Neural Optimal Transport

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Abstract

We present a novel neural-networks-based algorithm to compute optimal transport maps and plans for strong and weak transport costs. To justify the usage of neural networks, we prove that they are universal approximators of transport plans between probability distributions. We evaluate the performance of our optimal transport algorithm on toy examples and on the unpaired image-to-image style translation task.

1. Introduction

Solving optimal transport (OT) problems with neural networks has become widespread in machine learning tentatively starting with the introduction of the large-scale OT (Seguy et al., 2017) and the popular Wasserstein Generative Adversarial Network (Arjovsky et al., 2017, WGAN). The majority of existing methods compute the OT cost and use it as the loss function to update the generator in generative models (Gulrajani et al., 2017; Liu et al., 2019; Sanjabi et al., 2018; Petzka et al., 2017). Recently, (Rout et al., 2021; Daniels et al., 2021) have demonstrated that the OT plan itself can be used as a generative model providing comparable performance in practical tasks.

In this paper, we focus on the methods which compute the OT plan. Most recent methods (Korotin et al., 2021b; Rout et al., 2021) consider OT for the quadratic transport cost (the Wasserstein-2 distance, $W_2$) and recover a nonstochastic OT plan, i.e., a deterministic OT map. In general, it may not exist. (Daniels et al., 2021) recover the entropy-regularized stochastic plan, but the procedures for learning the plan and sampling from it are extremely time-consuming due to the necessity to learn score-based model and iterate the Langevin dynamic (Daniels et al., 2021, §6).

Contributions. We propose a novel algorithm to compute deterministic and stochastic OT plans with deep neural networks (§4.1, §4.2). Our algorithm works with weak and strong optimal transport costs (§2) and generalizes previously known scalable approaches (§3, §4.3). To reinforce

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![Unpaired style translation with our Algorithm 1.](image)

(a) Celeba (female) → anime, 128 × 128, deterministic ($W_2$).

(b) Outdoor → church, 128 × 128, deterministic ($W_2$).

(c) Handbags → shoes, 128 × 128, stochastic ($W_{2,1}$).
the usage of neural nets, we prove that they are universal approximators of stochastic transport plans (§4.4). We show that our algorithm recovers optimal plans fairly well and can be applied to large-scale computer vision tasks (§5).

Notations. We use $\mathcal{X}$, $\mathcal{Y}$, $\mathcal{Z}$ to denote Polish spaces and $\mathcal{P}(\mathcal{X})$, $\mathcal{P}(\mathcal{Y})$, $\mathcal{P}(\mathcal{Z})$ to denote the respective sets of probability distributions on them. We denote the set of probability distributions on $\mathcal{X} \times \mathcal{Y}$ with marginals $\mathcal{P}$ and $\mathcal{Q}$ by $\Pi(\mathcal{P}, \mathcal{Q})$. For a measurable map $T : \mathcal{X} \times \mathcal{Z} \rightarrow \mathcal{Y}$ (or $T : \mathcal{X} \rightarrow \mathcal{Y}$), we denote the associated push-forward operator by $T_\#$.

2. Preliminaries

In this section, we provide key concepts of optimal transport theory that we use in our paper. For a detailed overview, we refer to (Villani, 2008; Santambrogio, 2015; Gozlan et al., 2017; Backhoff-Veraguas et al., 2019).

Strong OT formulation. For distributions $\mathcal{P} \in \mathcal{P}(\mathcal{X})$, $\mathcal{Q} \in \mathcal{P}(\mathcal{Y})$ and a cost function $c : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$, Monge’s primal formulation of the optimal transport cost is

$$\text{Cost}(\mathcal{P}, \mathcal{Q}) \overset{\text{def}}{=} \inf_{T \in \Pi(\mathcal{P}, \mathcal{Q})} \int_{\mathcal{X}} c(x, T(x)) d\mathcal{P}(x),$$

(1)

where the minimum is taken over measurable functions (transport maps) $T : \mathcal{X} \rightarrow \mathcal{Y}$ that map $\mathcal{P}$ to $\mathcal{Q}$ (Figure 2). The optimal $T^*$ is called the optimal transport map.

![Figure 2: Monge’s formulation of optimal transport.](image)

Note that (1) is not symmetric, and this formulation does not allow mass splitting, i.e., for some $\mathcal{P}, \mathcal{Q} \in \mathcal{P}(\mathcal{X}), \mathcal{P}(\mathcal{Y})$, there may be no $T$ that satisfies $T_\# \mathcal{P} = \mathcal{Q}$. Thus, (Kantorovich, 1958) proposed the following relaxation (Figure 3):

$$\text{Cost}(\mathcal{P}, \mathcal{Q}) \overset{\text{def}}{=} \inf_{\pi \in \Pi(\mathcal{P}, \mathcal{Q})} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\pi(x, y),$$

(2)

where the minimum is taken over all transport plans $\pi$, i.e., distributions on $\mathcal{X} \times \mathcal{Y}$ whose marginals are $\mathcal{P}$ and $\mathcal{Q}$. The optimal $\pi^* \in \Pi(\mathcal{P}, \mathcal{Q})$ is called the optimal transport plan. If $\pi^*$ is of the form $|\text{id}, T^*|_\# \mathcal{P} \in \Pi(\mathcal{P}, \mathcal{Q})$ for some $T^*$, then $T^*$ minimizes (1). In this case, the plan is called deterministic. Otherwise, it is called stochastic (nondeterministic).

Two popular examples of OT costs for $\mathcal{X} = \mathcal{Y} = \mathbb{R}^D$ are the Wasserstein-1 and 2 ($\mathcal{W}_1$, $\mathcal{W}_2$), i.e., formulation (2) for $c(x, y) = \|x - y\|$ and $c(x, y) = \frac{1}{2}\|x - y\|^2$, respectively.

![Figure 3: Kantorovich’s formulation of optimal transport.](image)

Weak OT formulation (Gozlan et al., 2017). Let $C : \mathcal{X} \times \mathcal{P}(\mathcal{Y}) \rightarrow \mathbb{R}$ be a weak cost, i.e., a function which takes a point $x \in \mathcal{X}$ and a distribution of $y \in \mathcal{Y}$ as input. The weak optimal transport cost between $\mathcal{P}, \mathcal{Q}$ is

$$\text{Cost}(\mathcal{P}, \mathcal{Q}) \overset{\text{def}}{=} \inf_{\pi \in \Pi(\mathcal{P}, \mathcal{Q})} \int_{\mathcal{X}} C(x, \pi(\cdot|x)) d\pi(x),$$

(3)

where $\pi(\cdot|x)$ denotes the conditional distribution (Figure 4).

![Figure 4: Weak formulation of optimal transport.](image)

Note that (3) is a generalization of (2). Indeed, let

$$C(x, \mu) = \int_{\mathcal{Y}} c(x, y) d\mu(y)$$

(4)

For cost (4), the weak formulation (3) becomes strong (2).

An example of a weak OT cost for $\mathcal{X} = \mathcal{Y} = \mathbb{R}^D$ is the $\gamma$-weak ($\gamma \geq 0$) Wasserstein-2 ($\mathcal{W}_2$), i.e., (3) with

$$C(x, \mu) = \int_{\mathcal{Y}} \frac{1}{2}\|x - y\|^2 d\mu(y) - \frac{\gamma}{2} \text{Var}(\mu)$$

(5)

For $\gamma = 0$, the transport cost (5) is strong, i.e., $\mathcal{W}_2 = \mathcal{W}_{2,0}$.

Existence and duality. Throughout the paper, we consider weak costs $C(x, \mu)$ which are lower bounded, lower semicontinuous and convex in $\mu$. Under these assumptions, (Backhoff-Veraguas et al., 2019) prove that the minimizer $\pi^*$ of (3) always exists. With mild assumptions on $c$, strong costs (4) satisfy these assumptions. They are linear w.r.t. $\mu$ and, consequently, convex. The $\gamma$-weak quadratic cost (5) is also convex since the functional $\text{Var}(\mu)$ is concave in $\mu$.

For the costs in view, the dual form of (3) is

$$\text{Cost}(\mathcal{P}, \mathcal{Q}) = \sup_{f} \int_{\mathcal{X}} f^C(x) d\mathcal{P}(x) + \int_{\mathcal{Y}} f(y) d\mathcal{Q}(y),$$

(6)
where \( f \) are the lower-bounded continuous functions with not very rapid growth (Backhoff-Veraguas et al., 2019, Equation 1.2) and \( f^C \) is the weak \( C \)-transform of \( f \), i.e.,

\[
f^C(x) \equiv \inf_{\mu \in \mathcal{P}(\mathcal{Y})} \left\{ C(x, \mu) - \int \! f(y) \, d\mu(y) \right\}.
\] (7)

Note that for strong costs \( C \), the infimum is attained at any \( \mu \in \mathcal{P}(\mathcal{Y}) \) supported on the arg inf \( y \in \mathcal{Y} \{ c(x, y) - f(y) \} \) set. Therefore, it suffices to use the strong \( c \)-transform:

\[
f^C(x) = f^c(x) \equiv \inf_{y \in \mathcal{Y}} \{ c(x, y) - f(y) \}.
\] (8)

For strong costs (4), the formula (6) with (8) is the well known Kantorovich duality (Villani, 2008, §5).

Nonuniqueness. In general, an OT plan \( \pi^* \) is not unique, e.g., see (Peyré et al., 2019, Remark 2.3).

3. Related Work

In large-scale machine learning, OT costs are primarily used as the loss to learn generative models. Wasserstein GANs introduced by (Arjovsky et al., 2017; Gulrajani et al., 2017) are the most popular examples of this approach. However, these models are out of scope of our paper since they only compute the OT cost but not OT plans or maps. To compute OT plans (or maps) is a more challenging problem, and only a limited number of scalable methods to solve it have been developed.

We overview methods to compute OT plans (or maps) below. We emphasize that existing methods are designed only for strong OT formulation (2). Most of them search for a deterministic solution (1), i.e., for a map \( T^* \) rather than a stochastic plan \( \pi^* \), although \( T^* \) might not always exist.

To compute the OT plan (map), (Lu et al., 2020; Xie et al., 2019) approach the primal formulation (1) or (2). Their methods imply using generative models and yield complex optimization objectives with several adversarial regularizers, e.g., they are used to enforce the boundary condition \( (T^* P) = Q \). As a result, the methods are hard to setup since they require careful selection of hyperparameters.

In contrast, methods based on the dual formulation (6) have simpler optimization procedures. Most of such methods are designed for OT with the quadratic cost, i.e., the Wasserstein-2 distance \( (W_2^2) \). An overview and evaluation of these methods is provided in (Korotin et al., 2021b). Below we mention the issues of these methods.

Methods by (Taghvaei & Jalali, 2019; Makkuva et al., 2019; Korotin et al., 2021a;c) based on input-convex neural networks (ICNNs, see (Amos et al., 2017)) have solid theoretical justification, but do not provide sufficient performance in practical large-scale problems. Methods based on entropy regularized optimal transport (Genevay et al., 2016; Seguy et al., 2017; Daniels et al., 2021) recover regularized OT plan that is biased from the true one. Also, it is hard to sample from the plan or compute its density.

According to (Korotin et al., 2021b), the best performing approach is \( \text{[MM:R]} \), which is based on the minimax reformulation of (6). It recovers OT maps fairly well and has a good generative performance. The follow-up papers (Rout et al., 2021; Fan et al., 2020) test extensions of this approach for more general strong transport costs \( c(\cdot, \cdot) \). The key limitation of the approach is that it aims to recover a deterministic OT plan, i.e., map \( T^* \) which might not exist.

4. Algorithm for Learning OT Plans

In this section, we develop a novel neural algorithm to recover a solution \( \pi^* \) of OT problem (3). The following lemma will play an important role in our derivations.

**Lemma 1** (Existence of transport maps.). Let \( \mu \) and \( \nu \) be probability distributions on \( \mathbb{R}^M \) and \( \mathbb{R}^N \), respectively. Assume that \( \mu \) is atomless. Then there exists a measurable \( t : \mathbb{R}^M \to \mathbb{R}^N \) satisfying \( t_# \mu = \nu \).

**Proof.** (Santambrogio, 2015, Corollary 1.29) proves the fact for \( M = N \). The proof generalizes to \( M \neq N \). \( \square \)

For simplicity, throughout the paper we assume that \( \mathcal{P}, \mathcal{Q} \) are supported on subsets \( \mathcal{X} \subset \mathbb{R}^P, \mathcal{Y} \subset \mathbb{R}^Q \), respectively.

**4.1. Reformulation of the Dual Problem**

First, we reformulate the optimization in \( C \)-transform (7). For this, we introduce a subset \( \mathcal{Z} \subset \mathbb{R}^S \) with an atomless distribution \( S \) on it, e.g., \( S = \text{Uniform}(\{0, 1\}) \) or \( \mathcal{N}(0, 1) \).

**Lemma 2** (Reformulation of the \( C \)-transform).

\[
f^C(x) = \inf_t \left\{ C(x, t_# S) - \int \! f(t(z)) \, dS(z) \right\},
\] (9)

where the infimum is taken over all measurable \( t : \mathcal{Z} \to \mathcal{Y} \).

**Proof.** For all \( x \in \mathcal{X} \) and \( t : \mathcal{Z} \to \mathcal{Y} \),

\[
f^C(x) \leq C(x, t_# S) - \int \! f(t(z)) \, dS(z).
\] (10)

The inequality is straightforward: we substitute \( \mu = t_# S \) to (7) to upper bound \( f^C(x) \) and use the change of variables. Taking the infimum over \( t \) in (10), we obtain

\[
f^C(x) \leq \inf_t \left\{ C(x, t_# S) - \int \! f(t(z)) \, dS(z) \right\}.
\] (11)
Now let us turn (11) to an equality. We need to show that for every $\epsilon > 0$ there exists a map $t^* : Z \to \mathcal{Y}$ satisfying

$$f^C(x) + \epsilon \geq C(x, t^*_\# S) - \int_Z f(t^*(z)) dS(z). \quad (12)$$

By (7) and the definition of inf, $\exists \mu^* \in \mathcal{P}(\mathcal{Y})$ such that

$$f^C(x) + \epsilon \geq C(x, \mu^*) - \int_Y f(y) d\mu^*(y). \quad (13)$$

Thanks to Lemma 1, there exists a measurable $t^* : Z \to \mathcal{Y}$ such that $\mu^* = t^*_\# S$, i.e., (13) immediately yields (12).

Now we use Lemma 2 to get an analogous reformulation of the entire integral of $f^C$ in the dual form (6).

**Lemma 3 (Reformulation of the integrated C-transform).**

$$\inf \int X f^C(x) d\mathbb{P}(x) = \inf_{T} \int X \left( C(x, T(x, \cdot)_\# S) - \int_Z f(T(x, z)) dS(z) \right) d\mathbb{P}(x), \quad (14)$$

where the inner minimization is performed over all measurable functions $T : \mathcal{X} \times Z \to \mathcal{Y}$.

**Proof.** The lemma follows from the interchange between the infimum and integral provided by the Rockafellar’s interchange theorem (Rockafellar, 1976, Theorem 3A).

The theorem states that for a function $F : A \times B \to \mathbb{R}$ and a distribution $\nu$ on $A$,

$$\int B \inf_{a \in A} F(a, b) d\nu(a) = \inf_{H : A \to B} \int A F(a, H(a)) d\nu(a). \quad (15)$$

We apply (15), use $A = \mathcal{X}$, $\nu = \mathbb{P}$, and put $B$ to be the space of measurable functions $Z \to \mathcal{Y}$, and

$$F(a, b) = C(a, b_\# S) - \int Y f(y) d[b_\# S](y).$$

Consequently, we obtain that $\int X f^C(x) d\mathbb{P}(x)$ equals

$$\inf_{H} \int X \left( C(x, H(x)_\# S) - \int Y f(y) d[H(x)_\# S](y) \right) d\mathbb{P}(x). \quad (16)$$

Finally, we note that the optimization over functions $H : \mathcal{X} \to \{t : Z \to \mathcal{Y}\}$ equals the optimization over functions $T : \mathcal{X} \times Z \to \mathcal{Y}$. We put $T(x, z) = [H(x)](z)$, use the change of variables for $y = T(x, z)$ and derive (14) from (16).

Lemma 3 provides the way to represent the dual form (6) as a saddle point optimization problem. Namely, we have

**Corollary 1 (Minimax reformulation of the dual problem).**

$$\text{Cost}(\mathbb{P}, \mathbb{Q}) = \sup_{f} \inf_{T} L(f, T), \quad (17)$$

where the functional $L$ is defined by

$$L(f, T) \overset{def}{=} \int Y f(y) d\mathbb{Q}(y) + \int X \left( C(x, T(x, \cdot)_\# S) - \int Z f(T(x, z)) dS(z) \right) d\mathbb{P}(x). \quad (18)$$

**Proof.** It suffices to substitute (14) into (6).

We say that functions $T : \mathcal{X} \times Z \to \mathcal{Y}$ are stochastic maps. If a map $T$ is independent of $z$, i.e., for all $(x, z) \in \mathcal{X} \times Z$ we have $T(x, z) \equiv T(x)$, we say the map is deterministic.

Our idea behind the introduced notation is the following. An optimal transport plan $\pi^*$ might be nondeterministic, i.e., there might not exist a deterministic function $T : \mathcal{X} \to \mathcal{Y}$ which satisfies $\pi^* = [id_\mathcal{X}, T]_\# \mathbb{P}$. However, each transport plan $\pi \in \Pi(\mathbb{P}, \mathbb{Q})$ can be represented implicitly through a stochastic function $T : \mathcal{X} \times Z \to \mathcal{Y}$. This fact is known as noise outsourcing (Kallenberg, 1997, Theorem 5.10) for $Z = [0, 1] \subset \mathbb{R}$ and atomless $S \in \mathcal{P}(Z)$. We visualize the idea in Figure 5. For a plan $\pi$, there might exist multiple stochastic maps $T$ which represent it.

![Figure 5: Stochastic function $T(x, z)$ representing a transport plan. The function’s input is $x \in \mathcal{X}$ and $z \sim S$.](image)

For a pair of probability distributions $\mathbb{P}, \mathbb{Q}$, we say that $T^*$ is a stochastic optimal transport map if it realizes some optimal transport plan $\pi^*$. We prove that such maps solve the inner problem in (17) for optimal potentials $f^*$.

**Lemma 4.** For any potential $f^*$ which attains the optimal value of (6), and for any stochastic map $T^*$ which realizes some optimal transport plan $\pi^*$,

$$T^* \in \arg \inf_{T} L(f^*, T). \quad (19)$$
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Proof. Let \( \pi^* \) be the OT plan realized by \( T^* \). We derive
\[
\int \int f^*(T^*(x, z)) dS(z) dP(x) = \int \int f^*(y) d\pi^*(y|x) d\pi^*(x) = \int \int f^*(y) d\pi^*(x, y) = \int f^*(y) d\mathbb{Q}(y),
\]
where we use change of variables for \( y = T^*(x, z) \) and the property \( d\pi^*(x) = dP(x) \). Now assume that
\[
T^* \notin \arg \inf_T L(f^*, T).
\]
In this case, from the definition (18) we conclude that \( L(f^*, T^*) > \text{Cost}(P, Q) \). However, substituting (20) into (18), we see that
\[
\mathcal{L}(f^*, T^*) = \int C(x, T^*(x, \cdot) \# S) dP(x) = \text{Cost}(P, Q),
\]
which is a contradiction. That is, (21) is wrong. \( \square \)

Thanks to our Lemma 4, one may solve the saddle point problem (17) and extract an optimal stochastic transport map \( T^* \) from its solution \( (f^*, T^*) \). In general, the \( \arg \inf \) set for \( f^* \) may contain not only the optimal stochastic transport maps but other stochastic functions as well.

4.2. Practical Optimization Procedure

To approach the problem (17) in practice, we use neural networks \( T_k : \mathbb{R}^P \times S \rightarrow \mathbb{R}^Q \) and \( f_\omega : \mathbb{R}^Q \rightarrow \mathbb{R} \) to parametrize \( T \) and \( f \), respectively. We train their parameters with the stochastic gradient ascent-descent (SGAD) by using random batches from distributions \( P, Q, S \). The optimization procedure is detailed in Algorithm 1.

Our Algorithm 1 requires an empirical estimator \( \hat{C} \) for \( C(x, T(x, \cdot)) \# S \). If the transport cost is strong (4), it is straightforward to use the following unbiased Monte-Carlo estimator from a random batch \( Z \sim S \):
\[
\hat{C}(x, T(x, z)) \overset{\text{def}}{=} \frac{1}{|Z|} \sum_{z \in Z} \|x - T(x, z)\|^2 - \frac{\gamma}{2} \hat{\sigma}^2,
\]
where \( \hat{\sigma}^2 \) is the (corrected) batch variance
\[
\hat{\sigma}^2 = \frac{1}{|Z| - 1} \sum_{z \in Z} \|T(x, z) - \frac{1}{|Z|} \sum_{z \in Z} T(x, z)\|^2.
\]

For unbiased estimation of strong costs (22), it is enough to sample a single noise vector, i.e., \( |Z| = 1 \). To estimate the \( \gamma \)-weak quadratic cost (23), one needs at least \( |Z| \geq 2 \) since the estimation of the variance \( \hat{\sigma}^2 \) of the batch is needed.

4.3. Relation to Prior Works

Our algorithm (1) recovers stochastic OT plans for weak costs (3). It generalizes previously known algorithms which learn deterministic maps for strong transport costs (4). When the cost is strong (4) and transport map \( T \) is restricted to be deterministic \( T(x, z) \equiv T(x) \), our Algorithm 1 yields minimax solutions [MM:R], which was discussed in (Korotin et al., 2021b, §2) for the quadratic cost \( \frac{1}{2} \|x - y\|^2 \) and further developed by (Rout et al., 2021) for the \( Q \)-embedded negative inner product cost \( -Q(x, y) \) and (Fan et al., 2020) for some other strong costs \( c(x, y) \).

Algorithm 1: Neural optimal transport (NOT)

Input: distributions \( P, Q, S \) accessible by samples;
  - mapping network \( T_0 : \mathbb{R}^P \times S \rightarrow \mathbb{R}^Q \);
  - potential network \( f_\omega : \mathbb{R}^Q \rightarrow \mathbb{R} \);
  - number of inner iterations \( K_T \);
  - (weak) cost \( C : X \times P(Y) \rightarrow \mathbb{R} \);
Output: learned stochastic OT map \( T_k \) representing an OT plan between distributions \( P, Q \);

repeat
  Sample batches \( Y \sim Q, X \sim P \);
  For each \( x \in X \) sample batch \( Z_x \sim S \);
    \( \mathcal{L}_f \leftarrow \frac{1}{|X|} \sum_{x \in X} \sum_{z \in Z_x} f_\omega(T_0(x, z)) - \frac{1}{|Y|} \sum_{y \in Y} f_\omega(y) \);
  Update \( \omega \) by using \( \frac{\partial \mathcal{L}_f}{\partial \omega} \);
for \( K_T = 1, 2, \ldots K_T \) do
  Sample batches \( X \sim P \);
  For each \( x \in X \) sample batch \( Z_x \sim S \);
    \( \mathcal{L}_T \leftarrow \frac{1}{|X|} \sum_{x \in X} \left[ \hat{C}(x, T_0(x, Z_x)) - \frac{1}{|Z_x|} \sum_{z \in Z_x} f_\omega(T_0(x, z)) \right] \);
  Update \( \theta \) by using \( \frac{\partial \mathcal{L}_T}{\partial \theta} \);
until not converged;

Monte-Carlo estimator is straightforward to derive:
\[
\hat{C}(x, T(x, z)) \overset{\text{def}}{=} \frac{1}{2|Z|} \sum_{z \in Z} \|x - T(x, z)\|^2 - \frac{\gamma}{2} \hat{\sigma}^2,
\]
4.4. Universal Approximation with Neural Networks

In this section, we show that it is possible to approximate stochastic transport maps with neural networks.

**Theorem 1** (Neural networks are universal approximators of stochastic transport maps). Assume that \( \mathcal{X}, \mathcal{Z} \) are compact and \( \mathcal{Q} \) has finite second moment. Let \( T \) be a stochastic map from \( \mathbb{P} \) to \( \mathcal{Q} \) (not necessarily optimal). Then for any nonpolynomial activation function and for any \( \epsilon > 0 \), there exists a neural network \( T_\theta : \mathbb{R}^P \times \mathbb{R}^S \to \mathbb{R}^Q \) satisfying

\[
\|T_\theta - T\|_{L^2}^2 \leq \epsilon,
\]

where \( L^2 = L^2(\mathbb{P} \times \mathbb{S}, \mathcal{X} \times \mathcal{Z} \to \mathbb{R}^Q) \) is the space of quadratically integrable w.r.t. \( \mathbb{P} \times \mathbb{S} \) functions \( \mathcal{X} \times \mathcal{Z} \to \mathbb{R}^Q \). Consequently, the network \( T_\theta \) satisfies

\[
\mathbb{W}_2^2((T_\theta)_\#(\mathbb{P} \times \mathbb{S}), \mathcal{Q}) \leq \epsilon,
\]

i.e., it generates a distribution which is \( \epsilon \)-close to \( \mathcal{Q} \) in \( \mathbb{W}_2^2 \).

**Proof.** The squared norm \( \|T\|_{L^2}^2 \) is equal to the second moment of \( \mathcal{Q} \) since \( T \) pushes \( \mathbb{P} \times \mathbb{S} \) to \( \mathcal{Q} \). The distribution \( \mathcal{Q} \) has finite second moment, and, consequently, \( T \in L^2 \). Thanks to (Folland, 1999, Proposition 7.9), the continuous functions \( C^0(\mathcal{X} \times \mathcal{Z} \to \mathbb{R}^Q) \) are dense in \( L^2 \). According to (Kidger & Lyons, 2020, Theorem 3.2), the neural networks \( \mathbb{R}^P \times \mathbb{R}^S \to \mathbb{R}^Q \) with nonpolynomial activation are dense in \( C^0(\mathcal{X} \times \mathcal{Z} \to \mathbb{R}^Q) \) w.r.t. \( L^\infty \) norm and, consequently, w.r.t. \( L^2 \) norm. Combining these results yields that neural networks are dense in \( L^2 \), and for every \( \epsilon > 0 \) there necessarily exists network \( T_\theta \) satisfying (24). For this network \( T_\theta \), (25) follows from (Korotin et al., 2021a, Lemma A.2).

Our Theorem 1 states that neural networks can approximate stochastic maps in \( L^2 \) norm. However, it should be taken into account that such continuous networks \( T_\theta \) theoretically may be highly irregular and hard to learn in practice.

5. Evaluation

We conduct tests on toy 2D distributions in Appendix B. In this section, we test our algorithm on an unpaired image-to-image style translation task. We perform comparison with popular existing style transfer methods in Appendix C. The code is written in PyTorch framework and will be made public together with all the trained translation models.

**Image datasets.** We use the following publicly available datasets as \( \mathbb{P}, \mathcal{Q} \): aligned anime faces\(^2\), celebrity faces (Liu et al., 2015), shoes (Yu & Grauman, 2014), Amazon handbags, churches from LSUN dataset (Yu et al., 2015), outdoor images from the MIT places database (Zhou et al., 2014). The size of datasets varies from 50K to 500K images.

**Pre-processing.** We beforehand rescale anime face images to 512 × 512, and do 256 × 256 crop with the center located 14 pixels above the image center to get the face. Next, for all these datasets, we rescale RGB channels to \([-1, 1]\] and resize images to the required size (64 × 64 or 128 × 128). We do not apply any augmentations to data.

**Train-test split.** We pick 90% of each dataset for training. The rest 10% are considered as test. All the results presented here are exclusively for test images, i.e., unseen data.

**Neural networks.** We use WGAN-QC discriminator’s ResNet architecture (Liu et al., 2019) for potential \( f \). We use UNet\(^3\) (Ronneberger et al., 2015) as the stochastic transport map \( T(x, z) \). The noise \( z \) is simply an additional 4th input channel (RGBZ), i.e., the dimension of the noise equals the entire image size (64 × 64 or 128 × 128). We use high-dimensional Gaussian noise with axis-wise \( \sigma = 0.1 \).

**Transport costs.** We experiment with the strong (\( \gamma = 0 \)) and \( \gamma \)-weak (\( \gamma > 0 \)) quadratic costs. Testing other costs might be interesting practically, but these two costs already provide promising practical performance.

**Other training details** are given in Appendix D.

5.1. Preliminary Evaluation

In the preliminary experiments with strong cost (\( \gamma = 0 \)), we noted that \( T(x, z) \) becomes independent of \( z \). For a fixed potential \( f \) and a point \( x \), the map \( T(x, \cdot) \) learns to be the map pushing distribution \( \mathcal{S} \) to some arg inf distribution \( \mu \) of (7). For strong costs, there are suitable degenerate distributions \( \mu \), see the discussion around (8). Thus, for \( T \) it becomes unnecessary to keep any dependence on \( z \), as it simply discards it and learns a deterministic map \( T(x, z) = T(x) \). We call this behavior a **conditional collapse**.

Importantly, for the \( \gamma \)-weak cost (\( \gamma > 0 \)), we noted a different behavior. In the experiments on real data, the stochastic map \( T(x, z) \) did not collapse conditionally. To explain this, we substitute (5) into (3) to obtain

\[
\mathbb{W}_2^2(\mathbb{P}, \mathcal{Q}) = \inf_{\pi \in \Pi(\mathbb{P}, \mathcal{Q})} \left[ \int_{\mathcal{X} \times \mathcal{Y}} \frac{1}{2} \|x - y\|^2 d\pi(x, y) - \gamma \cdot \int_{\mathcal{X}} \frac{1}{2} \text{Var}(\pi(y|x)) d\pi(x) \right].
\]

The first term is analogous to the strong cost (\( \mathbb{W}_2 = \mathbb{W}_2^0 \)), while the additional second term stimulates the OT plan to be stochastic, i.e., to have high conditional variance.

Taking into account our preliminary findings, we perform

\[^{2}\text{kaggle.com/reitanaka/alignedanimefaces}\]

\[^{3}\text{github.com/milesial/Pytorch-UNet}\]
two types of experiments. In §5.2, we learn deterministic (one-to-one) translation maps \( T(x) \) for the strong cost \( (\gamma = 0) \), i.e., do not add \( z \)-channel. In §5.3, we learn stochastic (one-to-many) maps \( T(x, z) \) for the \( \gamma \)-weak cost \( (\gamma > 0) \). For completeness, in Appendix A, we study how varying \( \gamma \) affects the diversity of samples.

### 5.2. One-to-one Translation with Optimal Maps

We learn deterministic OT maps between various pairs of datasets. We provide the results in Figures 1a, 1b and 6. Extra results are given in Appendix E. Being optimal, our translation map \( \tilde{T}(x) \) tries to minimally change the image content \( x \) in the \( L^2 \) pixel space. This results in preserving certain features during translation.

In \( shoes \leftrightarrow handbags \) (Figures 6b, 6a), the image color and texture of the pushforward samples reflects those of input samples. In \( celeba (female) \leftrightarrow anime \) (Figures 1a, 6c, 6d), head forms, hairstyles are mostly similar for input and output images. The hair in anime is usually bigger than that in celeba. Thus, when translating \( celeba \rightarrow female \), the anime hair inherits the color from the celebrity image background. In \( outdoor \rightarrow churches \) (Figure 1b), the ground and the sky are preserved, in \( celeba (male) \rightarrow celeba (female) \) (Figure 6e) – the face does not change. We also provide results for translation in the case when the input and output domains are significantly different, see \( anime \rightarrow shoes \) (Figure 6f).

#### Related work

Existing unpaired translation models, such as CycleGAN (Zhu et al., 2017) or UNIT (Liu et al., 2017), typically have complex adversarial optimization objectives endowed with additional losses such as cycle-consistency. As a result, the models require simultaneous optimization of multiple generator, discriminator, encoder networks. Importantly, vanilla CycleGAN searches for a random transfer map by default and is not capable of preserving certain attributes, e.g., the color, see (Lu et al., 2019, Figure 5b). To handle this issue, imposing extra losses is required (Benaim & Wolf, 2017; Kim et al., 2017), which further complicates optimization and hyperparameter selection. In contrast, our approach has a straightforward optimization objective (17); we optimize only 2 networks (potential \( f \) and map \( T \)).

### 5.3. One-to-many Translation with Optimal Plans

We learn stochastic OT maps between various pairs of datasets for the \( \gamma \)-weak quadratic cost. The parameter \( \gamma \) equals \( \frac{2}{3} \) or 1 in the experiments. We provide the results in Figures 1c and 7. Extended results and examples of interpolation in the conditional latent space are given in
Appendix E. Similar to §5.2, the stochastic map \( \tilde{T}(x, z) \) preserves the attributes of input image. This time, the map is capable of producing multiple outputs.

Related work. Transforming a one-to-one learning pipeline to one-to-many is nontrivial. Simply adding additional noise input leads to conditional collapse (Zhang, 2018). This is resolved by AugCycleGAN (Almahairi et al., 2018) and M-UNIT (Huang et al., 2018), but their optimization objectives are much more complicated than vanilla one-to-one versions. We again emphasize that we optimize only 2 networks \( f, T \) in the straightforward objective (17).

6. Discussion

Computational complexity. The time and memory complexity of training deterministic OT maps \( T(x) \) is comparable to that of training usual generative models for style transfer. Our networks converge in 1-3 days on a Tesla V100 GPU (16 GB); wall-clock times depend on the datasets and the image sizes. Training stochastic \( T(x, z) \) is harder since we sample multiple random \( z \) per \( x \) (we use \(|Z| = 4\)). Thus, we learn stochastic maps on \( 4 \times \) Tesla V100 GPUs.

Potential impact. Our method is a generic tool to align probability distributions with deterministic and stochastic maps. Beside unpaired style transfer, we expect our approach to be applied to other one-to-one and one-to-many unpaired learning tasks as well (image restoration, domain adaptation, etc.) and improve existing models in those fields. However, it should be taken into account that OT maps we learn might be suitable not for all unpaired tasks.

Limitations. Our method searches for a solution \((f^*, T^*)\) of a saddle point problem (17) and extracts the stochastic OT map \( T^* \) from it. We highlight after Lemma 4 and in §5.1 that not all \( T^* \) are optimal stochastic OT maps. For strong costs, the issue leads to the conditional collapse. Studying
saddle points of (17) and arg inf sets (19) is an important challenge to address in the further research.

**Reproducibility.** We provide the source code for all experiments and will release the checkpoints for all models of §5. The details are given in README.MD.

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A. Variance-Similarity Trade-off

In this section, we study the effect of the parameter $\gamma$ on the structure of the learned stochastic map for the $\gamma$-weak quadratic cost. We consider handbags $\rightarrow$ shoes translation ($64 \times 64$) and test $\gamma \in \{0, \frac{1}{3}, \frac{2}{3}, 1\}$. The results are shown in Figure 8.

![Figure 8: Stochastic Handbags $\rightarrow$ shoes translation with the $\gamma$-weak quadratic cost for various values $\gamma$.](image)

**Discussion.** For $\gamma = 0$ there is no variety in produced samples (Figure 8a), i.e., the conditional collapse happens. With the increase of $\gamma$ (Figures 8b, 8c), the variety of samples increases and the style of the input images is mostly preserved. For $\gamma = 1$ (Figure 8d), the variety of samples is very high but many of them do not preserve the style of the input image. That is, parameter $\gamma$ can be viewed as the trade-off parameter balancing the variance of samples and their similarity to the input.

B. Toy 2D experiments

In this section, we conduct experiments with our Algorithm 1 on toy 2D distributions $P, Q$, i.e., $P = Q = 2$.

**Strong quadratic cost ($\gamma = 0$).** As we noted in §5.1 and Appendix A, for the strong quadratic cost, our method tends to learn deterministic maps $T(x, z) = T(x)$ which are independent of the noise input $z$. For deterministic maps $T(x)$, our method yields $\lfloor$MM:R$\rfloor$ method which has been evaluated in the recent Wasserstein-2 benchmark by (Korotin et al., 2021b). The authors show that the method recovers OT maps well on synthetic high-dimensional pairs $P, Q$ with known ground truth OT maps. Thus, for brevity, we do not include toy experiments with our method for the strong quadratic cost.
Weak quadratic cost ($\gamma > 0$). The analysis of computed transport plans for weak costs is challenging due to the lack of nontrivial pairs $P, Q$ with known ground truth OT plan $\pi^\star$. The situation is even worsened by the nonuniqueness of $\pi^\star$.

To cope with this issue, we consider the weak quadratic cost with $\gamma = 1$. For this cost, one may derive

$$C(x, \mu) = \int \frac{1}{2} \|x - y\|^2 d\mu(y) - \frac{1}{2} \text{Var}(\mu) = \frac{1}{2} \|x - \int y d\mu(y)\|^2.$$  \hfill (26)

For cost (26) and a pair $P, Q$, (Gozlan & Juillet, 2020, Theorem 1.2) states that there exists a $P$-unique (up to a constant) convex $\psi : \mathbb{R}^P \to \mathbb{R}$ such that every OT plan $\pi^\star$ satisfies $\nabla \psi(x) = \int y d\pi^\star(y|x)$. Besides, $\nabla \psi : \mathbb{R}^P \to \mathbb{R}^P$ is 1-Lipschitz.

Let $\hat{T}(x, z)$ be the stochastic map recovered by our Algorithm 1, and let $\hat{\pi}$ be the corresponding plan. Let

$$T(x) \overset{def}{=} \int y d\hat{\pi}(y|x) = \int_z \hat{T}(x, z) dS(z).$$  \hfill (27)

Due to the above mentioned characterization of OT plans, $T(x)$ should look like a gradient $\nabla \psi(x)$ of some convex function $\psi(x)$ and should nearly be a contraction. We check that this approximately holds on 2D toy examples.

Datasets. We test 2 pairs of distributions $P, Q$: Gaussian $\to$ Mixture of 8 Gaussians; Gaussian $\to$ Swiss roll.

Neural Networks. We use multi-layer perceptrons as $f_\omega, T_\theta$ with 3 hidden layers of 100 neurons and ReLU nonlinearity. The input of the stochastic map $T_\theta(x, z)$ is $2 + 2 = 4$ dimensional. The two first dimensions represent the input $x \in \mathbb{R}^2$ while the other dimensions represent the noise $z \sim S$. We employ a Gaussian noise with $\sigma = 0.1$.

Discussion. We provide qualitative results in Figures 9 and 10. In both cases, the pushforward distribution $\hat{T}_\#(P \times S)$ matches the desired target distribution $Q$ (Figures 9c and 10c). Figures 9e and 10e show how the mass of points $x \sim P$
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(a) Input distribution $P$.

(b) Target distribution $Q$.

(c) Fitted distribution $\hat{T}(P \times S) \approx Q$.

(d) Map $\hat{T}(x) = \int \hat{T}(x, z) dS(z)$.

(e) Learned stochastic map $\hat{T}(x, z)$.

Figure 10: Gaussian $\rightarrow$ Swiss Roll, learned stochastic OT map for the 1-weak quadratic cost.

is split by the stochastic map. The average maps $\hat{T}(x)$ indeed look like contractions: points $x$ near zero roughly satisfy $\hat{T}(x) \approx x$, while the points that are far from zero move closer to zero (Figures 9d and 10d).

Testing that $\hat{T}$ roughly equals a gradient of some convex function $\psi$ is much harder. That is, we check a slightly weaker necessary condition. The gradients of convex functions are cycle monotone (Rockafellar, 1966). Cycle monotonicity yields that for $x_1 \neq x_2$ the segments $[x_1, \nabla \psi(x_1)]$ and $[x_2, \nabla \psi(x_2)]$ do not intersect in the inner points (Villani, 2008, §8).

Visually, we see that in Figures 9d and 10d the segments $[x, \hat{T}(x)]$ do not intersect for different $x$, which is good.

C. Comparison with Style Transfer Methods

We compare our Algorithm 1 with popular models for unpaired style transfer. We consider handbags $\rightarrow$ shoes style translation $(64 \times 64)$. For quantitative comparison, we compute Frechet Inception Distance$^5$ (Heusel et al., 2017, FID) of the mapped test handbags subset w.r.t. the test shoes subset. The scores of our method and alternatives are given in Table 1.

| Type       | One-to-one | One-to-many |
|------------|------------|-------------|
| Method     | DiscoGAN   | Cycle GAN   | NOT (ours) | AugCycleGAN | MUNIT | NOT (ours) |
| FID       | 22.42      | 16.00       | 13.77      | 18.84 $\pm$ 0.11 | 15.76 $\pm$ 0.11 | 13.44 $\pm$ 0.12 |

Table 1: Test FID of the considered style translation methods.

$^4$For the sake of clarity, we slightly reformulated the actual property of the cycle monotone maps. For details, consult (Villani, 2008).

$^5$github.com/mseitzer/pytorch-fid
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**Comparison with One-to-one Methods.** We compare our method with CycleGAN (Zhu et al., 2017) and DiscoGAN (Kim et al., 2017). The translated images are shown in Figure 11.

![Translated Images](image)

(a) NOT (ours, $W_2$)

(b) DiscoGAN

(c) CycleGAN

Figure 11: Handbags $\rightarrow$ shoes translation, one-to-one maps learned by the methods in view.

**Comparison with One-to-many Methods.** We compare our method with AugCycleGAN (Almahairi et al., 2018) and MUNIT (Huang et al., 2018). The translated images are shown in Figure 12.

![Translated Images](image)

(a) NOT (ours, $W_{2,3}$)

(b) MUNIT

(c) AugCycleGAN

Figure 12: Handbags $\rightarrow$ shoes translation, one-to-many maps learned by the methods in view.

**Discussion.** Existing one-to-one methods visually preserve the style during translation comparably to our method (Figure 11). Alternative one-to-many methods do not preserve the style at all (Figure 12). FID scores of all the models are comparable.

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6 [github.com/eriklindernoren/PyTorch-GAN/tree/master/implementations/cyclegan](https://github.com/eriklindernoren/PyTorch-GAN/tree/master/implementations/cyclegan)

7 [github.com/eriklindernoren/PyTorch-GAN/tree/master/implementations/discogan](https://github.com/eriklindernoren/PyTorch-GAN/tree/master/implementations/discogan)

8 [github.com/aalmah/augmented_cyclegan](https://github.com/aalmah/augmented_cyclegan)

9 [github.com/NVlabs/MUNIT](https://github.com/NVlabs/MUNIT)
D. Experimental Details

We use the Adam optimizer (Kingma & Ba, 2014) with the default betas for both $T_\theta$ and $f_\omega$. The learning rate is $lr = 1 \cdot 10^{-4}$. The batch size is $|X| = 64$. The number of inner iterations is $k_T = 10$. When training with the weak cost (5), we sample $|Z_x| = 4$ noise samples per each image $x$ in batch. In toy experiments, we do 10K total iterations of $f_\omega$ update. In the experiments with style translation, our Algorithm 1 converges in $\approx 30$-40K iterations for most datasets.

**Dynamic weak cost.** In style translation for the $\gamma$-weak cost, we train the algorithm with the gradually changing $\gamma$. Starting from $\gamma = 0$, we linearly increase it to the desired value ($\frac{2}{3}$ or 1) during 25K first iterations of $f_\omega$.

**Stability of training.** In several cases, we noted that the optimization fluctuates around the saddle points and diverges. An analogous behavior of saddle point methods for OT has been observed by (Korotin et al., 2021b). Improving stability and convergence of the optimization is a promising avenue for the future work.

E. Additional Experimental Results

(a) Celeba (female) $\rightarrow$ anime translation, $128 \times 128$.

(b) Outdoor $\rightarrow$ church, $128 \times 128$.

(c) Handbags $\rightarrow$ shoes, $128 \times 128$.

(d) Shoes $\rightarrow$ handbags, $128 \times 128$.

Figure 13: Style translation with OT maps ($\mathbb{W}_2$). Additional examples (part 1).
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(a) Celeba (female) $\rightarrow$ anime translation, $64 \times 64$.

(b) Anime $\rightarrow$ celeba (female) translation, $64 \times 64$.

(c) Celeba (male) $\rightarrow$ celeba (female) translation, $64 \times 64$.

(d) Anime $\rightarrow$ shoes translation, $64 \times 64$.

Figure 14: Style translation with OT maps ($\mathcal{W}_2$). Additional examples (part 2).
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(a) Input images \( x \) and random translated examples \( T(x, z) \).

(b) Interpolation in the conditional latent space, \( z = (1 - \alpha)z_1 + \alpha z_2 \).

Figure 15: Celeba (female) → anime, 128 × 128, stochastic. Additional examples.
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(a) Input images $x$ and random translated examples $T(x, z)$.

(b) Interpolation in the conditional latent space, $z = (1 - \alpha) z_1 + \alpha z_2$.

Figure 16: Outdoor $\rightarrow$ church, $128 \times 128$, stochastic. Additional examples.
(a) Input images $x$ and random translated examples $T(x, z)$.

(b) Interpolation in the conditional latent space, $z = (1 - \alpha)z_1 + \alpha z_2$.

Figure 17: Handbags → shoes translation, 128 × 128, stochastic. Additional examples.
Neural Optimal Transport

(a) Input images $x$ and random translated examples $T(x, z)$.

(b) Interpolation in the conditional latent space, $z = (1 - \alpha)z_1 + \alpha z_2$.

Figure 18: Anime $\rightarrow$ celeba (female) translation, $64 \times 64$, stochastic. Additional examples.
Neural Optimal Transport

(a) Input images $x$ and random translated examples $T(x, z)$.

(b) Interpolation in the conditional latent space, $z = (1 - \alpha)z_1 + \alpha z_2$.

Figure 19: Anime → shoes translation, $64 \times 64$, stochastic. Additional examples.
Neural Optimal Transport

(a) Input images $x$ and random translated examples $T(x, z)$.

(b) Interpolation in the conditional latent space, $z = (1 - \alpha)z_1 + \alpha z_2$.

Figure 20: Shoes $\rightarrow$ handbags, $64 \times 64$, stochastic. Additional examples.