

Proximal Algorithms in Wasserstein Space

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Abstract

This report investigates a basic type of fully backward optimization method – Wasserstein Proximal Algorithm (also known as JKO scheme), in the space of probability measure. Theoretically, we compare the proximal algorithm in Wasserstein Space with its counterpart in Euclidean space to provide some intuitive understanding and some existing convergence rate analysis. We also provide the proof for "geodesic convexity + quadratic growth \Rightarrow linear convergence". The main contribution is we proved proximal algorithm in Wasserstein space with merely (uniform) LSI can ensure linear convergence. Experimentally, we verify the convergence result of Wasserstein Proximal Algorithms in some simple cases and explore its performance on a two-layer neural network.

1 Introduction

The task of minimizing a functional over the space of probability distributions is common in machine learning, especially in the field of mean-field dynamics of a two-layer neural network [CB18] and generative modeling [Che+24].

Mean-Field Limit - A Particle Perspective. Assume we have a two-layer NN,

$$f(\theta; x) = \frac{1}{m} \sum \varphi(\theta_i; x) = \int \varphi(\theta; x) d\rho_m(\theta) \quad (1)$$

where $\theta_i = (a_i, w_i)$ with $a_i \in \mathbb{R}, w_i \in \mathbb{R}^{d-1}$, $x \in \mathbb{R}^{d-1}$, $y \in \mathbb{R}$, $\rho_m = \frac{1}{m} \sum \delta_{\theta_i}$ and $\varphi(\theta) = a\phi(b^T x)$. Consider a dataset $(x, y) \sim p(x, y)$ and a convex loss $l(\cdot)$,

$$\begin{aligned} R(\rho_m) &= \mathbb{E}_{(x, y) \sim p} l(f(\theta, x), y) \\ &= \mathbb{E}_{(x, y) \sim p} l\left(\int \varphi(\theta; x) d\rho_m(\theta), y\right) \end{aligned} \quad (2)$$

and if we assume $m \rightarrow \infty$, we can formulate the optimization of two-layer NN as,

$$\min_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} R(\mu)$$

which is an optimization problem on space of probability measures.

1.1 The Contributions

In this report, we focus on the comparison between the Forward algorithm and Backward Algorithm in Wasserstein Space. We first verify the convergence result of Wasserstein Proximal Algorithms in Langevin dynamics and focus on its performance on two-layer NN optimization.

1.2 The Notations

Let $\mathcal{P}_2(\mathbb{R}^d)$ be the space of probability measure with the finite second moment. The \mathcal{W}_2 distance is defined as the square root of,

$$\mathcal{W}_2(\mu, v)^2 = \min_{\gamma \in \Pi(\mu, v)} \int \|x - y\|^2 d\gamma(x, y)$$

where $\Pi(\mu, v) \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d)$ whose marginals are μ and v respectively. For a measurable map $T : \mathbb{R}^d \rightarrow \mathbb{R}^d$, let $T_\#$ be its pushforward.

Note that \mathcal{W}_2 space is not a flat metric space, but is positively curved. We define that F is convex along geodesics defined as: for every $\rho_0, \rho_1 \in \mathcal{P}_2(\mathbb{R}^d)$, F is λ -convex if

$$F(\rho_t) \leq (1-t)F(\rho_0) + tF(\rho_1) - \frac{1}{2}\lambda(1-t)t\mathcal{W}_2(\rho_0, \rho_1)$$

where ρ_t is the constant speed shortest curve, and can be identified as $((1-t)Id + tT)_\# \rho_0$ when $\rho_0 \ll \mathcal{L}(\mathbb{R}^d)$.

$\lambda = 0$ refers to normal geodesically convexity, and $\lambda > 0$ is called as strongly geodesically convexity.

We also refer to [AGS05] for the concept of convexity along generalized geodesics. Notice that,

$$\text{If } F : \mathcal{P}_2^a(\mathbb{R}^d) \rightarrow \mathbb{R}, \text{ Convexity along generalized geodesics} \Rightarrow \text{Convexity along geodesic}$$

We also have similar implication under $F : \mathcal{P}_2^a(\mathbb{R}^d)$. However, the definition for convexity along generalized geodesic is stronger in this case [AGS05].

Let $F : \mathcal{P}_2^a(\mathbb{R}^d) \rightarrow \mathbb{R}$ be lower semicontinuous and lower bounded. We say that $\xi \in L_2(\rho; \mathbb{R}^d)$ belongs to the Frechet subdifferential $\partial F(\rho)$ of F at ρ if for any $\rho' \in \mathcal{P}_2^a(\mathbb{R}^d)$,

$$F(\rho') \geq F(\rho) + \int_{\mathbb{R}^d} \langle \xi, T_{\rho}^{\rho'}(\theta) - \theta \rangle d\rho(\theta) + o(\mathcal{W}_2(\rho, \rho'))$$

If $\xi \in \partial F(\rho)$ satisfies the following for any transport map T ,

$$F(T_\# \rho) \geq F(\rho) + \int_{\mathbb{R}^d} \langle \xi, T(\theta) - \theta \rangle d\rho(\theta) + o(\|T - Id\|_{L_2(\rho; \mathbb{R}^d)})$$

then it is called strong subdifferential. $\nabla \frac{\delta F}{\delta \rho}(\rho)$ is strong differential where $\frac{\delta F}{\delta \rho}(\rho) : \mathbb{R}^d \rightarrow \mathbb{R}$ is first variation.

2 Related Works

2.1 Forward and Backward Algorithms in Wasserstein Space

Assume we have a functional $F : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, our goal is

$$\min_{\rho \in \mathcal{P}_2(\mathbb{R}^d)} F(\rho)$$

Forward Algorithm in Wasserstein Space.

$$\rho_{k+1} = (I - \eta \nabla \frac{\delta F}{\delta \rho}(\rho_k))_\# \rho_k \quad (3)$$

where $\nabla \frac{\delta F}{\delta \rho}(\rho_k)$ is the Wasserstein differential. It might look difficult to understand at first, but we can understand it from the particle perspective of two-layer NN. If we have a ρ which is a discrete measure, we need to optimize loss $R(\rho)$, then Eqn. 3 can be understood as the gradient descent (GD) for two-layer NN:

$$\theta_i^{k+1} = \theta_i^k - m\eta \nabla R\left(\frac{1}{m} \sum \delta_{\theta_i^k}\right)$$

Backward Algorithm in Wasserstein Space. JKO scheme is proposed for the optimization in the space of probability measures [JKO98]

$$\rho_{k+1} = JKO_{\eta, F}(\rho_k) \quad (4)$$

where $JKO_{\eta, F}(\rho) = \operatorname{argmin}_{\rho} F(\rho) + \frac{1}{2\eta} \mathcal{W}^2(\rho, \rho_k)$. It is also known as Wasserstein Proximal Algorithm.

Wasserstein Gradient Flow (WGF). Intuitively, when $\eta \rightarrow 0$, both algorithms will converge to a continuity equation,

$$\partial_t \rho_t = \nabla \cdot \left(\rho_t \nabla \frac{\delta F}{\delta \rho} \right)$$

under certain conditions.

3 Convergence Rate Analysis

3.1 Convergence Rate in Euclidean Space

Before stepping into the optimization in Wasserstein Space, let's have a brief look at Euclidean space. Similarly, we have GD, implicit Euler scheme(Implicit GD), and gradient flow(GF).

Proposition 3.1. (Informal) *The Implicit GD shares a "similar" convergence rate as GF without requiring other assumptions, while GD requires smoothness to ensure the "approximation ability" of first-order approximation.*

Example 1. For instance, if function f is strongly convex, the GF and Implicit GD have linear convergence rates (see Appendix. A.1 for proof), while GD requires smoothness to demonstrate linear convergence which is proved in lectures of Optimization for ML. GF and Implicit GD share a sublinear convergence rate if f is only convex, while smoothness is required for GD to obtain a sublinear rate [Bec17].

Before closing this section, we want to revisit two condition that are essential for obtaining a linear convergence rate for optimizing functions.

$$f(\theta) - f(\theta^*) \geq \frac{1}{2\mu} \|\nabla f(\theta)\|^2 \quad (\text{PL inequality})$$

$$f(\theta) - f(\theta^*) \geq \frac{\mu}{2} \|\theta - \theta^*\|^2 \quad (\text{Quadratic Growth})$$

Simply speaking, QG + convexity \Rightarrow PL inequality \Rightarrow linear convergence.

3.2 Convergence Rate in Wasserstein Space

The Wasserstein space case is similar to Euclidean space. Now we consider,

$$F(\rho) = \int V d\rho + \int W(\theta_1, \theta_2) d\rho(\theta_1) d\rho(\theta_2) + \int h(\rho) \rho d\theta$$

The strong differential $\nabla \frac{\delta F}{\delta \rho}(\rho) : \mathbb{R}^d \rightarrow \mathbb{R}^d$

$$\nabla \frac{\delta F}{\delta \rho}(\rho) = \nabla \left(V + \log \rho + \int W(\theta_1, \cdot) d\rho(\theta_1) + \int W(\cdot, \theta_2) d\rho(\theta_2) \right)$$

Proposition 3.2. (Informal) *If F is strongly convex along generalized geodesics, then WGF of F and Backward Algorithm of F enjoy linear convergence¹.*

Lemma 3.3. *Assume we follow the update rule by Eqn. 4, we have the following two formulas,*

$$\frac{T_{\rho_k}^{\rho_{k-1}} - Id}{\eta} = \nabla \frac{\delta F}{\delta \rho}(\rho_k) = \nabla \left(V + \log \rho_k + \int W(\theta_1, \cdot) d\rho_k(\theta_1) + \int W(\cdot, \theta_2) d\rho_k(\theta_2) \right) \quad (5)$$

$$F(\rho_{k-1}) - F(\rho_k) \geq \frac{1}{2\eta} W_2^2(\rho_{k-1}, \rho_k) \quad (6)$$

Theorem 3.4. *Assume V and W convex, $\int h(\rho) d\theta$ is geodesically convex, F satisfies the following λ -quadratic growth condition,*

$$F(\rho) - F(\rho^*) \geq \frac{\lambda}{2} W_2^2(\rho, \rho^*)$$

then linear convergence of the proximal algorithm is guaranteed.

¹Detailed proof for discrete-time analysis can be found in [Che+24; YY23]. For continuous-time analysis, we can find proof for "geodesically strong convexity in $\mathcal{P}_2^a(\mathbb{R}^d) \Rightarrow$ linear convergence" in [FGA21].

Proof. By the geodesical convexity of F ,

$$\begin{aligned} F(\rho_k) - F(\rho^*) &\leq - \int \langle \nabla \frac{\delta F}{\delta \rho}(\rho_k), T_{\rho_k}^{\rho^*} - Id \rangle d\rho_k \\ &\leq W_2(\rho_k, \rho^*) \sqrt{\int \|\nabla \frac{\delta F}{\delta \rho}(\rho_k)\|^2 d\rho_k} \\ &\leq \frac{1}{\eta} W_2(\rho_k, \rho^*) W_2(\rho_k, \rho_{k-1}) \end{aligned}$$

where we use Eqn. 5 for the second " \leq ". Combined with the QG condition, we have

$$W_2(\rho_k, \rho^*) \leq \frac{2}{\lambda \eta} W_2(\rho_k, \rho_{k-1})$$

Thus

$$F(\rho_k) - F(\rho^*) \leq \frac{2}{\lambda \eta^2} W_2^2(\rho_k, \rho_{k-1})$$

With Eqn. 6,

$$\begin{aligned} F(\rho_{k-1}) - F(\rho_k) &\geq \frac{2}{\lambda \eta^3} (F(\rho_k) - F(\rho^*)) \\ F(\rho_{k-1}) - F(\rho^*) &\geq (1 + \frac{2}{\lambda \eta^3}) (F(\rho_k) - F(\rho^*)) \end{aligned}$$

□

Corollary 3.5. *If F is KL divergence, geodesically convex, and satisfies LSI inequality, then linear convergence is guaranteed for the proximal algorithm applied to F .*

Proof. LSI is equivalent to Talagrand inequality when V is convex, which directly leads to quadratic growth. □

The takeaway is: Backward Algorithm, as discretization of WGF, has fewer requirements on the property of functional. However, Forward Algorithm is easier to compute especially under the particle method setting, while computing the JKO scheme has no closed form in general. As Backward Algorithm is a better approximation for WGF, we would be more interested in its behavior.

Can this paper (Euclidean) [HLO] help with the analysis for semiconvex functional?

3.3 Langevin Dynamics under LSI Condition

Following Theorem 9 in [Che+22] which shows that only PL inequality can ensure the linear convergence of the proximal algorithm in Euclidean space, we try to apply the idea to Wasserstein space.

Theorem 3.6. *Assume we have a functional $F : \mathcal{P}_2^a(\mathbb{R}^d) \rightarrow \mathbb{R}$ and satisfying so-called PL inequality,*

$$\int \|\nabla \frac{\delta F}{\delta \rho}(\rho_t)\|^2 d\rho_t \geq 2\mu(F(\rho_t) - F_{min}) \quad (7)$$

for any ρ_t . Then the linear convergence of the corresponding JKO scheme with step size η is guaranteed.

Proof.

Step 1. Assume $\xi \in (0, \eta)$. We define a mapping (Moreau Envelope) with fixed $\tilde{\rho}$

$$G : (\xi, \tilde{\rho}) \rightarrow F_{\xi, \tilde{\rho}}(\rho_\xi)$$

where the following JKO scheme obtains ρ_ξ ,

$$\rho_\xi = \underset{\rho}{\operatorname{argmin}} F_{\xi, \tilde{\rho}}(\rho), \quad F_{\xi, \tilde{\rho}}(\rho) = F(\rho) + \frac{1}{2\xi} W_2^2(\rho, \tilde{\rho}) \quad (8)$$

The optimal condition for the Problem. 8 is:

$$\left(\nabla \frac{\delta F}{\delta \rho}(\rho_\xi) + \nabla \frac{\delta(\frac{1}{2\xi} W_2^2(\cdot, \tilde{\rho}))}{\delta \rho}(\rho_\xi) \right) = \nabla \frac{\delta F}{\delta \rho}(\rho_\xi) - \frac{T_{\rho_\xi}^{\tilde{\rho}} - Id}{\xi} = 0 \quad (9)$$

Step 2. Using Lemma. 3.7, we have the following

$$\begin{aligned} \partial_\xi F_{\xi, \tilde{\rho}}(\rho_\xi) &= \int \left(\nabla \frac{\delta F}{\delta \rho}(\rho_\xi) + \nabla \frac{\delta(\frac{1}{2\xi} W_2^2(\cdot, \tilde{\rho}))}{\delta \rho}(\rho_\xi) \right) v_\xi d\rho_\xi - \frac{1}{2\xi^2} W_2^2(\rho_\xi, \tilde{\rho}) \\ &= \int \underbrace{\left(\nabla \frac{\delta F}{\delta \rho}(\rho_\xi) - \frac{T_{\rho_\xi}^{\tilde{\rho}} - Id}{\xi} \right)}_0 v_\xi d\rho_\xi - \frac{1}{2\xi^2} W_2^2(\rho_\xi, \tilde{\rho}) \end{aligned}$$

where ρ_ξ evolves under v_ξ induced by the Moreau Envelope, not the Wasserstein Gradient Flow. However, it is mostly a formal computation. For more accurate proof, Hopf-Lax formula in Wasserstein space [AGS13] might be of great help.

Step 3. With $W_2^2(\rho_\xi, \tilde{\rho}) = \int \|T_{\rho_\xi}^{\tilde{\rho}} - Id\|^2 d\rho_\xi$

$$\begin{aligned} \partial_\xi F_{\xi, \tilde{\rho}}(\rho_\xi) &= -\frac{1}{2\xi(1+\mu\xi)} W_2^2(\rho_\xi, \tilde{\rho}) - \frac{1}{2(1+\mu\xi)\xi^2} W_2^2(\rho_\xi, \tilde{\rho}) \\ &\stackrel{\text{Eqn. 9}}{=} -\frac{1}{2\xi(1+\mu\xi)} W_2^2(\rho_\xi, \tilde{\rho}) - \frac{1}{2(1+\mu\xi)} \int \|\nabla \frac{\delta F}{\delta \rho}(\rho_\xi)\|^2 d\rho_\xi \\ &\stackrel{\text{Eqn. 7}}{\leq} -\frac{\mu}{2\xi(1+\mu\xi)} W_2^2(\rho_\xi, \tilde{\rho}) - \frac{\mu}{(1+\mu\xi)} (F(\rho_\xi) - F_{min}) \end{aligned}$$

Hence, we have

$$\partial_\xi (F_{\xi, \tilde{\rho}}(\rho_\xi) - F_{min}) \leq -\frac{\mu}{1+\mu\xi} (F_{\xi, \tilde{\rho}}(\rho_\xi) - F_{min}) \leq -\frac{\mu}{1+\mu\xi} (F(\tilde{\rho}) - F_{min})$$

Integrating both sides,

$$F_{\eta, \tilde{\rho}}(\rho_\eta) - F_{min} \leq (F(\tilde{\rho}) - F_{min}) \exp\left(-\int_0^\eta \frac{\mu}{1+\mu\xi} d\xi\right) = \frac{1}{1+\mu\eta} (F(\tilde{\rho}) - F_{min})$$

Thus we have,

$$\begin{aligned} \frac{1}{1+\mu\eta} (F(\tilde{\rho}) - F_{min}) &\geq F_{\eta, \tilde{\rho}}(\rho_\eta) - F_{min} = F(\rho_\eta) - F_{min} + \frac{1}{2\eta} W_2^2(\rho_\eta, \tilde{\rho}) \\ &= F(\rho_\eta) - F_{min} + \frac{\eta}{2} \int \|\nabla \frac{\delta F}{\delta \rho}(\rho_\xi)\|^2 d\rho_\xi = F(\rho_\eta) - F_{min} - \frac{\eta}{2} \frac{d}{d\eta} (F(\rho_\eta) - F_{min}) \\ &\geq (1+\mu\eta) (F(\rho_\eta) - F_{min}) \end{aligned}$$

□

Lemma 3.7 (Chain Rule). *Assume we have a general functional $Q : \mathcal{P}_2^a(\mathbb{R}^d) \rightarrow \mathbb{R}$ and $\partial \rho_t = -\nabla \cdot (\rho_t v_t)$. Under certain conditions, we have the following chain rule,*

$$\frac{d}{dt} Q(\rho_t) = \int \nabla \frac{\delta Q}{\delta \rho}(\rho_t) v_t d\rho_t$$

Case 1. If $v_t = -\nabla \frac{\delta Q}{\delta \rho}(\rho_t)$, then $\frac{d}{dt} Q(\rho_t) = -\int \|\nabla \frac{\delta Q}{\delta \rho}(\rho_t)\|^2 d\rho_t$.

Case 2. See step 2 of Theorem 3.6.

Corollary 3.8 ((Nonlinear) Langevin Dynamics under (uniform) LSI). *If the (uniform) LSI is satisfies, then linear convergence of (nonlinear) Langevin dynamics is ensured by the JKO scheme.*

Proof. Both LSI and uniform LSI leads to the PL inequality 7. We don't present the details here. \square

There are main two issues that I don't include in the proof of Theorem 3.6:

(1) **Can the JKO scheme admit a unique minimizer?**

Yes. For linear Langevin dynamics, $\int V d\rho$ is convex in the sense of linear combination (without convexity requirement on V), so is $W_2^2(\cdot, \tilde{\rho})$. $\int \log \rho d\rho$ is strictly convex, which leads to a unique minimizer.

For nonlinear Langevin dynamics induced by a two-layer Neural network, the whole JKO optimization term is also strictly convex in the linear combination sense.

(2) **Do we need to prove this Chain Rule? Especially for Case 2?** Yes, we should not take it for granted. But proving this chain rule for case 2 might be very technical. Its counterpart in Euclidean space should be the viscous solution to the Hamilton-Jacobi equation.

Theorem B.1 solves these problems above and indeed provide a strict proof!

4 Methods and Experiments

4.1 Backward Algorithm for Langevin Dynamics

Assume we have a function $V : \mathbb{R}^d \rightarrow \mathbb{R}$ and $\int e^{-V} = 1$ for simplicity, the Langevin dynamics is defined as:

$$d\theta_t = \nabla V(\theta_t)dt + \sqrt{2}dW_t$$

This stochastic differential equation can be viewed as a continuous limit of GD with Gaussian noise. The minimizing goal with respect to its continuity equation is,

$$F(\rho) = KL(\rho|e^{-V}) = \int V d\rho + \int \log \rho d\rho$$

where the negative entropy regularization comes from the Gaussian noise. When $e^{-V} = \mathcal{N}(0, I)$, $KL(\rho|e^{-V})$ is geodesically strongly convex but non-smooth because of the $\int \log \rho d\rho$. Thus, we utilize Backward Algorithm in these situations.

Experiments. We provide numerical experiments to illustrate the dynamical behavior of the Backward Algorithm, similar to [SKL21], where they simulated the Wasserstein Proximal Gradient method for Gaussian distribution².

If the initialization distribution and the target distribution are both Gaussian, then we have a closed form of the update [Wib18] and the update will maintain to be Gaussian. Also, we have closed for W_2 distance for two Gaussians known as Bures-Wasserstein distance. We set the initialization distribution to be $\mathcal{N}(0, 100 * I)$ to have the same mean as target distribution which can simplify the update rule as Example 5 in [Wib18], and set the step size $\eta = 0.1$ and iterations 50.

The linear convergence rate is clearly shown in Fig. 1.

4.2 Backward Algorithm for Two-Layer NN

Assume our goal is now:

$$F(\rho) = R(\rho) + \tau H(\rho) \tag{10}$$

where $R()$ is defined as Eqn. 2 and $H()$ is a regularized term. Similar to Langevin dynamics, $H(\rho) = \int \log \rho d\rho$ when we apply Gaussian Noisy GD:

$$\theta_i^{k+1} = \theta_i^k - \eta \nabla R(\frac{1}{m} \sum \delta_{\theta_i^k}) + \sqrt{2\eta\tau}z \tag{11}$$

where $z \sim \mathcal{N}(0, I)$. When $\tau \rightarrow 0$, Eqn. 11 be equivalent to WGF (the continuity equation) of Eqn. 10. under mild conditions [MMM19]. The main difference compared to previous discussion is, $F(\rho)$ for two-layer NN is convex in

²Similar to Proximal Gradient Methods in \mathbb{R}^d , it is a Forward-Backward method.

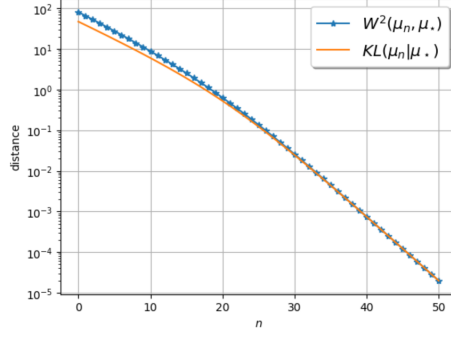


Figure 1: Linear Convergence of Wasserstein distance and KL objective.

the linear combination sense, while previous results like Proposition. 3.2 are based on convexity in the geodesic sense.

Thus, we are interested in: **How would the Backward Algorithm perform in this setting? What is the influence of noise regularization on Forward Algorithms and Backward Algorithms?**

Methods. By the fully backward proximal algorithm, we hope to find T^k such that $T^k \rho_k = \rho_{k+1}$, where ρ_{k+1} minimize the JKO scheme.

$$T^{k+1} = \underset{T}{\operatorname{argmin}} R(T_{\#}\rho_k) + \tau H(T_{\#}\rho_k) + \frac{1}{2\eta} \int \|T(x) - x\|^2 d\rho_k$$

We can estimate the problem using functional approximation,

$$\begin{aligned} T^{k+1} = \underset{T}{\operatorname{argmin}} \quad & \mathbb{E}_{(x,y) \sim p(x,y)} \left\| \frac{1}{m} \sum_{i=1}^m \varphi(\theta_i^k, x) - y \right\|^2 \\ & - \frac{\tau}{m} \sum_{i=1}^m \log |\det \nabla T(\theta_i^k)| + \frac{1}{2m\eta} \sum_{i=1}^m \|T(\theta_i^k) - \theta_i^k\|^2 \end{aligned}$$

where we utilized the change of variable formula [Mok+21]. The idea of functional approximation is to learn one optimal transport map T^k for each iteration.

Experiments. We set the dimension of θ_i to be $d = 3$, number of particles $m = 100$, discretized step size $\eta = 0.1$. We choose activation function $\phi()$ to be $\tanh()$ in Eqn. 1, and create a dataset of size 80 by $y = \beta^T x$, where β is fixed and generated with standard Gaussian and x are sampled from standard Gaussian. For the estimation of negative entropy $H(\rho)$, we utilize the nearest neighbor estimator [KL87].

For the training of the T map, we choose a NN of the form $g(\theta) = W_2 \sigma(W_1 \theta)$, where $W_1 \in \mathbb{R}^{q \times d}$, $W_2 \in \mathbb{R}^{d \times q}$ where $q = 1000$. We use GD optimizer and set the learning rate to be 0.002 and iterations to be 200.

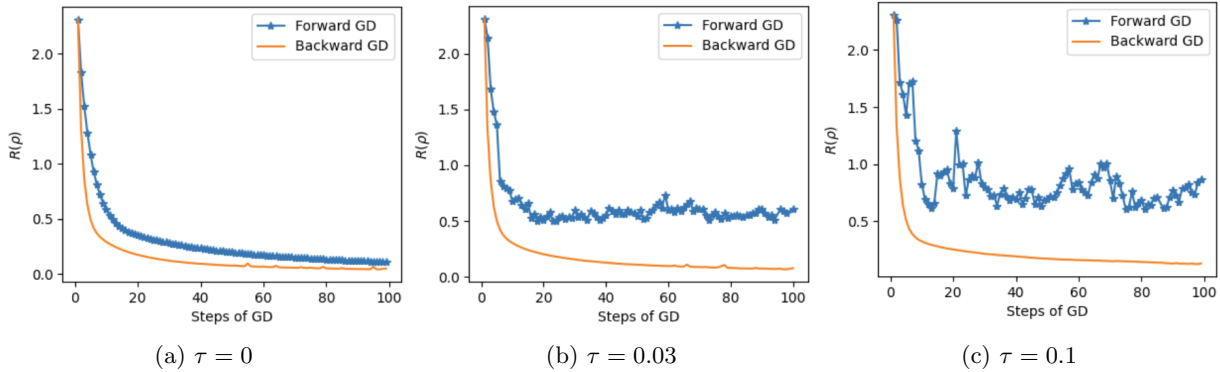


Figure 2: Evolution of $R(\rho)$ for Two-layer NN with $d = 3$, $m = 100$, and $\tanh()$ activation.

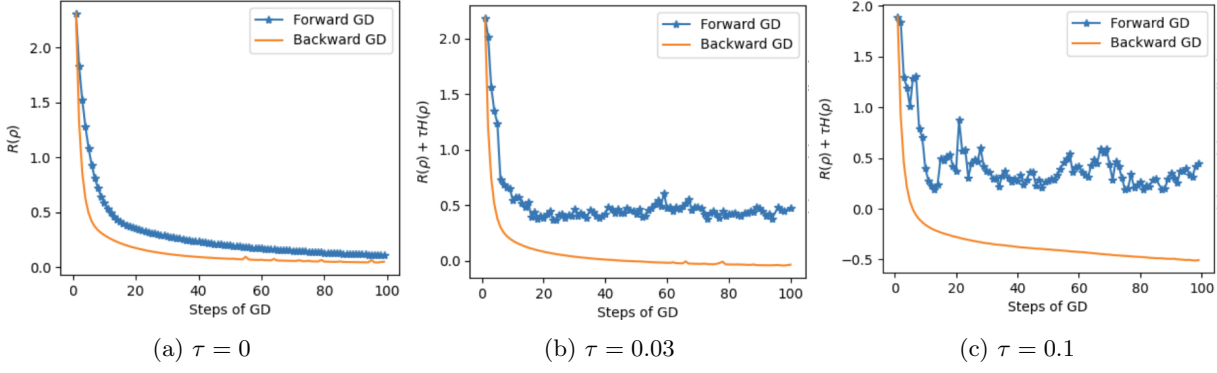


Figure 3: Evolution of $R(\rho) + \tau H(\rho)$ for Two-layer NN with $d = 3$, $m = 100$, and $\tanh()$ activation.

Convergence speed of Backward Algorithm and Forward Algorithm without Gaussian Noise. From Fig. 2 we observe that both Forward and Backward methods can optimize the goal either with or without Gaussian noise. The Backward Algorithm seems to enjoy a faster convergence rate at the beginning of the training, which is a natural benefit from the JKO scheme, as the backward formulation doesn't explicitly constrain the step size and serves a certain local search role.

Convergence Rate Conjecture. The experiments seem to demonstrate a sublinear/linear convergence rate for both algorithms. However, there is no convergence rate result for two-layer NN optimization, which is only convex in linear combination sense. Though there are some global convergence results [CB18; MMM19].

Influence of Noise Regularization. From Fig. 2 and Fig. 3 we can observe that the Backward Algorithm is less sensitive to the Gaussian noise regularization in the aspect of optimizing $R(\rho)$ and $R(\rho) + \tau H(\rho)$.

5 Conclusion

In this project, we applied the Backward Algorithm in Wasserstein Space to a two-layer Neural Network and compared its performance with the Forward Algorithm. The main contribution is we proved proximal algorithm in length space (Euclidean and Wasserstein Space is our main concern in our literature) can ensure linear convergence under merely PL inequality.

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A Convergence Rate in Euclidean Space

A.1 With only Convexity

Now we consider a continuous gradient flow,

$$\frac{d\theta_t}{dt} = -\nabla f(\theta_t)$$

Proposition A.1. *Consider f convex, then GF of f enjoys a sublinear convergence rate.*

Proof.

$$\begin{aligned}\frac{d}{dt} \frac{1}{2} \|\theta_t - \theta^*\|^2 &= -\nabla f(\theta_t)^T (\theta_t - \theta^*) \leq f(\theta^*) - f(\theta_t) \\ f(\theta_t) - f(\theta^*) &\leq -\frac{d}{dt} \frac{1}{2} \|\theta_t - \theta^*\|^2\end{aligned}$$

Take integral of both sides,

$$\frac{1}{T} \int_0^T f(\theta_t) dt - f(\theta^*) \leq \frac{1}{2T} (\|\theta_0 - \theta^*\|^2 - \|\theta_T - \theta^*\|^2)$$

Using Jensen inequality,

$$f\left(\frac{1}{T} \int_0^T \theta_t dt\right) - f(\theta^*) \leq \frac{1}{2T} \|\theta_0 - \theta^*\|^2$$

Therefore, we obtain a $O(1/T)$ convergence rate. \square

Proposition A.2. *Consider f convex, then the Implicit GD of f enjoys a sublinear convergence rate.*

Proof. Firstly, we have the update rule,

$$\theta_{k+1} = \theta_k - \eta \nabla f(\theta_{k+1})$$

then we have the following two potentially useful formula.

Formula 1.

$$f(\theta^*) - f(\theta_k) \geq \nabla f(\theta_k)^T (\theta^* - \theta_k)$$

Equivalently,

$$f(\theta_k) - f(\theta^*) \leq \nabla f(\theta_k)^T (\theta_k - \theta^*)$$

Formula 2.

$$\begin{aligned}f(\theta_k) - f(\theta_{k+1}) &\geq \nabla f(\theta_{k+1})^T (\theta_k - \theta_{k+1}) \\ &= \eta \|\nabla f(\theta_{k+1})\|^2\end{aligned}$$

By the second one, we have,

$$f(\theta_0) - f(\theta_K) \geq \eta \sum_{k=0}^{K-1} \|\nabla f(\theta_{k+1})\|^2$$

Formula 3.

Now we want to explore the third useful one. However the following expansion doesn't work well

$$\begin{aligned}\|\theta_{k+1} - \theta^*\|^2 &= \|\theta_k - \theta^*\|^2 + \eta^2 \|\nabla f(\theta_{k+1})\|^2 \\ &\quad - 2\eta \nabla f(\theta_{k+1})^T (\theta_k - \theta^*)\end{aligned}$$

Thus we switch to,

$$\begin{aligned}\|\theta_k - \theta^*\|^2 &= \|\theta_{k+1} - \theta^*\|^2 + \eta^2 \|\nabla f(\theta_{k+1})\|^2 \\ &\quad + 2\eta \nabla f(\theta_{k+1})^T (\theta_{k+1} - \theta^*)\end{aligned}$$

Thus we have,

$$\begin{aligned}\|\theta_{k+1} - \theta^*\|^2 - \|\theta_k - \theta^*\|^2 &\leq -\eta^2 \|\nabla f(\theta_{k+1})\|^2 - 2\eta (f(\theta_{k+1}) - f(\theta^*)) \\ &\leq 2\eta (f(\theta^*) - f(\theta_{k+1}))\end{aligned}$$

Therefore,

$$f(\theta_{k+1}) - f(\theta^*) \leq \frac{1}{2\eta} (\|\theta_k - \theta^*\|^2 - \|\theta_{k+1} - \theta^*\|^2)$$

Using Jensen inequality,

$$\begin{aligned}f\left(\frac{1}{K} \sum_0^{K-1} \theta_{k+1}\right) - f(\theta^*) &\leq \frac{1}{K} \sum [f(\theta_{k+1}) - f(\theta^*)] \\ &\leq \frac{1}{2\eta K} \|\theta_0 - \theta^*\|^2\end{aligned}$$

We actually only used Formula 1 and Formula 3. \square

A.2 With Strong Convexity

Proposition A.3. *Consider f strongly convex and differentiable, then GF of f enjoys linear convergence.*

Proof. By strong convexity,

$$f(\theta) \geq f(\theta_t) + \nabla \langle f(\theta_t), \theta - \theta_t \rangle + \frac{\mu}{2} \|\theta - \theta_t\|^2 \quad (12)$$

Minimize both sides,

$$f(\theta^*) \geq f(\theta_t) - \frac{1}{2\mu} \|\nabla f(\theta_t)\|^2$$

where we let $\theta = \theta_t - \frac{1}{\mu} \nabla f(\theta_t)$ in RHS of Eqn. 12. Thus we will obtain,

$$\frac{df(\theta_t)}{dt} = -\|\nabla f(\theta_t)\|^2 \leq -2\mu (f(\theta_t) - f(\theta^*))$$

Therefore,

$$f(\theta_t) - f(\theta^*) \leq e^{-2\mu t} (f(\theta_0) - f(\theta^*))$$

□

Proposition A.4. *If f is strongly convex (assume it is also differentiable), then the Implicit GD enjoys linear convergence.*

Proof. Firstly, we have the update rule,

$$\theta_{k+1} = \theta_k - \eta \nabla f(\theta_{k+1})$$

By strong convexity,

$$f(\theta_k) \geq f(\theta_{k+1}) + \langle \nabla f(\theta_{k+1}), \theta_k - \theta_{k+1} \rangle + \frac{\mu}{2} \|\theta_k - \theta_{k+1}\|^2$$

Let $\eta = \frac{C}{\mu}$,

$$\begin{aligned} f(\theta_{k+1}) - f(\theta_k) &\leq -\eta \|\nabla f(\theta_{k+1})\|^2 - \frac{\mu\eta^2}{2} \|\nabla f(\theta_{k+1})\|^2 \\ &= -\left(\frac{C^2 + 2C}{2\mu}\right) \|\nabla f(\theta_{k+1})\|^2 \end{aligned}$$

Since we have $f(\theta^*) \geq f(\theta_{k+1}) - \frac{1}{2\mu} \|\nabla f(\theta_{k+1})\|^2$,

$$f(\theta_{k+1}) - f(\theta_k) \leq (C^2 + 2C)(f(\theta^*) - f(\theta_{k+1}))$$

Simply, we let $C^2 + 2C = 1$,

$$f(\theta_{k+1}) - f(\theta^*) \leq \frac{1}{2} (f(\theta_k) - f(\theta^*))$$

which implies linear convergence. □

A.3 With only PL Inequality

With only PL inequality without convexity, the linear convergence of continuous GF can be proved, which is suggested by the proof of Prop. A.3. However, for discrete-time analysis, it is shown in [Che+22] until recently for linear convergence under discrete-time. However, the proof in [Che+22] is not strict; thus, we provide more careful proof here.

Basically, we rely on two lemma here, one is the classical result that the Hopf-Lax formula satisfies the HJ equation if the initial f is Lipschitz continuous and H is convex and $\lim_{\|\theta\| \rightarrow \infty} \frac{H(\theta)}{\|\theta\|} = \infty$;

$$\begin{cases} \partial_t u(\theta, t) + H(D_\theta u(\theta, t)) = 0 \\ u(\theta, 0) = f(\theta) \end{cases} \quad (13)$$

the other is a much stronger theorem from [AGS13] but specifically for $H = \frac{1}{2} \|\cdot\|^2$.

Theorem A.5 (Linear Convergence under PL inequality and L -Smoothness). *If f is L -smooth and satisfies PL inequality,*

$$\|\nabla f(\theta)\|^2 \geq 2\mu (f(\theta) - f(\theta^*))$$

then linear convergence is guaranteed with $\eta \leq 1/L$.

Proof. The main idea in this proof, is to avoid the "chain rule" with $\dot{\theta}_\xi$. We define

$$u(\theta, \xi) = \min_{\theta_\xi \in \mathbb{R}^d} f(\theta_\xi) + \frac{1}{2\xi} \|\theta_\xi - \theta\|^2$$

Firstly, we will show that if f is $(-L)$ -semiconvex, then $u(\cdot, \xi)$ is convex for any fixed $\xi \in (0, 1/L)$. Define

$$g(\theta, \beta) = f(\beta) + \frac{1}{2\xi} \|\beta - \theta\|^2$$

It is obvious that g is convex in θ and β . By Theorem 2.18 in [Bec17], partial minimization over a convex function is still convex. Thus similar to Theorem 5.30 in [Bec17], we can show that

$$\nabla_\theta u(\theta, \xi)(\theta) = \nabla^* \left(\frac{1}{2\xi} \|\theta - \text{prox}_{f, \xi}(\theta)\|^2 \right) = \frac{1}{\xi} \|\theta - \text{prox}_{f, \xi}(\theta)\| \quad (14)$$

where $\text{prox}_{f, \xi}(\theta) = \text{argmin}_{\theta_\xi \in \mathbb{R}^d} f(\theta_\xi) + \frac{1}{2\xi} \|\theta_\xi - \theta\|^2$ and ∇^* denotes gradient operation for θ but ignore the prox part.

Now we have $u(\theta, \xi)$ is **differentiable everywhere** in θ for fixed t . With this result, and some localization techniques, we should be able to prove that $U(\theta, \xi)$ satisfies HJ equation using the idea from Theorem 6 in Section 3.3.2 in [Eva22]. And therefore, We can plug Eqn. 14 into Eqn. 13. \square

B One General Strong Theorem

Theorem B.1 (Linear Convergence under only PL inequality). *By Proposition 3.1 and Proposition 3.3 in [AGS13], for any fixed θ which belongs to a general length space,*

$$\partial_t u(\theta, \xi) + \frac{1}{2\xi^2} d(\text{prox}_{f, \xi}(\theta), \theta)^2 = 0$$

holds for $t \in (0, \infty)$ except for at most countable exceptions. Thus, we can easily have linear convergence for the proximal algorithm in length space with PL inequality satisfied, using the proof in step 3 of Theorem 3.6.