$\theta_{k+1} = \theta_k - h\nabla\mathcal{L}(\theta_k)$$

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- Convexity of $\mathcal{L}$ ensures convergence of the continuous time flow to the minimum
- Smoothness of $\mathcal{L}$ ensures that the discretization is asymptotically unbiased (i.e, converges to the minimum)

Optimization over Measures

Problem Setup: Minimizing KL Divergence

Minimize KL divergence over probability measures $\mu \in \mathcal{P}(\mathbb{R}^d)$:

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

where $\pi(x) \propto e^{-V(x)}$ is the target measure. If μ has density ρ w.r.t. Lebesgue measure, this is equivalent to minimizing:

$$F(\mu) = \int V d\mu + \int \rho \log \rho \, dx + \mathrm{const}$$

This involves the negative entropy $-H(\mu) = \int \rho \log \rho \, dx$.

Optimization over Measures

Wasserstein Gradient Flow

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Discretization Challenge: Non-Smoothness?

The entropy term $H(\mu)$ behaves poorly. The function $x \mapsto x \log x$ has derivative $1 + \log x$, which blows up as $x \to 0^+$.

$$-H(\mu) = \int \mu(x) \log \mu(x) dx$$

This inherent non-smoothness (at the boundary of the space of measures) makes naive discretization of the corresponding gradient flow challenging. Smoothness conditions on V (e.g., $\nabla^2 V \leq \beta I$) are needed, but the entropy itself poses problems.

Example: L1 Regularization

Problem Setup

Consider minimizing a smooth loss plus an L1 penalty (LASSO):

$$\min_{\theta \in \mathbb{R}^d} \mathcal{L}(\theta) + \lambda \|\theta\|_1$$

The L1 norm promotes sparsity but is non-differentiable at $\theta_i = 0$.

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Problem with Naive Gradient Descent

A simple gradient step is ill-defined due to the non-differentiability:

$$\theta_{k+1} = \theta_k - h\nabla\mathcal{L}(\theta_k) - h\nabla(\lambda\|\theta_k\|_1) \quad \text{(Problematic! } \nabla\|\cdot\|_1 \text{ undefined)}$$

Proximal Gradient Descent

Algorithm: Proximal Gradient Descent

Split the objective into smooth ($\mathcal{L}$) and non-smooth ($\lambda\|\cdot\|_1$) parts.

Alternate between:

1. Gradient step on the smooth part:

$$\theta_{k+1/2} = \theta_k - h\nabla\mathcal{L}(\theta_k)$$

2. Proximal step on the non-smooth part:

$$\theta_{k+1} = \operatorname*{prox}_{h\lambda\|\cdot\|_1}\left(\theta_{k+1/2}\right)$$

Proximal Operator Definition

The proximal operator is defined as the solution to a small optimization problem:

$$\operatorname{prox}_g(z) = \arg\min_{\theta} \left\{ g(\theta) + \frac{1}{2}\|\theta - z\|^2 \right\}$$

For $g(\theta) = \gamma\|\theta\|_1$, this becomes:

$$\operatorname{prox}_{\gamma\|\cdot\|_1}(z) = \arg\min_{\theta\in\mathbb{R}^d} \left\{ \gamma\|\theta\|_1 + \frac{1}{2}\|\theta - z\|^2 \right\}$$

This has a closed-form solution: the *soft-thresholding* operator.

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$$(\operatorname{prox}_{\gamma\|\cdot\|_1}(z))_i = \operatorname{sign}(z_i)\max(|z_i| - \gamma, 0)$$

This allows handling non-smooth terms rigorously and often efficiently.

Extension to Measures: Proximal Entropy

Goal

Apply the proximal idea to minimize functionals involving entropy $H(\mu)$, like the KL divergence.

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Proximal Operator for Entropy (JKO Scheme Idea)

Define a proximal operator for the entropy functional $H(\mu)$:

$$\underset{hH}{\operatorname{prox}}(\mu_k) = \arg\min_{\nu \in \mathcal{P}(\mathbb{R}^d)} \left\{ H(\nu) + \frac{1}{2h} W_2^2(\nu, \mu_k) \right\}$$

where W_2 is the 2-Wasserstein distance. This finds a measure ν that balances minimizing entropy (spreading out) and staying close to μ_k in the Wasserstein sense.

Extension to Measures: Proximal Entropy

Challenge

This step defines the celebrated Jordan-Kinderlehrer-Otto (JKO) scheme, a variational approach to gradient flows in Wasserstein space. However, computing this proximal step is generally very difficult. "Not very nice". Alternatives like convolution methods can also be complex.

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So, how do we sample ??

Langevin Diffusion SDE

Goal

Sample from a target distribution $\pi(x) \propto e^{-V(x)}$.

Continuous Time Process: Langevin SDE

Consider the Stochastic Differential Equation (SDE):

$$dX_t = \underbrace{-\nabla V(X_t)dt}_{\text{Drift towards minimum}} + \underbrace{\sqrt{2}dB_t}_{\text{Random diffusion}}$$

where B_t is standard Brownian motion.

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Stationary Distribution

Under suitable conditions on V, the unique stationary (equilibrium) distribution of the process X_t is exactly the target distribution $\pi(x) \propto e^{-V(x)}$.

Problem: Euler-Maruyama Discretization (ULA)

Discrete Approximation: Unadjusted Langevin Algorithm (ULA)

Apply the simplest time discretization (Euler-Maruyama) to the Langevin SDE:

$$X_{k+1} = X_k - h\nabla V(X_k) + \sqrt{2h}Z_k, \quad Z_k \sim \mathcal{N}(0, I)$$

This is computationally simple: take a gradient step and add Gaussian noise.

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Issue: Discretization Bias

For any step size $h > 0$, the Markov chain generated by ULA does **not** have π as its exact stationary distribution.

$$\pi_{ULA}^{(h)} \neq \pi$$

The error $||\pi_{ULA}^{(h)} - \pi||_{W_2}$ depends on h. Achieving high accuracy requires very small h, which is inefficient.

Solution: Metropolis-Adjusted Langevin Algorithm (MALA)

Idea

Use the ULA step as a proposal mechanism within a Metropolis-Hastings framework to correct the discretization bias.

Solution: Metropolis-Adjusted Langevin Algorithm (MALA)

Theorem 1 (MALA Algorithm)

Given current state X_k:

1. **Propose:** *Generate a candidate Y using one ULA step:*

$$Y = X_k - h\nabla V(X_k) + \sqrt{2h}\,Z_k, \quad Z_k \sim \mathcal{N}(0, I).$$

2. **Accept/Reject:** *Accept Y with probability $\alpha(X_k, Y)$:*

$$\alpha(X_k, Y) = \min\left\{1, \frac{\pi(Y)\,q(Y, X_k)}{\pi(X_k)\,q(X_k, Y)}\right\},$$

where $q(x, y) \propto \exp\left(-\frac{\|y-(x-h\nabla V(x))\|^2}{4h}\right)$ is the proposal transition density.

3. **Update:** *If accepted, $X_{k+1} = Y$; otherwise, $X_{k+1} = X_k$.*

Solution: Metropolis-Adjusted Langevin Algorithm (MALA)

Key Property: The MALA Markov chain has **exactly** $\pi(x) \propto e^{-V(x)}$ as its invariant distribution for **any** step size $h > 0$. (Though acceptance rate decreases for large h).

Connection to Metropolized HMC

Literature

Appendix A of *[Logsmooth Gradient Concentration and Tighter Runtimes for Metropolized Hamiltonian Monte Carlo, Lee et. al. '20]* establishes an equivalence.

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Equivalence Result

A specific variant of Metropolized Hamiltonian Monte Carlo (MHMC) using exactly **one** leapfrog integration step is **algorithmically equivalent** to MALA.

- Both generate proposals of the form:

  $$Y = X_k - c\nabla V(X_k) + \mathcal{N}(0, \sigma^2 I)$$

  (with constants matched appropriately).
- Both use a Metropolis-Hastings correction based on the target π.

Connection to Metropolized HMC

Implication

Rigorous analysis and theoretical guarantees (like mixing time bounds) derived for 1-step MHMC directly apply to MALA.

Theorem: Mixing Time of MALA

Theorem 2 (Mixing of Metropolized Langevin Dynamics (via MHMC))

Let $V : \mathbb{R}^d \to \mathbb{R}$ be L-smooth ($\nabla^2 V \preceq LI$) and μ-strongly convex ($\nabla^2 V \succeq \mu I$). Let $\kappa = L/\mu \geq 1$ be the condition number. Target distribution is $\pi(x) \propto e^{-V(x)}$. Assume initialization $X_0 \sim \mathcal{N}(x^*, L^{-1}I)$, where x^* minimizes V.
Then there exists $C > 0$ such that for k iterations where

$$k = O\left(\kappa\, d \log\left(\frac{\kappa}{\epsilon}\right) \log\left(d \log \frac{\kappa}{\epsilon}\right) \log\left(\log \frac{\kappa}{\epsilon}\right)\right) = \tilde{O}(\kappa d)$$

the distribution ρ_k of X_k satisfies Total Variation distance:

$$\|\rho_k - \pi\|_{TV} \leq \epsilon.$$

($\tilde{O}$ hides logarithmic factors in $\kappa, d, 1/\epsilon$).

Theorem: Mixing Time of MALA (Discussion)

Remark

The previous theorem shows that MALA achieves ϵ-accuracy in sampling π after $\tilde{O}(\kappa d)$ steps. This is efficient, but the dependence on the condition number κ can be problematic if κ is large.

The Problem of Large κ

Recap

The mixing time of MALA scales as $\tilde{O}(\kappa d)$.

Challenge: Ill-Conditioned Problems

If the potential V is poorly conditioned (e.g., features have vastly different scales), $\kappa = L/\mu$ can be very large. This makes the $\tilde{O}(\kappa d)$ mixing time prohibitive.

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Goal

Can we modify the sampling approach to mitigate the dependence on the original κ?

Sampling :: Optimization Analogies

To solve this problem, we would like to draw some analogies with optimization.

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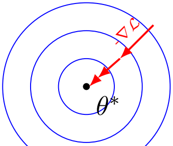
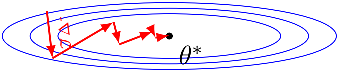
Note that sampling from $\pi \propto e^{-V(x)}$ is equivalent to optimization of a certain functional (specifically, $\int V d\mu + \int \frac{d\mu}{d\lambda} \log \frac{d\mu}{d\lambda}$) over the space of measures.

Sampling :: Optimization Analogies

Sampling	**Optimization**
$\pi(x) \propto e^{-V(x)}$	$\min_\theta \mathcal{L}(\theta)$
Ill-Conditioned Density $\kappa_V = L/\mu \gg 1$ Elongated contours $\implies$ Slow Mixing (ULA/MALA)	**Ill-Conditioned Objective** $\kappa_{\mathcal{L}} = L/\mu \gg 1$ Elongated level sets $\implies$ Slow Convergence (GD)
Well-conditioned ($\kappa \approx 1$)  	Ill-conditioned ($\kappa \gg 1$) 

Sampling :: Optimization Analogies

- We have already dealt with a rather extreme case of ill-conditioned objective earlier: $\int V d\mu + \int \frac{d\mu}{d\lambda} \log \frac{d\mu}{d\lambda}$.

- Specifically, the entropy term $\int \frac{d\mu}{d\lambda} \log \frac{d\mu}{d\lambda}$ is non-smooth, making its condition number infinity!

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- Specifically, the entropy term $\int \frac{d\mu}{d\lambda} \log \frac{d\mu}{d\lambda}$ is non-smooth, making its condition number infinity!

- The way we dealt with this was to use the **proximal operator**.

Proximal Methods Comparison

Sampling	**Optimization**
Proximal Sampler (Gibbs) Step: $X \sim p(x \mid y)$ where $p(x \mid y) \propto e^{-V(x)-\frac{1}{2h}\Vert x-y\Vert^2}$ Mode is $\text{prox}_{hV}(y)$ Benefit: Uses well-conditioned $V_y(x) = V(x) + \frac{1}{2h}\Vert x-y\Vert^2$	**Proximal Gradient Desc.** Update: $\theta_{k+1} = \text{prox}_{hg}(\theta_k - h\nabla f(\theta_k))$ for min $f(\theta) + g(\theta)$ Benefit: Handles non-smooth $g(\theta)$
(Leveraging proximal structure $\min_x\{Func(x) + \frac{1}{2\lambda}\Vert x-z\Vert^2\}$ *)*	

Proximal Sampling Algorithm

Augmented Target Distribution

Define a joint distribution $\boldsymbol{\pi}$ on $(x, y) \in \mathbb{R}^d \times \mathbb{R}^d$:

$$\boldsymbol{\pi}(x, y) \propto \exp\left(-V(x) - \frac{1}{2h}\|y - x\|^2\right)$$

Note: The marginal distribution of x under $\boldsymbol{\pi}$ is the original target $\pi(x) \propto e^{-V(x)}$. $\int \boldsymbol{\pi}(x, y)dy \propto e^{-V(x)}$.

Proximal Sampling Algorithm

Proximal Sampler (Gibbs Sampling on π)

Iterate the following steps:

1. Given $X_k = x$, sample $Y_{k+1} \sim \boldsymbol{\pi}^{Y|X=x}$:

$$Y_{k+1} \sim \mathcal{N}(x, hI) \quad \text{(Simple Gaussian step)}$$

2. Given $Y_{k+1} = y$, sample $X_{k+1} \sim \boldsymbol{\pi}^{X|Y=y}$:

$$\boldsymbol{\pi}^{X|Y=y}(x) \propto \exp\left(-V(x) - \frac{1}{2h}\|y - x\|^2\right) \quad \text{(RGO Sampling)}$$

This Gibbs sampler targets $\boldsymbol{\pi}$, so the X samples marginally target π.

Theorem: Improved Conditioning

Implementing Step 2: Sampling from RGO

Step 2 requires sampling from $\exp(-V_y(x))$, where the potential is modified:

$$V_y(x) = V(x) + \frac{1}{2h}\|y - x\|^2$$

We can use MALA (or another sampler) for this sub-problem.

Theorem: Improved Conditioning

Condition Number Improvement

Let $\mu I \preceq \nabla^2 V(x) \preceq LI$. The Hessian of the modified potential $V_y(x)$ is:

$$\nabla^2 V_y(x) = \nabla^2 V(x) + \frac{1}{h} I$$

The condition number κ_y for the sub-problem is: $\kappa_y = \frac{L+1/h}{\mu+1/h}$

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Limiting Behavior

As the proximal parameter $h \to 0$:

$$\lim_{h \to 0} \kappa_y = \lim_{h \to 0} \frac{hL + 1}{h\mu + 1} = \frac{1}{1} = 1$$

For small h, the condition number of the MALA sub-problem becomes $\kappa_y \approx 1$, regardless of the original $\kappa = L/\mu$.

Conclusion: Benefits of Proximal Sampling

Key Idea

Proximal sampling alternates between:

1. A simple Gaussian step $Y \sim \mathcal{N}(X, hI)$.
2. Sampling X from a modified potential $V_y(x) = V(x) + \frac{1}{2h}\|y - x\|^2$.

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Advantage

The second step (sampling from $\exp(-V_y)$) can be done using MALA. Crucially, the potential $V_y(x)$ has a much better condition number $\kappa_y \approx 1$ for small h.

Conclusion: Benefits of Proximal Sampling

Result

Applying Theorem 2 to the MALA sub-problem suggests its mixing time is $\tilde{O}(\kappa_y d) \approx \tilde{O}(d)$. This removes the potentially large factor κ from the MALA iterations within the proximal sampler. Proximal sampling offers a way to efficiently sample from ill-conditioned distributions $\pi \propto e^{-V}$ by solving a sequence of well-conditioned sub-problems.