GENERATIVE MODELING WITH OPTIMAL TRANSPORT MAPS

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ABSTRACT

With the discovery of Wasserstein GANs, Optimal Transport (OT) has become a powerful tool for large-scale generative modelings tasks. In these tasks, OT cost is typically used as the loss for GANs. In contrast to this approach, we show that the OT map itself can be used as the generative model, providing comparable performance. While previous analogous approaches consider OT maps in the latent spaces, we consider OT in the ambient space, e.g. high-dimensional images. First, we derive a min-max optimization algorithm to compute OT maps for the quadratic cost (Wasserstein-2 distance). Next, we extend the approach to the case when input and output distributions are located in the spaces of unequal dimension and derive error bounds for the computed OT map. We evaluate the algorithm in image generation and in unpaired image restoration. In particular, we consider denoising, colorization, and inpainting, where the optimality of the restoration map is a desired attribute, since the output (restored) image is expected to be close to the input (degraded) one.

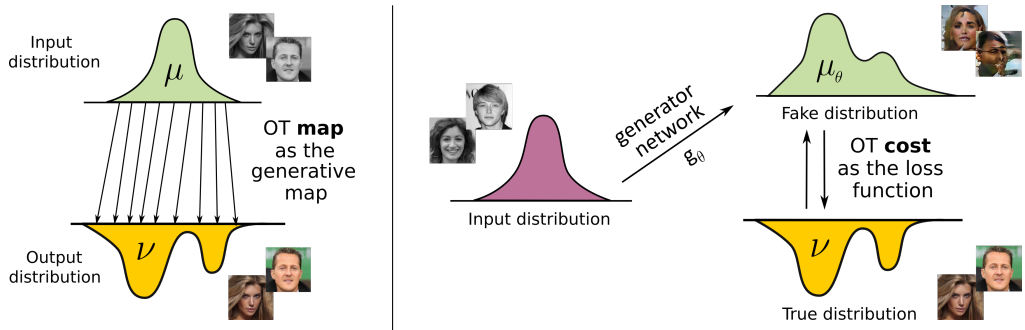
1 INTRODUCTION

Since the discovery Generative Adversarial Networks (GANs, Goodfellow et al. (2014)), there has been a surge in generative modeling (Radford et al., 2016; Arjovsky et al., 2017; Brock et al., 2019; Karras et al., 2019). In the past few years, Optimal Transport (OT, Villani (2008)) theory has been pivotal in addressing important issues of generative models. In particular, the usage of Wasserstein distance has improved diversity (Arjovsky et al., 2017; Gulrajani et al., 2017), convergence (Sanjabi et al., 2018), and stability (Miyato et al., 2018; Kim et al., 2021) of GANs.

Generative models based on OT can be split into two classes based on the function OT performs. First, the **optimal transport cost serves as the loss** for generative models, see Figure 1b. This is the most prevalent class of methods which includes WGAN (Arjovsky et al., 2017) and its modifications: WGAN-GP (Gulrajani et al., 2017), WGAN-LP (Petzka et al., 2018), and WGAN-QC (Liu et al., 2019). Second, the **optimal transport map is used as the generative model** itself, see Figure 1a. Such approaches include LSOT (Seguy et al., 2018), AE-OT (An et al., 2020a), ICNN-OT (Makkuva et al., 2020), W2GN (Korotin et al., 2021a). Models of the first class have been well-studied, but limited attention has been paid to the second class. Existing approaches of the second class primarily consider **OT maps in latent spaces** of pre-trained autoencoders (AE), see Figure 3, and do not produce practical applications in high-dimensional ambient spaces. The performance of these methods in generative modeling depends on the underlying AE. For this reason, solving OT in the latent space does not necessarily guarantee superior performance in generative modeling.

The focus of our paper is the second class of OT-based models using OT map as the generative map. Finding an optimal mapping is motivated by its ability to preserve specific attributes of the input samples, a desired property in unpaired learning. For example, in unpaired image-to-image translation, the learner has to fit a map between two data distributions while preserving the image content. CycleGAN-based models (Zhu et al., 2017) are widely used for this purpose. However, they typically have complex optimization objectives consisting of several losses (Amodio & Krishnaswamy, 2019; Lu et al., 2019) in order to make the fitted map preserve the required attributes.

The main contributions of this paper are as follows:



(a) OT map as the generative model.

(b) OT cost as the loss for the generative model.

Figure 1: Two existing approaches to use optimal transport in generative models.

1. We propose an end-to-end algorithm (§4.3) to fit OT maps for the quadratic cost (Wasserstein-2 distance) between distributions located on the spaces of equal dimensions (§4.1) and extend the method to unequal dimensions as well (§4.2). We prove error bounds for the method (§4.4).
2. We demonstrate large-scale applications of OT maps in popular computer vision tasks. We consider image generation (§5.1) and image enhancement (§5.2) tasks.

The OT map obtained by our method can be directly used in large-scale computer vision problems which is in high contrast to previous related methods relying on autoencoders and OT maps in the latent space. Importantly, the performance and computational complexity of our method is comparable to OT-based generative models using OT cost as the loss.

Notations. We use $\mathcal{X}$ and $\mathcal{Y}$ to denote two complete metric spaces, $\mu(x)$ and $\nu(y)$ to denote probability measures on $\mathcal{X}$ and $\mathcal{Y}$, respectively. For a measure μ its support is represented by $Supp(\mu)$. For a measurable map $T : \mathcal{X} \to \mathcal{Y}$, $T_{\#}\mu$ denotes the push-forward measure of μ, i.e. the measure for which any measurable set $E \subset \mathcal{Y}$ satisfies $T_{\#}\mu(E) = \mu(T^{-1}(E))$. For a vector x, $\|x\|$ denotes its Euclidean norm. We use $\langle x, y\rangle$ to denote the inner product between vectors x and y. We use $\Pi(\mu, \nu)$ to denote the set of joint probability measures on $\mathcal{X} \times \mathcal{Y}$ whose marginals are μ and ν respectively (couplings). For a function $f : \mathbb{R}^D \to \mathbb{R} \cup \{\pm\infty\}$ its Legendre-Fenchel transform (convex conjugate) is $\overline{f}(y) = \sup_{x\in\mathbb{R}^D}\{\langle x, y\rangle - f(x)\}$. It is convex, even if f is not.

2 Background on Optimal Transport

Consider a cost of transportation, $c : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ defined over the product space of $\mathcal{X}$ and $\mathcal{Y}$.

Monge's Formulation. The *optimal transport cost* between μ and ν for ground cost $c(\cdot, \cdot)$ is

$$\text{Cost}(\mu, \nu) \stackrel{def}{=} \inf_{T_{\#}\mu=\nu} \int_{\mathcal{X}} c\left(x, T(x)\right) d\mu(x), \tag{1}$$

see Figure 2. The map T^* attaining the infimum of (1) is called the *optimal transport map*. Monge's formulation does not allow splitting. For example, when μ is a Dirac measure and ν is a non-Dirac measure, the feasible set of equation (1) is empty. This issue is addressed by Kantorovich (1942).

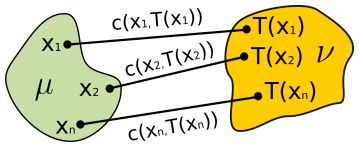


Figure 2: Monge's OT.

Kantorovich's Relaxation. Instead of asking to which particular point $y \in \mathcal{Y}$ should all the probability mass of x be moved, Kantorovich (1948) asks how the mass of x should be distributed among all $y \in \mathcal{Y}$. Formally, a transport coupling is sought over a transport map and the OT cost is given by:

$$\text{Cost}(\mu, \nu) \stackrel{def}{=} \inf_{\pi\in\Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} c\left(x, y\right) d\pi(x, y). \tag{2}$$

The coupling π^* attaining the infimum of (2) is called the *optimal transport plan*. Unlike the formulation of (1), the formulation of (2) is well-posed, and with mild assumptions on spaces $\mathcal{X}, \mathcal{Y}$ and

ground cost $c(\cdot,\cdot)$, the minimizer π^* of (2) always exists (Villani, 2008, Theorem 4.1). In particular, if π^* is deterministic, i.e. $\pi^* = [\mathrm{id}_{\mathcal{X}}, T^*]_{\#}\mu$ for some $T^* : \mathcal{X} \to \mathcal{Y}$, then T^* minimizes of (1).

Duality. The dual form of (2) is given by (Kantorovich, 1948):

$$\mathrm{Cost}(\mu,\nu) = \sup_{(u,v)} \left\{ \int_{\mathcal{X}} u(x) d\mu(x) + \int_{\mathcal{Y}} v(y) d\nu(y) \colon u(x) + v(y) \leq c(x,y) \right\}, \tag{3}$$

with $u \in \mathcal{L}^1(\mu)$, $v \in \mathcal{L}^1(\nu)$ called Kantorovich *potentials*. For $u : \mathcal{X} \to \mathbb{R}$ and $v : \mathcal{Y} \to \mathbb{R}$ define their c-transforms by $u^c(x) = \inf_{x \in \mathcal{X}} \{c(x,y) - u(x)\}$ and $v^c(x) = \inf_{y \in \mathcal{Y}} \{c(x,y) - v(y)\}$ respectively. Using c-transform, (3) is reformulated as (Villani, 2008, §5)

$$\mathrm{Cost}(\mu,\nu) = \sup_{v} \left\{ \int_{\mathcal{X}} v^c(x) d\mu(x) + \int_{\mathcal{Y}} v(y) d\nu(y) \right\} = \sup_{u} \left\{ \int_{\mathcal{X}} u(x) d\mu(x) + \int_{\mathcal{Y}} u^c(y) d\nu(y) \right\}. \tag{4}$$

Primal-dual relationship. For certain ground costs $c(\cdot,\cdot)$, the primal solution T^* of (1) can be recovered from the dual solution u^* of (3). For example, if $\mathcal{X} = \mathcal{Y} = \mathbb{R}^D$, $c(x,y) = h(x-y)$ with strictly convex $h : \mathbb{R}^D \to \mathbb{R}$ and μ is absolutely continuous supported on the compact set, then

$$T^*(x) = x - (\nabla h)^{-1}\big(u^*(x)\big), \tag{5}$$

see (Santambrogio, 2015, Theorem 1.17). For general costs, see (Villani, 2008, Theorem 10.28).

3 Optimal Transport in Generative Models

Optimal transport cost as the loss (Figure 1b). Starting with the works of Arjovsky & Bottou (2017); Arjovsky et al. (2017), the usage of OT cost as the loss has become the major way to apply OT for generative modeling. In this setting, given data distribution ν and fake distribution μ_θ, the goal is to minimize $\mathrm{Cost}(\mu_\theta, \nu)$ w.r.t. parameters θ. Typically, μ_θ is a pushforward distribution of some given distribution, e.g. $\mathcal{N}(0, I)$, via generator network g_θ.

The *Wasserstein-1* distance ($\mathcal{W}_1$), i.e. the transport cost for ground cost $c(x,y) = \|x-y\|$, is the most practically prevalent example of such a loss. Models based on this loss are known as Wasserstein GANs (WGANs). They estimate $\mathcal{W}_1(\mu_\theta, \nu)$ based on the dual form as given by (4). For $\mathcal{W}_1$, the optimal potentials u^*, v^* of (4) satisfy $u^* = -v^*$ where u^* is a 1-Lipschitz function (Villani, 2008, Case 5.16). As a result, to compute $\mathcal{W}_1$, one needs to optimize the following simplified form:

$$\mathcal{W}_1(\mu_\theta, \nu) = \sup_{\|u\|_L \leq 1} \left\{ \int_{\mathcal{X}} u(x) d\mu_\theta(x) - \int_{\mathcal{Y}} u(y) d\nu(y) \right\}. \tag{6}$$

In WGANs, potential u is called the *discriminator*. Optimization of (6) reduces constrained optimization of (4) with two potentials u, v to optimization of only one discriminator u. In practice, enforcing the Lipschitz constraint on u is challenging. Most methods to do this are regularization-based, e.g. they use gradient penalty (Gulrajani et al., 2017, WGAN-GP) and Lipschitz penalty (Petzka et al., 2018, WGAN-LP). Other methods enforce Lipschitz property via incorporating certain hard restrictions on the discriminator's architecture (Anil et al., 2019; Tanielian & Biau, 2021).

General transport costs (other than $\mathcal{W}_1$) can also be used as the loss for generative models. They are less popular since they do not have a dual form reducing to a single potential function similar to (6) for $\mathcal{W}_1$. Consequently, the challenging estimation of c-transform u^c is needed. To avoid this, Sanjabi et al. (2018) consider dual form of (3) with two potentials u, v instead form (4) with one u and softly enforce condition $u(x) + v(y) \leq c(x,y)$ via entropy or quadratic regularization. Nhan Dam et al. (2019) use dual form of (4) and amortized optimization to compute u^c via an additional neural network. Both methods work for general $c(\cdot,\cdot)$, though the authors test them for $c(x,y) = \|x-y\|$ only, i.e. $\mathcal{W}_1$ distance. Mallasto et al. (2019) propose a fast way to approximate the c-transform and test the approach (WGAN-(q,p)) with several costs, in particular, the *Wasserstein-2* distance ($\mathcal{W}_2$), i.e. the transport cost for the quadratic ground cost $c(x,y) = \frac{1}{2}\|x-y\|^2$. Specifically for $\mathcal{W}_2$, Liu et al. (2019) approximate c-transform via a linear program (WGAN-QC).

A fruitful branch of OT-based losses for generative models comes from modified versions of OT cost, such as Sinkhorn (Genevay et al., 2018), sliced (Deshpande et al., 2018) and minibatch (Fatras et al., 2019) OT distances. They typically have lower sample complexity than usual OT and can be

accurately estimated from random mini-batches without using dual forms such as (3). In practice, these approaches usually learn the ground OT cost $c(\cdot, \cdot)$ adversarially.

OPTIMAL TRANSPORT MAP AS THE GENERATIVE MAP (Figure 1a). Methods to compute the OT map (plan) are less common in comparison to those computing the cost. Recovering the map from the primal form (1) or (2) usually yields complex optimization objectives containing several adversarial terms (Xie et al., 2019; Liu et al., 2021; Lu et al., 2020). Such procedures require careful hyperparameter choice. This needs to be addressed before using these methods in practice.

Primal-dual relationship (§2) makes it possible to recover the OT map via solving the dual form (3). Dual-form based methods primarily consider $\mathcal{W}_2$ cost due to its nice theoretical properties and relation to convex functions (Brenier, 1991). In the semi-discrete case (μ is continuous, ν is discrete), An et al. (2020a) and Lei et al. (2019) compute the dual potential and the OT map by using the Alexandroff theory and convex geometry. For the continuous case, Seguy et al. (2018) use the entropy (quadratic) regularization to recover the dual potentials and extract OT map from them via the barycenteric projection. Taghvaei & Jalali (2019), Makkuva et al. (2020), Korotin et al. (2021a) employ input-convex neural networks (ICNNs, see Amos et al. (2017)) to parametrize potentials in the dual problem and recover OT maps by using their gradients.

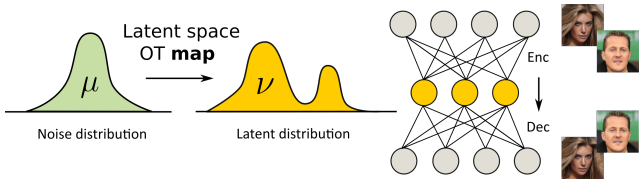


Figure 3: The existing most prevalent approach to use OT maps in generative models.

The aforementioned dual form methods compute OT maps in **LATENT SPACES** for problems such as domain adaptation and latent space mass transport, see Figure 3. OT maps in high-dimensional ambient spaces, e.g. natural images, are usually not considered. Recent evaluation of continuous OT methods for $\mathcal{W}_2$ (Korotin et al., 2021b) reveals their crucial limitations, which negatively affect their scalability, such as poor expressiveness of ICNN architectures or bias due to regularization.

4 END-TO-END SOLUTION TO LEARN OPTIMAL MAPS

4.1 EQUAL DIMENSIONS OF INPUT AND OUTPUT DISTRIBUTIONS

In this section, we use $\mathcal{X} = \mathcal{Y} = \mathbb{R}^D$ and consider the Wasserstein-2 distance ($\mathcal{W}_2$), i.e. the optimal transport for the quadratic ground cost $c(x, y) = \frac{1}{2}\|x - y\|^2$. We consider distributions μ, ν with finite second moments. We assume that for measures μ, ν in view there *exists* a *unique* OT plan π^* minimizing (3) and it is deterministic, i.e. $\pi^* = [\text{id}_{\mathbb{R}^D}, T^*]_{\#}\mu$. Here T^* is an OT map which minimizes (1). Previous related works (Makkuva et al., 2020; Korotin et al., 2021a) assumed the absolute continuity of μ which implied the existence and uniqueness of T^* (Brenier, 1991).

Let $\psi(y) \stackrel{def}{=} \frac{1}{2}\|y\|^2 - v(y)$, where v is the potentials of (4). Note that

$$v^c(x) = \inf_{y \in \mathbb{R}^D} \left\{ \frac{1}{2}\|x - y\|^2 - v(y) \right\} = \frac{1}{2}\|x\|^2 - \sup_{y \in \mathbb{R}^D} \{\langle x, y \rangle - \psi(y)\} = \frac{1}{2}\|x\|^2 - \overline{\psi}(x). \quad (7)$$

Therefore, (4) is equivalent to

$$\mathcal{W}_2^2(\mu, \nu) = \int_{\mathcal{X}} \frac{\|x\|^2}{2} d\mu(x) + \int_{\mathcal{Y}} \frac{\|y\|^2}{2} d\nu(x) + \sup_{\psi} \left\{ -\int_{\mathcal{X}} \overline{\psi}(x) d\mu(x) - \int_{\mathcal{Y}} \psi(y) d\nu(y) \right\} = \quad (8)$$

$$\text{Const}(\mu, \nu) - \inf_{\psi} \left\{ \int_{\mathcal{X}} \overline{\psi}(x) d\mu(x) + \int_{\mathcal{Y}} \psi(y) d\nu(y) \right\} = \quad (9)$$

$$\text{Const}(\mu, \nu) - \inf_{\psi} \left\{ \int_{\mathcal{X}} \sup_{y \in \mathbb{R}^D} \{\langle x, y \rangle - \psi(y)\} \, d\mu(x) + \int_{\mathcal{Y}} \psi(y) d\nu(y) \right\} = \quad (10)$$

$$\text{Const}(\mu,\nu) - \inf_{\psi}\left\{\int_{\mathcal{X}} \sup_{T}\left\{\langle x, T(x)\rangle - \psi\big(T(x)\big)\right\} d\mu(x) + \int_{\mathcal{Y}} \psi(y) d\nu(y)\right\} \quad (11)$$

where between lines (10) and (11) we replace the optimization over $x \in \mathbb{R}^D$ with the equivalent optimization over functions $T : \mathbb{R}^D \to \mathbb{R}^D$.

Lemma 4.1. *Let T^* be the OT map from μ to ν. For every optimal potential ψ^* we have:*

$$T^* \in \arg\sup_{T} \int_{\mathcal{X}} \left\{\langle x, T(x)\rangle - \psi^*\big(T(x)\big)\right\} d\mu(x). \quad (12)$$

We prove Lemma 4.1 in Appendix A.1. Thanks to the lemma, we may solve saddle point problem (11) and obtain OT map T^* from its solution (ψ^*, T^*). For general μ, ν the $\arg\sup_T$ set for optimal ψ^* might contain not only OT map T^*, but other functions as well. Working with real-world data in experiments (§5.2), we observe that despite this issue, optimization (11) still recovers T^*.

Relation to previous works. Using function T to approximate the c-transform was proposed by Nhan Dam et al. (2019) to estimate the Wasserstein loss in WGANs. For $\mathcal{W}_2$, the fact that T^* is the OT map was used by Makkuva et al. (2020); Korotin et al. (2021a) who primarily assumed continuous μ, ν and reduced (11) to convex ψ and $T = \nabla\phi$ for convex ϕ. Issues with non-uniqueness of solution of (12) were softened, but using ICNNs to parametrize ψ became necessary.

Korotin et al. demonstrated that ICNNs negatevily affect practical performance of OT and tested an unconstrained formulation similar to our (11). As per the evaluation, it provided the best empirical performance (see §4.5, Korotin et al. (2021b)). The method ⌊MM:R⌉ they consider parametrizes $\frac{1}{2}\|\cdot\|^2 - \psi(\cdot)$ by a neural network, while we directly parametrize $\psi(\cdot)$ by a neural network.

Recent work by Fan et al. (2021) exploits formulation similar to (11) for general costs $c(\cdot,\cdot)$. While their formulation leads to a max-min scheme with general costs (Fan et al., 2021, Theorem 3), our approach gives rise to a min-max method for quadratic cost. In particular, we extend the formualtion to learn OT maps between unequal dimensions, see the next subsection.

4.2 Unequal Dimensions of Input and Output Distributions

Consider the case when $\mathcal{X} = \mathbb{R}^H$ and $\mathcal{Y} = \mathbb{R}^D$ have different dimensions, i.e. $H \neq D$. In order to map the probability distribution μ to ν, a straightforward solution is to embed $\mathcal{X}$ to $\mathcal{Y}$ via *some* $Q : \mathcal{X} \to \mathcal{Y}$ and then to fit the OT map between $Q_{\#}\mu$ and ν for quadratic cost on $\mathcal{Y} = \mathbb{R}^D$. In this case, the optimization objective becomes

$$\inf_{\psi}\sup_{T}\left\{\int_{\mathcal{X}} \left\{\langle Q(x), T\big(Q(x)\big)\rangle - \psi\Big(T\big(Q(x)\big)\Big)\right\} d\mu(x) + \int_{\mathcal{Y}} \psi(y) d\nu(y)\right\} \quad (13)$$

with the optimal T^* recovering the OT map from $Q_{\#}\mu$ to ν. For equal dimensions $H = D$ and identity embedding $Q(x) \equiv x$ expression (13) reduces to optimization (11) up to a constant.

Instead of a optimization (13) over functions $T : Q(\mathcal{X}) \to \mathcal{Y}$, we propose to consider optimization directly over generative mappings $G : \mathcal{X} \to \mathcal{Y}$:

$$\mathcal{L}(\psi, G) \stackrel{def}{=} \inf_{\psi}\sup_{G}\left\{\int_{\mathcal{X}} \left\{\langle Q(x), G(x)\rangle - \psi\big(G(x)\big)\right\} d\mu(x) + \int_{\mathcal{Y}} \psi(y) d\nu(y)\right\} \quad (14)$$

Our following lemma establishes connections between (14) and OT between unequal dimensions:

Lemma 4.2. *Assume that exists a unique deterministic OT plan between $Q_{\#}\mu$ and ν and it is deterministic, i.e. $[id_{\mathbb{R}^D}, T^*]_{\#}(Q_{\#}\mu)$. Then $G^*(x) = T^*\big(Q(x)\big)$ is the OT map between μ and ν for the Q-**embedded quadratic cost** $c(x,y) = \frac{1}{2}\|Q(x) - y\|^2$. Moreover, for every optimal potential ψ^* of problem (14) it holds:*

$$G^* \in \arg\sup_{G} \int_{\mathcal{X}} \left\{\langle Q(x), G(x)\rangle - \psi^*\big(G(x)\big)\right\} d\mu(x). \quad (15)$$

We prove Lemma 4.2 in Appendix A.2. Analogously to Lemma 4.1, it provides a way to compute the OT map G^* for Q-embedded quadratic cost between distributions μ and ν via solving saddle point problem (14). Note the situation with non-uniqueness of $\arg\sup_G$ is similar to §4.1.

Relation to previous works. In practice, learning OT maps directly between spaces of unequal dimensions was considered in the work by (Fan et al., 2021, §5.2) but only on toy examples. We demonstrate that our method works well in large-scale generative modeling tasks (§5.1). Theoretical properties of OT maps for embedded costs are studied, e.g. in (Pass, 2010; McCann & Pass, 2020).

4.3 Practical Optimization Procedure

To optimize functional (14), we approximate $G : \mathbb{R}^H \to \mathbb{R}^D$ and $\psi : \mathbb{R}^D \to \mathbb{R}$ with neural networks G_θ, ψ_ω and optimize their parameters via stochastic gradient descent-ascent (SGAD) by using mini-batches from μ, ν. The practical optimization procedure is given in Algorithm 1 below. Following the usual practice in GANs, we add small gradient penalty (Gulrajani et al., 2017) on potential ψ_ω for better stability. The penalty in not included in Algorithm 1 to keep it simple.

Algorithm 1: Learning the optimal transport map between unequal dimensions.

Input : Input distribution μ on $\mathcal{X} = \mathbb{R}^H$; output distribution ν on $\mathcal{Y} = \mathbb{R}^D$;
generator network $G_\theta : \mathbb{R}^H \to \mathbb{R}^D$; potential network $\psi_\omega : \mathbb{R}^D \to \mathbb{R}$;
number of iterations per network: K_G, K_ψ; embedding $Q : \mathcal{X} \to \mathcal{Y}$;
Output: Trained generator G_θ representing OT map from μ to ν;

1 **repeat**
2 **for** $k_\psi \leftarrow 1$ to K_ψ **do**
3   Draw batch $X \sim \mu$ and $Y \sim \nu$;
4   $\mathcal{L}_\psi \leftarrow \frac{1}{|Y|}\sum_{y\in Y}\psi_\omega(y) - \frac{1}{|X|}\sum_{x\in X}\psi_\omega\big(G_\theta(x)\big)$;
5   Update ω by using $\frac{\partial \mathcal{L}_\psi}{\partial \omega}$ to minimize $\mathcal{L}_\psi$;
6 **for** $k_G \leftarrow 1$ to K_G **do**
7   Draw batch $X \sim \mu$;
8   $\mathcal{L}_G \leftarrow \frac{1}{|X|}\sum_{x\in X}\big[\psi\big(G(x)\big) - \langle Q(x), G_\theta(x)\rangle\big]$;
9   Update θ by using $\frac{\partial \mathcal{L}_G}{\partial \theta}$ to minimize $\mathcal{L}_G$;
10 **until** not converged;
11 **return** G_θ

Relation to previous works. WGAN by Arjovsky & Bottou (2017) uses $\mathcal{W}_1$ as the loss to update generator while we solve a diferent task – we fit generator G to be the OT map for Q-embedded quadratic cost. Despite this, our algorithm 1 has similarities with WGAN's training. The update of ψ (line 4) coincides with discriminator's update in WGAN. The update of generator G (line 8) differs from WGAN's update by term $-\langle Q(\cdot), G_\theta(\cdot)\rangle$. Besides, in WGAN the optimization is $\inf_G \sup_D$, while we have $\inf_\psi \sup_G$, i.e. the generator in our case is the solution of the inner problem.

4.4 Error Analysis

Given a pair $(\hat{\psi}, \hat{G})$ approximately solving (14), a natural question to ask is how good is the recovered OT map $\hat{G}$. In this subsection, we provide a bound on the difference between G^* and $\hat{G}$ based on the duality gaps for solving outer and inner optimization problems.

We emphasize that initial optimization (8), and, as the result, optimizations (10), (11), (13), (14) can be reduced to optimization over *convex* functions ψ, see (Villani, 2008, Case 5.17). Our theorem below assumes convexity of $\hat{\psi}$ although it might not hold in practice since in practice $\hat{\psi}$ is a network.

Theorem 4.3. *Assume that $\hat{\psi}$ is β-strongly convex ($\beta > 0$) and $\hat{G} : \mathbb{R}^H \to \mathbb{R}^D$. Define*

$$\epsilon_1 = \sup_G \mathcal{L}(\hat{\psi}, G) - \mathcal{L}(\hat{\psi}, \hat{G}) \qquad \textit{and} \qquad \epsilon_2 = \sup_G \mathcal{L}(\hat{\psi}, G) - \inf_\psi \sup_G \mathcal{L}(\psi, G)$$

Then the following bound holds true for the OT map G^* from μ to ν:

$$2 \cdot \mathcal{W}_2^2(\hat{G}_\sharp \mu, \nu) \leq \int_{\mathcal{X}} \|\hat{G}(x) - G^*(x)\|^2 d\mu(x) \leq \frac{2}{\beta}(\sqrt{\epsilon_1} + \sqrt{\epsilon_2})^2. \tag{16}$$

We prove Theorem 4.3 in Appendix A.3. The duality gaps upper bound $L^2(\mu)$ norm between computed $\hat{G}$ and true G^* maps, and the $\mathcal{W}_2^2$ between true ν and generated (fake) distribution $\hat{G}_\sharp\mu$.

Relation to previous works. Makkuva et al. (2020); Korotin et al. (2021a) prove related bounds for $\mathcal{W}_2$ with μ, ν located on the spaces of the same dimension. Our result holds for unequal dimensions.

5 Experiments

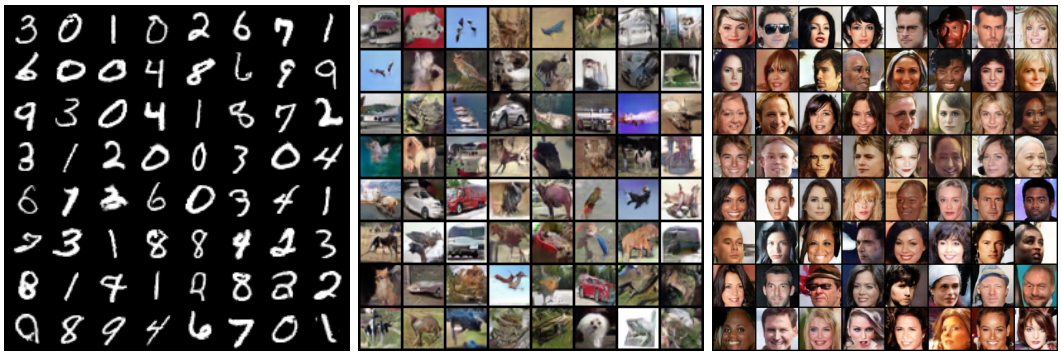
We evaluate our algorithm in generative modeling of data distribution from noise distribution (§5.1) and unpaired image restoration task (§5.2). Technical details are given in Appendix B.

5.1 Modeling Data distribution from Noise Distribution

In this subsection, μ is a 128-dimensional normal noise and ν the high-dimensional data distribution.

Let the images from ν be of size $w \times h$ with c channels. As the embedding $Q : \mathcal{X} \to \mathcal{Y}$ we use a *naive* upscaling of a noise. For $x \in \mathbb{R}^{128}$ we represent it as 1-channel 16×8 image, stack c copies over channel dimension and bicubically upscale it to the size $w \times h$ of data images from ν.

We test our method on MNIST (LeCun et al., 1998), CIFAR10 (Krizhevsky et al., 2009), and CelebA (Liu et al., 2015) image datasets. In Figure 4, we show random samples generated by our approach, namely **Optimal Transport Modeling** (OTM). To quantify the results, in Tables 1 and 2 we give the inception (Salimans et al., 2016) and FID (Heusel et al., 2017) scores of generated samples. Similar to (Song & Ermon, 2019, Appendix B.2), we compute them on 50K real and generated samples.



(a) MNIST, 28×28, grayscale (b) CIFAR10, 32×32, RGB (c) CelebA, 64×64, RGB

Figure 4: Randomly generated MNIST, CIFAR10, and CelebA samples by our method (OTM).

For comparison, we include the scores of existing generative models of three types: (1) OT map as the generative model; (2) OT cost as the loss; (3) not OT-based. Note that models of the first type compute OT in the *latent space* of an autoencoder, which is a contrast to our approach. According to our evaluation, the performance of our method is better or comparable to existing alternatives.

Table 1: Results on CIFAR10 dataset.

Model	**Related Work**	**Inception** ↑	**FID** ↓
PixelIQN	Ostrovski et al. (2018)	5.29	49.46
BEGAN	Berthelot et al. (2017)	5.62	-
EBM	Du & Mordatch (2019)	6.02	40.58
DCGAN	Radford et al. (2016)	6.64±0.14	37.70
NCSN	Song & Ermon (2019)	8.87±0.12	25.32
WGAN	Arjovsky et al. (2017)	-	55.2
WGAN-GP	Gulrajani et al. (2017)	6.49±0.09	39.40
3P-WGAN	Nhan Dam et al. (2019)	7.38 ± 0.08	28.8
AE-OT	An et al. (2020a)	-	28.5
AE-OT-GAN	An et al. (2020b)	-	17.1
OTM	Ours	7.41±0.11	20.69

Table 2: Results on CelebA dataset.

Model	**Related Work**	**FID** ↓
DCGAN	Radford et al. (2016)	52.0
DRAGAN	Kodali et al. (2017)	42.3
BEGAN	Berthelot et al. (2017)	38.9
3P-WGAN	Nhan Dam et al. (2019)	62.1
WGAN	Arjovsky et al. (2017)	41.3
WGAN-GP	Gulrajani et al. (2017)	30.0
WGAN-QC	Liu et al. (2019)	12.9
AE-OT	An et al. (2020a)	28.6
AE-OT-GAN	An et al. (2020b)	7.8
OTM	Ours	7.7

5.2 UNPAIRED IMAGE RESTORATION

In this subsection, we consider unpaired image restoration tasks on CelebA faces dataset. In this case, input distribution μ consists of degraded images, while ν are clean images. In all the cases, embedding Q is a straightforward identity embedding $Q(x) \equiv x$.

In image restoration, optimality of the restoration map is desired since the output (restored) image is expected to be close to the input (degraded) one minimizing the transport cost. Note that GANs do not seek for an optimal mapping. However, in practice, due to implicit inductive biases such as convolutional architectures, still tend to fit low transport cost mappings (Bézenac et al., 2021).

The experimental setup is shown in Figure 5. We split the dataset in 3 parts A, B, C containing 90K, 90K, 22K samples respectively. To each image we apply the degradation transform (decolorization, noising or occlusion) and obtain the degraded dataset containing of 3 respective parts A, B, C. For *unpaired* training we use part A of degraded and part B of clean images. For testing, we use parts C.

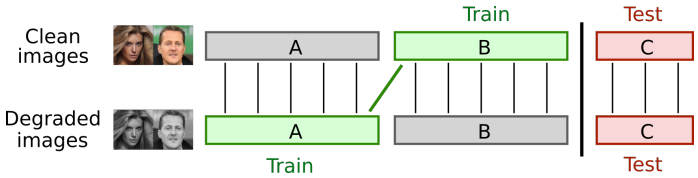


Figure 5: The training/testing scheme that we use for unpaired restoration tasks.

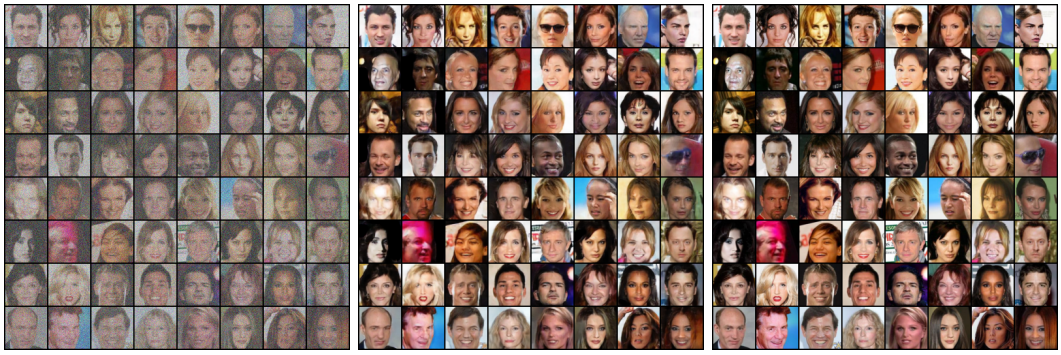
To quantify the results we compute FID of restored images w.r.t. clean images of part C. The scores for denoising, inpainting and colorization are given in Table 3, details of each experiment and qualitative results are given below.

Model	**Denoising**	**Inpainting**	**Colorization**
Input	166.59	47.65	36.51
WGAN-GP	21.86	48.99	15.46
OTM (ours)	10.95	9.96	6.37

Table 3: FID↓ on test part C in image restoration experiments.

As the baseline, we include WGAN-GP. For fair comparison, we fit it using *exactly* the same hyperparameters as in our method. This is possible due to the similarities between our method and WGAN-GP's training procedure, see discussion in §4.3.

Denoising. To create noisy images, we add white normal noise with $\sigma = 0.3$ to each pixel. Figure 6 illustrates image denoising using our OTM approach on the test part of the dataset.



(a) Noisy samples. (b) Push-forward samples. (c) Original samples.

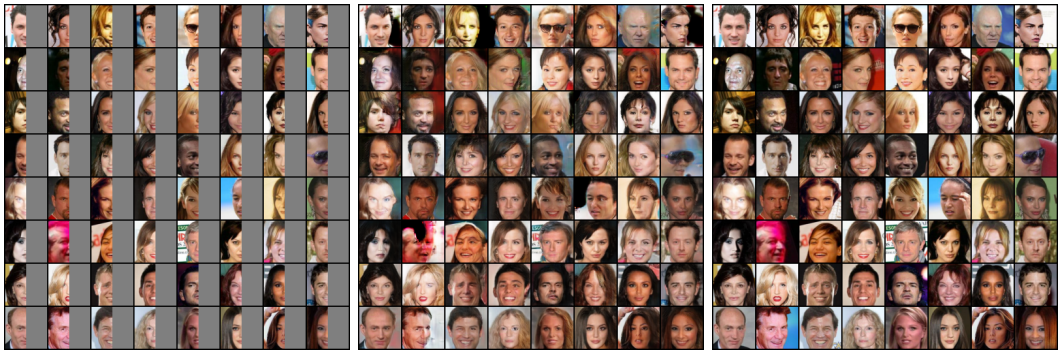
Figure 6: OTM for image denoising on test C part of CelebA, 64×64.

Colorization. To create grayscale images, we average the RGB values of each pixel. Figure 7 illustrates image colorization using our OTM on the test part of the dataset.

(a) Grayscale samples. (b) Push-forward samples. (c) Original samples.

Figure 7: OTM for image colorization on test C part of CelebA, 64×64.

Inpainting. To create incomplete images, we replace the right half of each clean image with zero. Figure 8 illustrates image inpainting using our OTM on the test part of the dataset.



(a) Occluded samples. (b) Push-forward samples. (c) Original samples.

Figure 8: OTM for image inpainting on test C part of CelebA, 64×64.

6 Conclusion

Our method fits OT maps for the embedded quadratic transport cost between probability distributions. Unlike predecessors, it scales well to high dimensions producing applications of OT maps directly in ambient spaces, such as spaces of images. The performance is comparable to other existing generative models while the complexity of training is similar to that of popular WGANs.

Limitations. For distributions μ, ν we assume existence of the OT map between them. In practice, this might not hold for all real-world μ, ν. Working with equal dimensions, we focus the quadratic ground cost $\frac{1}{2}\|x-y\|^2$. Nevertheless, our approach extends to other costs $c(\cdot,\cdot)$, see Fan et al. (2021). When the dimensions are unequal, we restrict our analysis to *embedded* quadratic cost $\frac{1}{2}\|Q(x)-y\|^2$ where Q equalizes dimensions. Choosing the embedding Q might not be straightforward in some practical problems, but our evaluation (§5.1) shows that even naive choices of Q work well.

Potential Impact. Real-world image restoration problems often do not have paired datasets limiting the application of supervised techniques. In these practical unpaired learning problems, we expect our optimal transport approach to improve the existing models.

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