Universal Neural Optimal Transport

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Abstract

Optimal Transport (OT) problems are a cornerstone of many applications, but solving them is computationally expensive. To address this problem, we propose UNOT (Universal Neural Optimal Transport), a novel framework capable of accurately predicting (entropic) OT distances and plans between discrete measures of variable resolution for a given cost function. UNOT builds on Fourier Neural Operators, a universal class of neural networks that map between function spaces and that are discretization-invariant, which enables our network to process measures of varying sizes. The network is trained adversarially using a second, generating network and a self-supervised bootstrapping loss. We theoretically justify the use of FNOs, prove that our generator is universal, and that minimizing the bootstrapping loss provably minimizes the ground truth loss. Through extensive experiments, we show that our network not only accurately predicts optimal transport distances and plans across a wide range of datasets, but also captures the geometry of the Wasserstein space correctly. Furthermore, we show that our network can be used as a state-of-the-art initialization for the Sinkhorn algorithm, significantly outperforming existing approaches.

1. Introduction

Optimal Transport (Villani, 2009; Peyré & Cuturi, 2019) plays an increasing role in various areas in machine learning, such as domain adaptation (Courty et al., 2017), single-cell genomics (Schiebinger et al., 2019), imitation learning (Dadashi et al., 2020), imaging (Schmitz et al., 2018), dataset adaptation (Alvarez-Melis & Fusi, 2019), and signal processing (Kolouri et al., 2017). Often, an entropic regularizer is added, as this allows efficient computation of the solution via the Sinkhorn algorithm (Cuturi, 2013). The entropic OT problem between probability measures $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$ on Polish spaces $X, Y$, given a cost function $c : X \times Y \rightarrow \mathbb{R} \cup \{\infty\}$, is defined as

$$\text{OT}_\epsilon(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times Y} c \, d\pi - \epsilon KL(\pi || \mu \otimes \nu), \quad (1)$$

where $\Pi(\mu, \nu)$ is the set of all transport plans (i.e. measures on $X \times Y$ that admit $\mu$ resp. $\nu$ as their marginals), $KL(\pi || \mu \otimes \nu) = \int \log(\pi/\mu \otimes \nu) d\pi$ is the KL divergence of $\pi$ from $\mu \otimes \nu$, and $\epsilon > 0$ is a regularizing coefficient.1

Many of these applications require solving problem (1) repeatedly, such as in single-cell perturbations (Bunne et al., 2022; 2023b,a), Natural Language Processing (Xu et al., 2018), flow matching with OT couplings (Tong et al., 2024; Pooladian et al., 2023), or even seismology (Engquist & Froese, 2013). However, solving OT problems is computationally expensive, and fast approximation methods are an active area of research. Variations of the transport problem, such as (generalized) sliced Wasserstein distances (Kolouri et al., 2015; 2019) reduce computational complexity at the

1For a background on OT, see Appendix A.
cost of accuracy via random projections. Two previous works are aimed at predicting good initializations for the Sinkhorn algorithm, which can iteratively solve problem (1). In (Thornton & Cuturi, 2022), initializations are computed from OT problems between Gaussians. (Amos et al., 2022) train a neural network to predict transport plans and costs via the entropic dual OT problem (Section 2). While their framework shares some similarities with ours (see Section 3.1), can accurately predict the OT cost and plan associated with problem (1). To this end, we leverage Fourier Neural Operators (FNOs) (Kovachki et al., 2024), a discretization-invariant class of neural networks that can process inputs of variable sizes. An FNO $\mathcal{G}_\theta$ is trained to predict a solution to the dual OT problem (Section 2) given two measures $(\mu, \nu)$ from which the primal problem (1) can be solved. Training is self-supervised with an adversarial generator $\mathcal{G}_\theta$ which creates training distributions $\mathcal{G}_\theta(z) = (\mu, \nu)$ from $z \sim \rho_z = \mathcal{N}(0, I)$ (see Section 3.4). We want to highlight that in contrast to most neural OT frameworks, such as Discrete Optimal Transport. We give a brief overview of optimal transport, and how it relates to UNOT. For a more thorough introduction, see Appendix A.1 or (Peyré & Cuturi, 2019; Villani, 2009).

Notation. We write vectors in bold and matrices in capitals. $1_n \in \mathbb{R}^n$ denotes the vector where all entries are equal to 1, $\Delta^{n-1}$ the $n$-1 dimensional simplex in $\mathbb{R}^n$, and all elements in $\Delta^{n-1}$ with positive entries are denoted by $\Delta^{n-1}_{>0}$. $\mathcal{P}(X)$ denotes the space of probability measures on $X$, and $\mathcal{P}_p(X)$ the set of probability measures with finite $p$-th moments. For $\mu \in \mathcal{P}(X)$ and a map $T$, we denote by $T \# \mu$ the pushforward of $\mu$ under $T$, i.e. the measure $\mu \circ T^{-1}$.

2. Background

Unregularized Optimal Transport. The unregularized problem takes the form $\inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times Y} c(x, y) d\pi(x, y)$, akin to (1) without the regularization term. In the case where $X = Y$, $c(x, y) = d(x, y)^p$ for $p \geq 1$ and a metric $d$ on $X$, the Wasserstein-$p$ distance is defined as

$$W_p(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \left( \int_{X \times X} d(x, y)^p d\pi(x, y) \right)^{\frac{1}{p}},$$

which is indeed a distance on the space $\mathcal{P}_p(X)$ of Borel measures with finite $p$-th moments (Villani, 2009).

Dual Optimal Transport Problem. The regularized Kantorovich problem (1) admits a dual formulation:

$$\sup_{f \in L_1(\mu), g \in L_1(\nu)} \int_X f(x) d\mu(x) + \int_Y g(y) d\nu(y) - \ell^*(f, g),$$

where

$$\ell^*(f, g) = \epsilon \int_{X \times Y} e^{\frac{1}{\epsilon}(f(x) + g(y) - c(x, y))} - 1 d\mu(x) d\nu(y).$$

It can be shown that if $c \in L_1(\mu \otimes \nu)$, the values of the primal (1) and the dual (3) coincide (Nutz, 2022).

Discrete Optimal Transport. We want to apply UNOT to discretizations of measures $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$ (see Section 3.1). To this end, consider measures $\mu$ and $\nu$ that are supported on finitely many points $x_1, \ldots, x_m \in X$, $y_1, \ldots, y_n \in Y$ resp. i.e., $\mu = \sum_{i=1}^m a_i \delta_{x_i}$ and $\nu = \sum_{j=1}^n b_j \delta_{y_j}$. By abusing notation, we can write $\mu \in \mathbb{R}^m_\geq$ and $\nu \in \mathbb{R}^n_\geq$. Note that the dual potentials in problem (3) are elements in $L_1^\ast(\mu)$ resp. $L_1^\ast(\nu)$, hence we can abuse notation again and consider the potentials $f \in \mathbb{R}^m$ and $g \in \mathbb{R}^n$ to be vectors as well. This point of view gives rise to discrete optimal transport. We set $C \in \mathbb{R}^{m \times n}$ via $C_{ij} = c(x_i, y_j)$, and view

\[\text{Whenever we view a discrete measure or a function as a vector, we will use bold characters.}\]
transport plans as matrices \( \Pi \in \mathbb{R}^{m \times n} \) (see Appendix A.1 for a more thorough introduction to discrete transport). The following proposition shows the plan \( \Pi \) can be recovered from the dual vectors \( f \) and \( g \) (Peyré & Cuturi, 2019).

**Proposition 1.** Define the Gibbs kernel \( K = \exp(-C/\epsilon) \). The unique solution \( \Pi \) of the discrete OT problem is given by

\[
\Pi = \text{diag}(u)K\text{diag}(v)
\]  

(4)

for two positive scaling vectors \( u \) and \( v \) unique up to a scaling constant (i.e. \( \lambda u,\frac{1}{\lambda}v \) for \( \lambda > 0 \)). Furthermore, \((u, v)\) are linked to a solution \((f, g)\) of the dual problem via

\[
(u, v) = \left( \exp\left(\frac{f}{\epsilon}\right), \exp\left(\frac{g}{\epsilon}\right) \right).
\]

In Section 3.1, we show how the solution to the entropic dual between discrete \((\mu_n, \nu_n)\) converges to the solution of the continuous dual (3) as \((\mu_n, \nu_n)\) converge to continuous measures \((\mu, \nu)\) in some way, which will be crucial for the design of our network \( S_\phi \).

### 2.2. The Sinkhorn Algorithm

The Sinkhorn Algorithm 1 can iteratively solve the discrete dual problem and was introduced in (Cuturi, 2013). It requires an initialization \( v^0 \in \mathbb{R}^n \), which is typically set to \( 1_n \), and \( \mu \) and \( \nu \) to be positive everywhere.

**Algorithm 1** Sinkhorn\((\mu, \nu > 0, K = \exp(-C/\epsilon), \epsilon, v^0)\)

1: for \( i = 0, \ldots, N \) do
2: \( u^{i+1} \leftarrow \mu / K u^i \)
3: \( v^{i+1} \leftarrow \nu / K^T v^{i+1} \)
4: end for
5: \( \Pi \leftarrow \text{diag}(u^i)K\text{diag}(v^i) \), \( \text{OT}_\epsilon(\mu, \nu) \leftarrow (C, \Pi) \)
6: return \( u, v, \Pi, \text{OT}_\epsilon(\mu, \nu) \)

In the algorithm, \( / \) is to be understood as element-wise division. Sinkhorn and Knopp (Sinkhorn & Knopp, 1967) showed that the iterates \( u^i \) and \( v^i \) from the algorithm converge to the vectors \( u \) and \( v \) from Proposition 1.

### 2.3. Predicting Dual Potentials

Given discrete measures \( \mu \) and \( \nu \), UNOT should ultimately be used to approximate the associated transport plan and cost. However, given an optimal dual potential \( v \), the corresponding potential \( u \) can be computed as

\[
 u = \mu / K v,
\]

(5)

which also holds at convergence of the Sinkhorn algorithm. Thus, solving for the \( m \times n \)-dimensional plan \( \Pi \) can be reduced to a \( n \)-dimensional problem over \( v \). Since computations in the log space tend to be more stable (Peyré & Cuturi, 2019), we will instead let UNOT predict the dual potential \( g = \epsilon \log(v) \), i.e.

\[
 S_\phi(\mu, \nu) = g, \quad \mu \in \mathcal{P}(\mathcal{X}), \nu \in \mathcal{P}(\mathcal{Y}).
\]

The prediction \( g \) can then be used to solve the entropic OT problem via the relationship (5) and Proposition 1, or to initialize the Sinkhorn algorithm via \( v^0 = \exp(g/\epsilon) \).

Note that the solution to the entropic dual is not unique, as can be seen from Proposition 1. How we deal with this fact is explained in section 3.4. However, when endowing \( \mathbb{R}^m \times \mathbb{R}^n \) with the equivalence relation \((u_1, v_1) \sim (u_2, v_2) \Leftrightarrow \exists \lambda > 0 : (\lambda u_1, 1/\lambda v_2) \) (i.e. accounting for the non-uniqueness of the solution of the dual), the map \((\mu, \nu) \mapsto v \), mapping two measures to the associated dual potential in the quotient space, is Lipschitz continuous (Carlier et al., 2022), which supports its learnability by a neural network.

### 3. Universal Neural Optimal Transport

Consider the optimal transport problem between two (greyscale) images, encoded as vectors in \( \mu_n, \nu_n \in \mathbb{R}^n \). These can be viewed as discrete measures on \( \mathcal{P}([0, 1]^2) \), which discretize continuous measures \( \mu, \nu \in \mathcal{P}([0, 1]^2) \), where the discretization depends on the resolution of the image, and the continuous measures correspond to the images at “infinite” resolution. UNOT should predict the corresponding dual potential \( g_n \in \mathbb{R}^n \) solving (3) independent of the resolution \( n \).

In Section 3.1, we establish a convergence result for the dual potentials as \( n \to \infty \), which justifies the use of Neural Operators (Kovachki et al., 2024) as a parametrization of \( S_\phi \); this is detailed in Section 3.2. Furthermore, as we want UNOT to work across datasets, we require a generator \( G_\theta \) that can provably generate any pair of distributions during training (Section 3.3). In Section 3.4, we construct an adversarial training objective for \( S_\phi \) and \( G_\theta \). Further details about hyperparameter and architecture choices can be found in Appendix C. The implementation and model weights are available at https://github.com/GregorKornhardt/UNOT.

#### 3.1. Convergence of Dual Potentials

In this section, we prove convergence of the discrete dual potentials \( g_n \) as \( n \) goes to infinity. For brevity, this section is kept informal; see Appendix B for a formal treatment. Assume now that \( \mathcal{X} = \mathcal{Y} \subseteq \mathbb{R}^N \) is compact, and \( c(x, y) = \|x - y\|^2_2 \), which gives rise to the Wasserstein-2
distance. For absolutely continuous $\mu, \nu \in \mathcal{P}(\mathcal{X})$, denote by $(\mu_n)_{n \in \mathbb{N}}, (\nu_n)_{n \in \mathbb{N}} \subset \mathcal{P}(\mathcal{X})$ discretizing sequences of $\mu$ and $\nu$ (formally defined in Appendix B). While a solution $(f_n, g_n)$ of the discrete dual problem between $\mu_n$ and $\nu_n$ is only defined for $\nu_n$ - a.e., it can be canonically extended to all of $\mathcal{X}$ (Feydy et al., 2018) (see Appendix B for details). The following proposition shows that the extended potentials $(f_n, g_n)$ converge to the solution $(f, g)$ of the continuous entropic problem between $\mu$ and $\nu$.

**Proposition 2. (Informal)** Let $(\mu_n)_{n \in \mathbb{N}}, (\nu_n)_{n \in \mathbb{N}}$ be discretizing sequences for absolutely continuous $\mu, \nu \in \mathcal{P}(\mathcal{X})$. Let $(f_n, g_n)$ be the (unique) extended dual potentials of $(\mu_n, \nu_n)$ such that $f_n(x_0) = 0$ for some $x_0 \in \mathcal{X}$ and all $n$. Let $(f, g)$ be the (unique) dual potentials of $(\mu, \nu)$ such that $f(x_0) = 0$. Then $f_n$ and $g_n$ converge uniformly to $f$ and $g$ on all of $\mathcal{X}$.

A formal version and its proof can be found in Appendix B. This proposition is crucial in designing our network $S_\theta$, as we discuss in the following section.

### 3.2. Fourier Neural Operators

Fourier Neural Operators (FNOs) (Kovachki et al., 2024) are neural networks mapping between infinite-dimensional function spaces, and are discretization-invariant, meaning they can process input and output functions at varying resolutions of the domain. More precisely, given an input function $u$ defined on some domain $\mathcal{U}$, $u$ can be encoded as a vector $u = [u_1, \ldots, u_n]$ corresponding to the value of $u$ at $n$ points in $\mathcal{U}$, where $n$ can vary; the same applies to the output. In Section 3.1, we showed that the dual potentials corresponding to measures $\mu_n$ and $\nu_n$ converge uniformly to the continuous potentials corresponding to the limiting distributions $\mu$ and $\nu$ as the resolution of $\mu_n$ and $\nu_n$ increases, hence FNOs are a natural architecture for our learning task. More details on FNOs can be found in Appendix A.5.

### 3.3. Generating Measures

UNOT is trained on pairs of distributions generated by a generator network $G_\theta$ of the following form:

$$G_\theta : \mathbb{R}^d \to \mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{X})$$

$$z \sim \rho_z \mapsto \mathcal{R} [\sigma (\text{NN}_\theta (z) + \lambda I_{d,d'} (z)) + \delta] ,$$

where $\rho_z = \mathcal{N}(0, I_d)$ is a Gaussian prior, $\text{NN}_\theta$ is a trainable neural network, $I_{d,d'}$ is an interpolation operator matching the generator’s output dimension $d'$ and acting as a skip connection reminiscent of ResNets (He et al., 2016), $\lambda > 0$ is a constant and $\sigma := \text{ReLU}$. $\delta > 0$ is a small constant needed to generate our targets with the Sinkhorn algorithm, as outlined in Section 3.4. $\mathcal{R}$ denotes renormalizing to two probability measures and downsampling them to random dimensions in a set range, such that $S_\theta$ trains on measures of varying resolutions, which is known to improve NO training (Li et al., 2024a). The generator is universal in the following sense:

**Theorem 3.** Let $0 < \lambda < 1$ and $G_\theta : \mathbb{R}^d \to \mathbb{R}^d$ be defined via

$$G_\theta (z) = \sigma (\text{NN}_\theta (z) + \lambda z) ,$$

where $z \sim \rho_z = \mathcal{N}(0, I_1)$, and where $\text{NN}_\theta : \mathbb{R}^d \to \mathbb{R}^d$ is Lipschitz continuous with $\text{Lip}(\text{NN}_\theta) = L < \lambda$. Then $G_\theta$ is Lipschitz continuous with $\text{Lip}(\sigma) < L + \lambda$, and for any $x \in \mathbb{R}^d_\geq 0$ it holds

$$\rho_{G_\theta \# \rho_z} (x) \geq \frac{1}{(L + \lambda)^d} \mathcal{N}(G_\theta^{-1}(x)|0, I) .$$

In other words, $G_\theta \# \rho_z$ has positive density at any non-negative $x \in \mathbb{R}^d_\geq 0$. This shows that any pair of discrete probability measures $(\mu, \nu)$ can be generated by $G_\theta$. A direct consequence of the theorem is an extension to functions that are compositions of functions $G_\theta$ as above, which covers a wide class of ResNets. Both proofs can be found in Appendix B.

**Corollary 4.** Let $G_\theta = G_{\theta_1} \circ \cdots \circ G_{\theta_n}$ be a composition of functions $G_{\theta_i}$, each of which is of the form as in Theorem 3. Let $z \sim \rho_z = \mathcal{N}(0, I_1)$. Then

$$\rho_{G_{\theta_1} \circ \cdots \circ G_{\theta_n} \circ \rho_z} (x) \geq \frac{1}{(L + \lambda)^{n d}} \mathcal{N}(G_{\theta_1}^{-1}(x)|0, I) .$$

Although the more general Corollary 4 is not needed for our purposes, it might be of independent interest to the research community. Note that the generator in Theorem 3 does not exactly match our generator’s architecture. A discussion of how the theorem relates to our setting, as well as further details on the generator, can be found in Appendix C.

![Generated pair of training samples (lighter=more mass).](image)

Figure 2 shows a pair of samples generated by $G_\theta$. The generator seems to layer highly structured shapes with more blurry ones. More examples can be found in Appendix D.1.

### 3.4. UNOT Training Algorithm

Given a pair of distributions $(\mu, \nu) = G_\theta (z)$ in this section, we will remove the subscript $n$ for clarity, $S_{\theta}(\mu, \nu) =: g_\theta$ should equal the true dual potential $g$.
associated with \( \mu \) and \( \nu \). Hence, we could simply compute the true potential \( g \) with the Sinkhorn algorithm and use \( L_2(g_{\phi}, g) := \| g_{\phi} - g \|_2^2 \) as our training loss. However, it would be prohibitively expensive to run the Sinkhorn algorithm until convergence. Hence, we instead employ a bootstrapping loss on the prediction \( g_{\phi} \). Let \( \tau_k : (\mu, \nu, g_{\phi}) \rightarrow g_{\tau_k} \) denote running the Sinkhorn algorithm on \( (\mu, \nu) \) with initialization \( v^0 = \exp(g_{\phi}/\epsilon) \) for a very small number of iterations \( k \), i.e., warmstarting the algorithm with the current prediction \( g_{\phi} \), and returning \( \epsilon \log v = g_{\phi} \). To ensure uniqueness and improve training, we shift \( g_{\tau_k} \) to have zero sum; this corresponds to the non-uniqueness of the dual potentials, see Proposition 1. We now prove that minimizing \( L_2(g_{\phi}, g_{\tau_k}) \) implies minimizing the ground truth loss \( L_2(g_{\phi}, g) \) against the true potential \( g \).

**Proposition 5.** For two discrete measures \((\mu, \nu)\) with \( n \) particles, let \( g \) be an optimal dual potential, \( g_{\phi} = S_\phi(\mu, \nu) \), and \( g_{\tau_k} = \tau_k(\mu, \nu, g_{\phi}) \). Without loss of generality, assume that \( \sum_i g_{\phi_i} = \sum_i g_{\tau_k} = 0 \). Then

\[
L_2(g_{\phi}, g) \leq c(K, k, n) L_2(g_{\phi}, g_{\tau_k})
\]

for some constant \( c(K, k, n) > 1 \) depending only on the Gibbs kernel \( K \), \( k \), and \( n \).

The proposition shows that minimizing \( L_2(g_{\phi}, g_{\tau_k}) \) implies minimizing \( L_2(g_{\phi}, g) \), i.e., the loss between the prediction and the ground truth potential. The proof is based on the Hilbert projective metric (Peyré & Cuturi, 2019) and can be found in Appendix B.

**Training objective.** Having defined the loss for \( S_\phi \), as well as the target generation procedure, the training objective for \( S_\phi \) and \( G_\theta \) consists of \( S_\phi \) trying to minimize the loss \( L_2(g_{\phi}, g) \), while \( G_\theta \) attempts to maximize it, similar to the training objective in GANs (Goodfellow et al., 2014). Putting everything together, our adversarial training objective for \( S_\phi \) and \( G_\theta \) reads

\[
\max_{\theta} \min_{\phi} \mathbb{E}_{z \sim p_z} \left[ L_2(\tau_k(G(z), S(G(z))), S_\phi(G_\theta(z))) \right],
\]

where \( S \) and \( G \) without subscripts denote no gradient tracking, as the target is not backpropagated through the training algorithm can be seen in Algorithm 2. In practice, training will be batched, which we omitted for clarity. Note that vectors \( g \) with subscripts \( \theta \) or \( \phi \) are backpropagated through with respect to these parameters, whereas target vectors (with subscript \( \tau_k \)) are not.

**Training Details.** We train with \( c(x, y) = \| x - y \|_2^2 \) being the squared Euclidean distance on the unit square, i.e., \( \mathcal{X} = [0, 1]^2 \). We train on 200M samples \( z \), and training samples \((\mu, \nu)\) are between \( 28 \times 28\)- and \( 64 \times 64\)-dimensional

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**Algorithm 2 UNOT Training Algorithm**

1: in cost \( c \), reg parameter \( \epsilon \), prior \( \rho_z \), learning rates \{\alpha_i\}_i, \{\beta_i\}_i \), Sinkhorn target generator \( \tau_k \)
2: for \( i = 1, 2, \ldots, T \) do
3: \( z \leftarrow \text{sample}(\rho_z) \)
4: \( (\mu, \nu) \leftarrow G_\theta(z) \)
5: for mini-batch \((\mu^b, \nu^b)\) in \((\mu, \nu)\) do
6: \( g_\phi \leftarrow S_\phi(\mu^b, \nu^b) \)
7: \( g_{\tau_k} \leftarrow \tau_k(\mu^b, \nu^b, g_\phi) \)
8: \( \phi \leftarrow \phi - \alpha_1 \nabla_\phi L_2(g_{\tau_k}, g_\phi) \)
9: end for
10: for mini-batch \( z^b \) in \( z \) do
11: \( (\mu_0, \nu_0) \leftarrow G_\theta(z^b) \)
12: \( g_\theta \leftarrow S_\phi(\mu_0, \nu_0) \)
13: \( g_{\tau_k} \leftarrow \tau_k(\mu_0, \nu_0, g_\phi) \)
14: \( \theta \leftarrow \theta + \beta_1 \nabla_\theta L_2(g_{\tau_k}, g_\theta) \)
15: end for
16: end for

(randomly downsampled in \( G_\theta \)). Training takes around 35h on an H100 GPU. \( S_\phi \) has 26M and \( G_\theta \) 272k parameters. We highlight that \( S_\phi \) is relatively small, such that its runtime vanishes compared to the runtime of even just a few Sinkhorn iterations, making it much cheaper to run than Sinkhorn (see Section 4). We set \( \alpha \) (the number of Sinkhorn iterations in \( \tau_k \)) to 5, and \( \epsilon = 0.01 \). Additional training details can be found in Appendix C.

### 4. Experiments

We demonstrate the performance of UNOT on various tasks, such as predicting transport distances, initializing the Sinkhorn algorithm, computing Sinkhorn divergence barycenters, and approximating Wasserstein geodesics. We view images as discrete distributions on the unit square, and test on MNIST \((28 \times 28)\), grayscale CIFAR10 \((28 \times 28)\), the teddy bear class from the Google Quick, Draw! dataset \((64 \times 64)\), and Labeled Faces in the Wild \((LFW, 64 \times 64)\), as well as cross-datasets CIFAR-MNIST and LFW-Bear (where \( \mu \) comes from one dataset and \( \nu \) from the other). Unless otherwise noted, we perform a single Sinkhorn iteration on \( g = S_\phi(\mu, \nu) \) in all experiments in order to compute the second potential \( f \). Errors are averaged over 500 samples. Additional experiments, including a sweep over input sizes \( 10 \times 10 \) to \( 64 \times 64 \), as well as variants of UNOT for fixed input dimension or variable \( \epsilon \) can be found in Appendix D.6.

#### 4.1. Predicting Transport Distances

We compare the convergence of the Sinkhorn algorithm in terms of relative error on the transport distance \( \text{OT} \), \((\mu, \nu)\) for our learned initialization \( v^0 = \exp(S_\phi(\mu, \nu)/\epsilon) \) to...
the default initialization $1_n$ and the Gaussian initialization from (Thornton & Cuturi, 2022), which is based on closed-form solutions for Gaussian distributions. We do not compare to (Amos et al., 2022), as their approach is inherently dataset dependent and breaks down when testing on out-of-distribution data.\footnote{We note that it should be possible to finetune UNOT on specific datasets as well; however, we have not tested this.} Figure 1 (Section 1) shows the relative error on $\text{OT}_\epsilon(\mu, \nu)$ after a single Sinkhorn iteration. Figure 3 shows the same quantity over the number of Sinkhorn iterations, demonstrating that UNOT can be used as a state-of-the-art initialization. Table 1 shows the average number of Sinkhorn iterations needed to achieve 0.01 relative error on $\text{OT}_\epsilon(\mu, \nu)$. In Table 2 we show the relative speedup achieved by initializing the Sinkhorn algorithm with UNOT. We achieve an average speedup of 1.8 on $28 \times 28$ datasets and 3.13 on $64 \times 64$ datasets. For comparison, the relative speedup achieved in (Amos et al., 2022) was 1.96 (for a model trained on a single $28 \times 28$ dataset).\footnote{We did not optimize the network $S_{\phi}$ for efficiency, and more efficient implementations likely exist. Note that FNOs process complex numbers, but PyTorch is heavily optimized for real number operations. With kernel support for complex numbers, UNOT will likely be much faster. In addition, computation times can vary significantly across different hardware.}

### 4.2. Sinkhorn Divergence Barycenters

The Wasserstein barycenter for a set of measures \( \{ \nu_1, \ldots, \nu_N \} \subset P_2(X) \) and \( \lambda \in \Delta^{n-1} \) is defined as

\[
\mu = \arg\min_{\mu \in P_2(X)} \sum_{i} \lambda_i W_2^\epsilon(\mu', \nu_i).
\]

(7)

To make this problem tractable, consider the Sinkhorn divergence barycenter

\[
\mu = \arg\min_{\mu \in P_2(X)} \sum_{i} \lambda_i \text{SD}_\epsilon(\mu', \nu_i),
\]

(8)

where the Sinkhorn divergence\footnote{It can be seen as a debiased version of $\text{OT}_\epsilon(\mu, \nu)$, and we use it as an approximation of the squared Wasserstein distance.} between $\mu$ and $\nu$ is

\[
\text{SD}_\epsilon(\mu, \nu) = \text{OT}_\epsilon(\mu, \nu) - \frac{1}{2} \text{OT}_\epsilon(\mu, \mu) - \frac{1}{2} \text{OT}_\epsilon(\nu, \nu).
\]

Now for discrete measures $\mu, \nu$, denote by $(f, g)$ the dual potentials for $\text{OT}_\epsilon(\mu, \nu)$, and by $p$ that for $\text{OT}_\epsilon(\mu, \mu)$, the gradient of (8) w.r.t $a$ is given by (cf. (Feydy et al., 2018)):

\[
\nabla_a \text{SD}_\epsilon(\mu, \nu) = f - p.
\]

(9)

Hence, we can solve (8) with (projected) gradient descent,
where \( S_{\phi} \) predicts \( f \) and \( p \) in (9). Further details and a pseudocode can be found in Appendix A.2. Figure 4 shows UNOT barycenters vs. the true barycenters (computed with the POT library) of between 5 and 10 MNIST samples of the same digit per barycenter. In Figure 5, we show barycenters computed between four shapes. UNOT accurately predicting barycenters demonstrates it captures the geometry of the Wasserstein space beyond predicting distances.

4.3. Calculating Geodesics

Let \( \mu, \nu \in P_2(\mathcal{X}) \) be two measures such that \( \nu = T_{\#} \mu \) for an optimal transport map \( T : \mathcal{X} \to \mathcal{X} \) (which exists for the non-entropic optimal transport problem under certain conditions, see Appendix A.1). The Wasserstein geodesic between \( \mu \) and \( \nu \), also called McCann interpolation, is the constant-speed geodesic between \( \mu \) and \( \nu \) and given by

\[
\mu_t : [0, 1] \to P_2(\mathcal{X}), \quad t \mapsto [(1 - t)I + tT]_{\#} \mu.
\]

It can be interpreted as the shortest path between \( \mu \) and \( \nu \). The Wasserstein barycenter (7) between \( \{\mu_i, (1 - t)\} \) and \( \{\nu, t\} \) (i.e. where \( 1 - t \) and \( t \) are the weights \( \lambda_i \) from equation (7)) turns out to be equal to \( \mu_t \) (Agueh & Carlier, 2011). This gives us two methods to approximate the Wasserstein geodesic between \( \mu \) and \( \nu \): Either by iteratively computing barycenters as in Section 4.2, or by computing the (entropic) transport plan from equation (4) as an approximation to \( T \) (we are leaving out some technicalities for brevity here, which can be found in Appendix A.3). We compare the geodesics computed by UNOT to the ground truth geodesic (obtained from the true OT plan), as well as to GeONet (Gracyk & Chen, 2024), a recently proposed framework that also uses Neural Operators to learn Wasserstein geodesics directly by parametrizing a coupled PDE system encoding the optimality conditions of the dynamic OT problem. Akin to (Amos et al., 2022), GeONet is inherently dataset dependent. Figure 7 shows the McCann interpolation between two MNIST digits using the ground truth OT plan, the OT plan computed by UNOT, barycenters computed by UNOT, and the GeONet geodesic. We see that while GeONet is trained to predict geodesics on MNIST, while UNOT does not train on geodesics, nor on MNIST, both geodesics computed by UNOT are significantly better than the GeONet geodesic.

4.4. Wasserstein on Wasserstein Distance

Oftentimes in machine learning, the distributions of interest are not images, but distributions over images, such as in generative modeling. In this experiment, we show that UNOT can successfully transport distributions over images as well. Let \( \hat{\mu}, \hat{\nu} \in P_2([0, 1]^2, W_2) \), i.e. the space of distributions over images equipped with the Wasserstein distance (and \( P([0, 1]^2) \) being equipped with \( c \), as usual). Denote by SD\(_c\)(\( \hat{\mu}, \hat{\nu} \)) the Sinkhorn divergence between \( \hat{\mu} \) and \( \hat{\nu} \), where we use SD\(_c\)(\( \mu, \nu \)) as the ground cost between \( \mu, \nu \in P_2([0, 1]^2) \) as an approximation of \( W_2^2(\mu, \nu) \). Writing \( \hat{\mu} = \frac{1}{n} \sum_{i} \delta_{\mu_i}, \quad \hat{\nu} = \frac{1}{n} \sum_{j} \delta_{\nu_j} \) for \( \mu_i, \nu_j \in P_2([0, 1]^2) \), we let UNOT approximate the particle flow \( \frac{\partial}{\partial t} \hat{\mu}_t = -\nabla_{\hat{\mu}_t} \text{SD}_c(\hat{\mu}_t, \hat{\nu}) \), for which a gradient can be derived in terms of the gradients of the Sinkhorn divergences SD\(_c\)(\( \mu_i, \nu_j \)), which are given by (9); more details can be found in Appendix A.4. In Figure 6, we plot the particle flow from Gaussian noise \( \hat{\mu} \) to a distribution \( \hat{\nu} \) over 10 images, where we visualize \( \hat{\mu} \) after every 10 gradient steps. We can see that the UNOT flow converges quickly.
Figure 7. McCann interpolations computed with the true OT plan, UNOT OT plan, UNOT barycenters, and GeONet (top to bottom).

5. Related Work

**Neural OT.** Various works deal with directly learning OT distances or maps in specific settings. Typically, neural approaches for learning OT distances aim at solving single instances of (high-dimensional) OT problems. In (Korotin et al., 2023), a maximin formulation for the dual problem is derived and two networks, parametrizing the transport plan and the dual potential resp., are trained adversarially. In (Bunne et al., 2023a), transport maps between continuous input distributions conditioned on a context variable are learned. Another interesting recent paper (Uscidda & Cuturi, 2023) suggests a universal regularizer, called the Monge gap, to learn OT maps and distances. Unlike these works, we focus on generalizing across OT problems.

**Initializing Sinkhorn.** There exist very little literature on initializing the Sinkhorn algorithm. (Thornton & Cuturi, 2022) propose using dual vectors recovered from the unregularized 1D optimal transport problem, or from closed-form transport maps in a Gaussian (mixture) setting, and were able to significantly speed up convergence. In (Amos et al., 2022), a learned approach is taken as well. They use a single network to predict the optimal dual potential \( f \) of the discrete dual problem, and their loss is simply the (negative) dual objective (3). This approach works well when training on low-dimensional datasets such as MNIST, and is elegant as it does not require ground truth potentials, i.e., is fully unsupervised, but it is not able to generalize to out-of-distribution data, and can also only be used for input measures of the same size as the training data.

**OT for Machine Learning.** Leveraging OT to formulate new machine learning methods has seen a surge in popularity in recent years, and it has been applied to a wide range of problems. Relevant works include the celebrated Wasserstein GAN (Arjovsky et al., 2017), multi-label learning (Frogner et al., 2015), inverse problems in physics (Engquist & Yang, 2019), or few-shot image classification to compute distances between images (Zhang et al., 2020). In flow matching OT can be used to straighten paths (Lipman et al., 2023; Tong et al., 2024; Pooladian et al., 2023). Approximating Wasserstein gradient flows with the JKO scheme is treated in (Alvarez-Melis & Fusi, 2021; Alvarez-Melis et al., 2022; Bunne et al., 2022; Choi et al., 2024). The theory of Wasserstein gradient flows has also been used to study learning dynamics in various settings, such as for overparametrized two-layer networks (Chizat & Bach, 2018) or simplified transformers (Geshkovski et al., 2024).

**Generative Adversarial Networks.** GANs (Goodfellow et al., 2014), like other types of generative models, aim at generating samples from a distribution \( \rho_{\text{data}} \), given access to a finite number of samples. In contrast, we do not have access to samples from the target distribution. However, our loss function (6) shares similarities with the adversarial GAN loss. Given prior samples \( z \sim \rho_z \) and data samples \( x \sim \rho_{\text{data}} \), the GAN objective for a generator \( G \) is

\[
\min_G \max_D \mathbb{E}_{x \sim \rho_{\text{data}}} \left[ \log D(x) \right] + \mathbb{E}_{z \sim \rho_z} \left[ \log (1 - D(G(z))) \right],
\]

where \( D \) is the discriminator, which predicts the probability that a sample came from the target distribution rather than the generator. Note that while our generator maximizes the objective, the GAN generator minimizes it.

6. Discussion

We presented UNOT, a neural OT solver based on Neural Operators capable of solving entropic transport problems for discrete input measures of varying resolutions that share an underlying cost function. To this end, we proposed a two-network approach, where one network generates training samples for the second network, and an adversarial training algorithm which enables our solver to generalize to various datasets at test time. To support our framework theoretically, we proved that the generator is universal, that our training objective minimizes the ground truth loss, and that a convergence result for the optimal dual potentials holds, which justifies the use of Neural Operators. UNOT predicts transport distances across a vast array of image datasets of varying resolutions up to \( 1-3\% \) relative error, and even approximates barycenters and geodesics in Wasserstein space by solving for the OT plan. Furthermore, we demonstrated that UNOT can be used as a state-of-the-art initialization for the Sinkhorn algorithm, achieving speedups of up to 3.46x. Current limitations are that the cost function \( c \) is constant and that UNOT does not extrapolate well to measures with significantly higher resolutions than the training samples. Scaling UNOT to higher resolutions, as well as applying it to other data modalities, possibly in higher dimensions than \( \mathbb{R}^2 \), are interesting directions for future research.
Universal Neural Optimal Transport

Impact Statement

This paper presents work whose goal is to advance the field of Machine Learning. There are many potential societal consequences of our work, as optimal transport has a vast range of applications, but none of these we feel must be specifically highlighted here.

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Universal Neural Optimal Transport

The Appendix is structured as follows: In Appendix A we give a more thorough background on OT, as well as additional technical details for our experiments on computing barycenters and geodesics. Appendix B contains all proofs omitted in the paper. In Appendix C, we provide additional training details, and Appendix D.1 contains additional experiments and materials.

A. Background

A.1. Optimal Transport

In this section, we recall some properties of optimal transport. First, we define the unregularized continuous problems for completeness.

**Problem A.1** (Kantorovich Optimal Transport Problem). For $\mu \in \mathcal{P}(\mathcal{X})$, $\nu \in \mathcal{P}(\mathcal{Y})$, and a cost $c : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \cup \{\infty\}$ the Kantorovich problem takes the form

$$\inf_{\pi \in \Pi(\mu, \nu)} \int c(x, y) \, d\pi(x, y)$$

The infimum in (10) is called the *transport cost*, and the minimizer $\pi$, if it exists, is the *optimal transport plan*.

The continuous dual problem is similar to the regularized dual (3). For a more thorough overview of OT, we refer the reader to (Villani, 2009; Peyrê & Cuturi, 2019; Chewi et al., 2024).

**Problem A.2** (Dual Optimal Transport Problem). For $\mu$, $\nu$ and $c$ as before, the dual problem reads

$$\sup_{f \in L^1(\mu), g \in L^1(\nu)} \int_{\mathcal{X}} f(x) \, d\mu(x) + \int_{\mathcal{Y}} g(y) \, d\nu(y),$$

where $f + g \leq c$ is to be understood as $f(x) + g(y) \leq c(x, y)$ for all $x, y$.

An important concept in optimal transport are *transport maps*.

**Definition A.3** (Transport Maps). A map $T : \mathcal{X} \to \mathcal{Y}$ is called a *transport map* between $\mu$ and $\nu$ if $\nu = T#\mu$. If there exists an optimal transport plan $\pi$ such that $\pi = (Id, T)#\mu$, $T$ is called an *optimal transport map*.

Of course, not every transport plan admits a transport map; however, every transport map yields an optimal transport plan via $\pi = (Id, T)#\mu$. For sufficient conditions for the existence of both transport plans and maps, we refer the reader to (Villani, 2009).

In the paper we mentioned that if $\mu$ and $\nu$ are supported on finitely many points, one can rewrite the problems A.1 and A.2 with vectors. We now define the discrete problems carefully.

**Problem A.4** (Discrete Optimal Transport Problem). For two discrete measures $\mu \in \Delta^{m-1}$ and $\nu \in \Delta^{n-1}$, and a cost matrix $C \in \mathbb{R}^{m \times n}$, the discrete OT problem is defined as

$$L(\mu, \nu) := \min_{\Pi \in \Pi(\mu, \nu)} \langle C, \Pi \rangle$$

Here, $\Pi(\mu, \nu)$ denotes the set of all transport plans between $\mu$ and $\nu$, i.e. matrices $\Pi \in \mathbb{R}_{\geq 0}^{m \times n}$ s.t. $\Pi 1_m = \mu$ and $\Pi^T 1_n = \nu$. The problem has a dual formulation:

**Problem A.5** (Dual Optimal Transport Problem).

$$D(\mu, \nu) := \max_{f \in \mathbb{R}^m, \, g \in \mathbb{R}^n} \langle f, \mu \rangle + \langle g, \nu \rangle$$

Here, $f + g \leq C$ is to be understood as $f_i + g_j \leq C_{ij}$ for all $i \in [m]$, $j \in [n]$. In the special case where $\mathcal{X} = \mathcal{Y}$ and $C$ corresponds to a metric, i.e. $C_{ij} = d(x_i, y_j)$, the Wasserstein distance of order $p$ between $\mu$ and $\nu$ for $p \in [1, \infty)$ is defined as:

$$W_p(\mu, \nu) = \left( \min_{\pi \in \Pi(\mu, \nu)} \sum_{i,j} C_{ij}^p \pi_{ij} \right)^{\frac{1}{p}}.$$
This definition coincides with the definition from the paper for continuous measures, if they are supported on finitely many points.

For completeness, we also state the entropically regularized primal and dual problem in the discrete case. The discrete problem is typically formulated with an entropy term instead of the KL divergence as in equation (1), but the two can be shown to be equivalent (Chewi et al., 2024).

**Definition A.6** (Entropy). For a matrix $P = [p_{ij}]_{ij} \in \mathbb{R}^{m \times n}$, we define its entropy $H(P)$ as

$$H(P) := -\sum_{i=1}^{m} \sum_{j=1}^{n} p_{ij} \log p_{ij}$$

if all entries are positive, and $H(P) := -\infty$ if at least one entry is negative. For entries $p_{ij} = 0$, we use the convention $0 \log 0 = 0$, as $x \log x \rightarrow 0$.

The entropic optimal transport problem is defined as follows.

**Problem A.7** (Entropic Discrete Optimal Transport Problem). For $\epsilon > 0$, the entropic optimal transport problem is defined as:

$$\text{OT}_\epsilon(\mu, \nu) := \min_{\Pi \in \Pi(\mu, \nu)} \langle C, \Pi \rangle - \epsilon H(\Pi).$$

Note that this is identical to the unregularized optimal transport problem, except that the unregularized one does not contain the regularization term $-\epsilon H(\Pi)$. As the objective in Problem A.7 is $\epsilon$-strongly convex, the problem admits a unique solution (Peyré & Cuturi, 2019).

The *Gibbs kernel* is defined as $K = \exp(-C/\epsilon)$. Then the entropic dual problem reads:

**Problem A.8** (Entropic Discrete Dual Problem).

$$\max_{f, \in \mathbb{R}^m, g, \in \mathbb{R}^n} \langle f, \mu \rangle + \langle g, \nu \rangle - \epsilon \left( \frac{e^{f}}{\epsilon}, K_\epsilon g \right).$$

Again, without the regularization term $-\epsilon \left( \frac{e^{f}}{\epsilon}, K_\epsilon g \right)$, this equals the regular optimal transport dual; note, however, that the unregularized dual is subject to the constraint $f + g \leq C$.

In both the continuous, as well as the discrete setting, there is duality, i.e. the optima of the primal and dual problems coincide. In addition, the optimizers are intrinsically linked, akin to Proposition 1 for the discrete entropic problem. We refer the reader to (Villani, 2009; Peyré & Cuturi, 2019) for more details.

**A.2. Calculating the Barycenter**

Recall the Sinkhorn divergence barycenter for a set of discrete measures $\{\nu_1, ..., \nu_N\} \subset \mathcal{P}_2(\mathcal{X})$,

$$\mu = \arg \min_{\mu' \in \mathcal{P}_2(\mathcal{X})} \sum_{i} \alpha_i \text{SD}_\epsilon(\mu', \nu_i).$$

For a solution $\langle f, g \rangle$ to the dual problem A.8 between two measures $\mu = \sum_i \alpha_i \delta_{x_i}$ and $\nu = \sum_j b_j \delta_{y_j}$, it holds

$$\text{SD}_\epsilon(\mu, \nu) = \langle \mu, f - p \rangle + \langle \nu, g - q \rangle,$$

see (Feydy et al., 2018). Here, $p$ and $q$ are the optimal potentials for $(\mu, \mu)$ and $(\nu, \nu)$ resp. (if both measures in the OT problem are the same, the dual potentials can be chosen to be equal).

From this identity, we immediately get

$$\nabla_a \text{SD}_\epsilon(\mu, \nu) = f - p.$$

Note that this is not a gradient with respect to the measure $\mu'$; instead, we view $\mu$ as a vector, and compute the gradient w.r.t. the entries in that vector. This means we essentially compute the barycenter on the discrete space $\{x_1, ..., x_n\}$. 


A pseudocode for how to approximate the Sinkhorn divergence barycenter with UNOT is given in Algorithm 3. Note that

Algorithm 3  

Barycenter Computation

1: in set of measures \( \{ \nu_i \}_i \subset \Delta^{n-1} \), initial \( \mu_0 \in \Delta^{n-1} \), weights \( \lambda \in \Delta^{n-1} \)
2: \( \mu \leftarrow \mu_0 \)
3: for \( i = 1, 2, \ldots, T \) do
4: \( p \leftarrow S_\phi(\mu, \mu) \)
5: for \( \nu_i \) in \( \{ \nu_i \}_i \) do
6: \( f_i \leftarrow S_\phi(\nu_i, \mu) \) //switch the order of the arguments to get \( f_i \) instead of \( g_i \)
7: end for
8: \( \mu \leftarrow \text{softmax}(\mu - \sum_i \lambda_i (f_i - p)) \)
9: end for

A pseudocode for how to approximate the Sinkhorn divergence barycenter with UNOT is given in Algorithm 3. Note that instead of using softmax to project back to probability measures, one could also just rescale; however, softmax proved better in practice.

**Barycenters can be far when Transport Distances are close.** We now give a simple example that illustrates that merely predicting transport distances accurately does not necessarily imply predicting barycenters accurately, at least in the nonregularized setting. Let \( \mu \) be the measure with mass 1/2 at the two points (0, 1) and (1, 0) in \( \mathbb{R}^2 \). Let \( \nu_1 \) be the measure with mass 1/2 at each of the points (−1, 0) and (1, −ε) for a small \( \epsilon > 0 \), and \( \nu_2 \) a measure with mass 1/2 at each of the two points (−1, 0) and (1, ε). Then as \( \epsilon \) goes to 0, the transport distances between \( \mu \) and \( \nu_1 \) resp. \( \mu \) and \( \nu_2 \) become arbitrarily close. However, the unique Wasserstein-p barycenter (for \( p > 1 \)) between \( \mu \) and \( \nu_1 \) has mass 1/2 at each of the points (−1/2, 1/2) and (1/2, −(1 + ε)/2), whereas the barycenter between \( \mu \) and \( \nu_2 \) has mass 1/2 at each of the points (−1/2, −1/2) and (1/2, (1 + ε)/2), so no matter how small \( \epsilon \) gets, the barycenters will always be far apart.

### A.3. Geodesics

In Section 4.3, we saw that the McCann interpolation between two measures \( \mu, \nu \in \mathcal{P}_2(\mathcal{X}) \) is a constant-speed geodesic. In this section, we provide additional background on constant-speed geodesics, and establish a connection between constant-speed geodesics in \( \mathcal{P}_2([0, 1]^2) \) and the notion of strong-\( \epsilon \) quasi-geodesics in the discretized space \( \mathcal{P}(\lfloor n \rfloor^2) \). This makes our approximation of geodesics as in Section 4.3 more rigorous.

First, we recall the definition of constant-speed geodesics.

**Definition A.9.** A curve \( \omega : [0, 1] \rightarrow (\mathcal{P}_2(\mathcal{X}), W_2) \) is called constant-speed geodesic between \( \omega(0) \) and \( \omega(1) \) if it satisfies

\[
W_2(\omega(t), \omega(s)) = |t - s|W_2(\omega(0), \omega(1)), \quad \forall t, s \in [0, 1].
\]

It turns out that for convex \( \mathcal{X} \subset \mathbb{R}^d \), constant-speed geodesics are equivalent to push-forwards under transport plans, and if the starting point \( \omega(0) \) is absolutely continuous, this is equal to the McCann interpolation.

**Theorem A.10.** Let \( \mathcal{X} \subset \mathbb{R}^d \) be convex. Then a curve \( \omega : [0, 1] \rightarrow (\mathcal{P}_2(\mathcal{X}), W_2) \) is a constant-speed geodesic between \( \omega(0) \) and \( \omega(1) \) if and only if it is of the form

\[
\omega(t) = (p_t)_# \pi
\]

for an optimal transport plan \( \pi \) between \( \omega(0) \) and \( \omega(1) \), where the interpolation \( p_t \) is given by \( p_t(x, y) = (1 - t)x + ty \). If, in addition, \( \omega(0) \) is absolutely continuous, then we can write

\[
\omega(t) = [(1 - t)I + tT]_# \omega(0)
\]

for an optimal transport map \( T \) from \( \omega(0) \) to \( \omega(1) \).

This theorem holds, in fact, for any Wasserstein-p space for \( p > 1 \), see (Santambrogio, 2016).

Now, denote by \( \mu_t \) the McCann interpolation between \( \mu \) and \( \nu \). As mentioned in Section 4.2, we can express \( \mu_t \) as the following barycenter:

\[
\mu_t = \arg \min_{\mu' \in \mathcal{P}_2(\mathcal{X})} \left( (1 - t)W_2^2(\mu', \mu) + tW_2^2(\mu', \nu) \right),
\]

where \( W_2(\mu, \nu) \) is the Wasserstein-2 distance between \( \mu \) and \( \nu \).
which we approximate by the Sinkhorn Divergence barycenter

$$
\mu_t = \arg \min_{\mu' \in \mathcal{P}_2(X)} \left( (1 - t) \text{SD}_\epsilon(\mu', \mu) + t \text{SD}_\epsilon(\mu', \nu) \right),
$$

(11)

which is justified by the fact that Sinkhorn Divergences converge to the OT cost as $\epsilon \to 0$, and that they are reliable loss functions, in the sense that weak convergence of a sequence of measures is equivalent to convergence of the Sinkhorn divergence, see (Feydy et al., 2018). As also shown in (Feydy et al., 2018), the gradient of the Sinkhorn Divergence w.r.t. the vector $a$, when writing a discrete measure $\mu$ as $\mu = \sum_i a_i \delta_{x_i}$, is given by

$$
\nabla_a \text{SD}_\epsilon(\mu, \nu) = f - p.
$$

(12)

However, if we now do a simple gradient descent on (11) using (12), we are not actually computing the barycenter on the space $\mathcal{P}_2(X)$ anymore, as we only consider gradients w.r.t. $a$, which does not allow particles to move, but merely to teleport mass to other particles. In particular, if $X$ is a discrete space, there exist no constant-speed geodesics between different points anymore, as can easily be seen from the following example. Let $\mu_0 = \delta_{x_0}$ and $\mu_1 = \delta_{x_1}$ be two Dirac measures for some $x_0, x_1 \in X$. Assume there would exist a constant speed geodesic $\omega$ joining $\mu_0$ and $\mu_1$. Then for $t > 0$,

$$
W_2(\omega(t), \omega(0)) = t W_2(\omega(1), \omega(0)).
$$

However, since the space is discrete, this implies that $x_0 = x_1$, i.e. the only constant-speed geodesics are constant. We therefore work with the following approximation of geodesics.

**Definition A.11** (Quasi-Isometry). Let $(X_1, d_1)$ and $(X_2, d_2)$ be metric spaces. $f : X_1 \to X_2$ is called a $(\lambda, \epsilon)$-quasi-isometry if there exist $\lambda \geq 0$ and $\epsilon > 0$ such that for all $x, y \in X_1$

$$
\frac{1}{\lambda} d_1(x, y) - \epsilon \leq d_2(f(x), f(y)) \leq \lambda d_1(x, y) + \epsilon.
$$

If in addition there exists a $C > 0$ such that for all $z \in X_2$ there exist an $x \in X_1$ such that $d_2(f(x), z) \leq C$, $f$ is called quasi-isometry.

We can then use this to define quasi-geodesics. (Bonciocat & Sturm, 2009) introduced a similar concept called h-rough geodesics, for which they just used the upper bound.

**Definition A.12** (Strong-$\epsilon$ Quasi-Geodesics). A strong-$\epsilon$ quasi-geodesic in a metric space $(X, d)$ is a map $\gamma : [0, 1] \to X$ such that for all $s, t \in [0, 1],$

$$
d(\gamma_0, \gamma_1)|t - s| - \epsilon \leq d(\gamma_s, \gamma_t) \leq d(\gamma_0, \gamma_1)|t - s| + \epsilon.
$$

Now let $X = [0, 1]^2$, and denote by $\left[ \frac{[n]}{n} \right] \subset [0, 1]^2$ the discrete space consisting of all $x_i$ of the form $x_i = \left( \frac{i}{2n}, \frac{j}{2n} \right) + k \left( \frac{1}{n}, 0 \right) + j \left( 0, \frac{1}{n} \right)$, for $k, j = 0, \ldots , n - 1$. We can then show that $(\mathcal{P}_2([0, 1]^2), W_2)$ is quasi-isometric to $(\mathcal{P}(\left[ \frac{[n]}{n} \right], W_2))$. 

**Proposition A.13.** The metric space $(\mathcal{P}_2([0, 1]^2), W_2)$ is $(1, \frac{1}{\sqrt{2n}})$-quasi-isometric to $(\mathcal{P}(\left[ \frac{[n]}{n} \right], W_2))$, i.e. there exist an $f : (\mathcal{P}_2([0, 1]^2), W_2) \to (\mathcal{P}(\left[ \frac{[n]}{n} \right], W_2))$ such that for all $\mu, \nu \in \mathcal{P}_2([0, 1])$ it holds that

$$
W_2(\mu, \nu) - \frac{1}{\sqrt{2n}} \leq W_2(f(\mu), f(\nu)) \leq W_2(\mu, \nu) + \frac{1}{\sqrt{2n}}.
$$

**Proof.** We split the space $[0, 1]^2$ into squares via $N(x_i) := (x_i + [-\frac{1}{2n}, \frac{1}{2n}]^2)$. We define $f : \mathcal{P}([0, 1]^2) \to \mathcal{P}(\left[ \frac{[n]}{n} \right])$ by

$$
f(\mu) = \sum_{x_i \in X} \left( \int_{N(x_i)} d\mu \right) \delta_{x_i}.
$$
By triangle inequality, we have
\[
W_2(f(\mu), f(\nu)) \leq W_2(\mu, \nu) + W_2(\mu, f(\mu)) + W_2(\nu, f(\nu))
\]
\[
W_2(\mu, \nu) \leq W_2(f(\mu), f(\nu)) + W_2(\mu, f(\mu)) + W_2(\nu, f(\nu))
\]
For any measure \( \mu \in \mathcal{P}([0, 1]) \), denoting by \( T : [0, 1]^2 \to \frac{[\|n\|^2}{n} \) the map that sends each point to the corresponding midpoint \( x_i \), we get
\[
W_2^2(\mu, f(\mu)) \leq \int_{[0,1]^2} |T(x) - x|^2 d\mu \leq \int_{[0,1]^2} \frac{2}{4n^2} d\mu = \frac{2}{4n^2}.
\]
Therefore we have a \((1, \frac{1}{\sqrt{2n}})\)-quasi-isometry between both spaces.

We also need to show that there exist a \( C > 0 \) such that for all \( \mu \in \mathcal{P}(\frac{[\|n\|^2}{n}) \) there exist a \( \nu \in \mathcal{P}([0, 1]) \) with
\[
W_2(f(\nu), \mu) < C.
\]
Choosing \( C = \frac{1}{\sqrt{2n}} \) and \( \nu = \mu \) concludes the proof.

We immediately get the following corollary.

**Corollary A.14.** Constant-speed geodesics \( \mathcal{P}_2([0, 1]^2) \) are strong-\( \epsilon \) quasi-geodesics in \( \mathcal{P}([\|n\|^2]/n) \).

This justifies doing gradient descent on (11) using the discrete space gradient (12) to approximate the geodesic, as we can approximate the constant-speed geodesic with a strong-\( \epsilon \)-quasi-geodesic in the discrete space.

### A.4. Wasserstein on Wasserstein Distance

In this section, we provide additional details on how to solve the particle flow
\[
\frac{\partial}{\partial t} \hat{\mu}_t = -\nabla_{\hat{\mu}_t} [SD_\epsilon(\hat{\mu}_t, \hat{\nu})] \tag{13}
\]
from Section 4.4. Recall that \( \hat{\mu}, \hat{\nu} \in \mathcal{P}_2(\mathcal{P}_2([0, 1]^2, c), W_2), \hat{\mu} = \frac{1}{n} \sum_i \delta_{\mu_i}, \hat{\nu} = \frac{1}{n} \sum_j \delta_{\nu_j} \) for \( \mu_i, \nu_j \in \mathcal{P}_2([0, 1]^2) \). From (Li et al., 2024b), we get that
\[
\frac{\partial SD_\epsilon(\hat{\mu}, \hat{\nu})}{\partial \mu_k} = \sum_j \frac{\partial SD_\epsilon(\mu_k, \nu_j)}{\partial \mu_k} \Pi_{kj},
\]
where \( \Pi \) is an optimal transport plan between \( \mu_k \) and \( \nu_j \). Now as in the previous section, we can approximate \( \frac{\partial SD_\epsilon(\mu_k, \nu_j)}{\partial \mu_k} = f_{kj} - p_k \), where \( f_{kj} \) is the dual potential from \( \text{OT}_\epsilon(\mu_k, \nu_j) \), and \( p_k \) that of \( \text{OT}_\epsilon(\mu_k, \mu_k) \). As before, we can approximate these gradients with UNOT, which lets us solve (13) with a simple gradient descent scheme, as shown in Section A.2.

### A.5. Neural Operators

The main breakthrough for Neural Operators came in the combination with approximating solutions to partial differential equations (PDEs) (Li et al., 2020; 2021; Goswami et al., 2022). Many problems, including PDEs, can be numerically solved by discretizing infinite-dimensional inputs and outputs. One of the main advantages of Neural Operators is that they can generalize over different grid discretizations, unlike traditional neural networks, which makes them particularly well-suited for solving PDEs, and they are universal approximators for continuous operators acting on Banach spaces (Kovachki et al., 2024). While our space \( \mathcal{P}([0, 1]^2) \) is not technically a Banach space, the space of finite signed measures with the total variation norm is, and \( \mathcal{P}([0, 1]^2) \) is a subset.

Our UNOT \( S_\phi \) is a mapping
\[
S_\phi : \mathcal{P}([0, 1]^2) \times \mathcal{P}([0, 1]^2) \to L^1([0, 1]^2)
\]
\[
(\mu, \nu) \mapsto Q \circ B_L \circ \ldots \circ B_1 \circ \mathcal{P}(\mu, \nu).
\]
Universal Neural Optimal Transport

\[
\begin{array}{cccccc}
\mu, \nu & \rightarrow & P & \rightarrow & \text{Layer 1} & \rightarrow & \cdots & \rightarrow & \text{Layer L} & \rightarrow & Q & \rightarrow & g
\end{array}
\]

\[\mathcal{F}^{-1}(N\mathcal{N}(\mathcal{F}(v))(x) + b(x))\]

\[\sigma\]

\[W\]

Figure 8. Fourier Neural Operator architecture, adapted from (Kovachki et al., 2024). The input measures \((\mu, \nu)\) are passed through a point-wise lifting operator \(P\) which is then followed by \(L\) Fourier operators and point-wise non-linearity operators. After the last Fourier layer, we project back to the output \(g\) with a point-wise operator \(Q\).

In contrast to (Kovachki et al., 2024) we found that a Fourier layer containing a neural network \(N\mathcal{N}\) instead of just a linear layer \(W\), i.e. \(\mathcal{F}^{-1}(N\mathcal{N}(\mathcal{F}(v))(x)\) instead of \(\mathcal{F}^{-1}(W \cdot \mathcal{F}(v))(x)\), worked better in practice. Our adapted Neural Operator is of the form:

- **Lifting** Using a 2D convolutional layer as a pointwise lifting map. The input is mapped from \(\{(\mu, \nu) : \mathcal{D} \rightarrow \mathbb{R}^2\} \mapsto \{v_0 : \mathcal{D} \rightarrow \mathbb{R}^{d_0}\}\). We choose \(d_{v_0} > 2\) such that it is a lifting.

- **Iterative Fourier Layer** For \(i = 0, \ldots, L - 1\) the hidden representation is mapping \(\{v_i : \mathcal{D}_i \rightarrow \mathbb{R}^{d_i}\} \mapsto \{v_{i+1} : \mathcal{D}_{d_{i+1}} \rightarrow \mathbb{R}^{d_{i+1}}\}\). In each layer \(B_i\) the input \(v_i\) is transformed in the Fourier space by the Fourier transform and applied to an MLP; afterwards, the inverse Fourier transform is used. We choose a constant hidden dim \(d_i = d_{i+1}\).

- **Projection** The projection \(Q\) is the analogue to the lifting layer, mapping the hidden representation to the output function \(\{v_L : \mathcal{D}_L \rightarrow \mathbb{R}^{d_L}\} \mapsto \{g : \mathcal{D}' \rightarrow \mathbb{R}\}\).

Details on hyperparameter choices can be found in Appendix C.
B. Proofs

This section contains all proofs, as well as further technical details omitted in the paper. For convenience, we restate the statements from the paper.

We start off by rigorously restating Proposition 2. Let $\mathcal{X} \subset \mathbb{R}^N$ be a compact set. We start off with a natural definition of discretization of a continuous measure, which applies, for example, to discrete images as discretizations of an underlying "ground truth" continuous image.

**Definition B.1 (Discretization of Measures).** Let $\mu \in \mathcal{P}(\mathcal{X})$ be an absolutely continuous measure, and let $X_n = \{x_1^n, \ldots, x_n^n\} \subset \mathcal{X}$. The discretization of $\mu$ on $X_n$ is defined as the measure $\mu_n \in \mathcal{P}(\mathcal{X})$ supported on $X_n$, where

$$\mu_n(x_i^n) = \int_{\Omega_i} d\mu,$$

with

$$\Omega_i^n = \{ x \in \mathcal{X} : \|x - x_i^n\| \leq \|x - y\| \forall y \in \mathcal{X} \}.$$

Note that the intersections $\Omega_i^n \cap \Omega_j^n$ have Lebesgue measure zero, so this is well-defined.

We cannot guarantee that an arbitrary sequence of discretizations $\mu_n$ converges weakly to $\mu$ as $n \to \infty$; simply consider the case where all the $x_i^n$ are identical for all $n$ and $i$. Hence, we need to ensure that the discretization is uniform over all of $\mathcal{X}$ in some way.

**Definition B.2 (Uniform Discretization).** Let $X_n = \{x_1^n, \ldots, x_n^n\}$ be subsets of $\mathcal{X}$ for all $n \in \mathbb{N}$. Then we call the sequence $(X_n)_{n \in \mathbb{N}}$ a uniform discretization of $\mathcal{X}$ if for all $x \in \mathcal{X}$,

$$\lim_{n \to \infty} \min_{1 \leq i \leq n} \|x - x_i^n\| = 0.$$

The following lemma holds.

**Lemma B.3 (Weak Convergence of Discretizations of Measures).** Let $\mu \in \mathcal{P}(\mathcal{X})$ be absolutely continuous, and $(\mu_n)_{n \in \mathbb{N}}$ be a sequence of discretizations of $\mu$ supported on a uniform discretization $(X_n)_{n \in \mathbb{N}}$ of $\mathcal{X}$. Then $\mu_n$ converges weakly to $\mu$.

**Proof.** Let $f \in C_b(\mathcal{X})$ be a test function. We have to show that

$$\int_{\mathcal{X}} f d\mu_n \xrightarrow{n \to \infty} \int_{\mathcal{X}} f d\mu.$$

Since $\mathcal{X}$ is compact and $f : \mathcal{X} \to \mathbb{R}$ is continuous, by the Heine–Cantor theorem $f$ is uniformly continuous. Hence, for every $\varepsilon > 0$ there exists $\delta > 0$ such that

$$\|x - y\| < \delta \quad \implies \quad |f(x) - f(y)| < \varepsilon \quad \text{for all } x, y \in \mathcal{X}.$$

Since

$$\sup_{x \in \mathcal{X}} \min_{1 \leq i \leq n} \|x - x_i^n\| \xrightarrow{n \to \infty} 0,$$

we can choose $n'$ such that for all $n \geq n'$,

$$\sup_{x \in \mathcal{X}} \min_{1 \leq i \leq n} \|x - x_i^n\| < \delta.$$

In particular, for each $x \in \mathcal{X}$, there is some $x_i^n \in X_n$ with $\|x - x_i^n\| < \delta$, giving

$$|f(x) - f(x_i^n)| < \varepsilon \quad \text{whenever } \|x - x_i^n\| < \delta. \quad (14)$$

Let

$$\Omega_i^n = \{ x \in \mathcal{X} : \|x - x_i^n\| \leq \|x - x_j^n\| \text{ for all } j = 1, \ldots, n \}$$
We can now state and prove a formal version of Proposition 2. We refer to (Santambrogio, 2015; Feydy et al., 2018) for more details.

Let

\[ \text{Theorem 3. (Feydy et al., 2018).} \]

(Lip)

In other words, \( \text{By Lemma B.3, we know that } f_n \rightarrow f \text{ and } g_n \rightarrow g \text{ on all of } X. \) We refer to (Santambrogio, 2015; Feydy et al., 2018) for more details.

We can now state and prove a formal version of Proposition 2.

**Proposition 2. (Formal)** Let \( (\mu_n)_{n \in \mathbb{N}}, (\nu_n)_{n \in \mathbb{N}} \) be discretizing sequences for absolutely continuous \( \mu, \nu \in \mathcal{P}(X) \), supported on a uniform discretization \( (X_n)_{n \in \mathbb{N}} \) of \( X \). Let \( (f_n, g_n) \) be the (unique) extended dual potentials of \( (\mu_n, \nu_n) \) such that \( f_n(x_0) = 0 \) for some \( x_0 \in X \) and all \( n \). Let \( (f, g) \) be the (unique) dual potentials of \( (\mu, \nu) \) such that \( f(x_0) = 0 \). Then \( f_n \) and \( g_n \) converge uniformly to \( f \) and \( g \) on all of \( X \).

**Proof.** By Lemma B.3, we know that \( \mu_n \rightarrow \mu \) and \( \nu_n \rightarrow \nu \). The statement now follows immediately from Proposition 13 in (Feydy et al., 2018).

**Theorem 3.** Let \( 0 < \lambda < 1 \) and \( G_\theta : \mathbb{R}^d \rightarrow \mathbb{R}^d \) be defined via

\[
G_\theta(z) = \sigma\left(\text{NN}_\theta(z) + \lambda z\right),
\]

where \( z \sim \rho_z = \mathcal{N}(0, I) \), and where \( \text{NN}_\theta : \mathbb{R}^d \rightarrow \mathbb{R}^d \) is Lipschitz continuous with \( \text{Lip}(\text{NN}_\theta) = L < \lambda \). Then \( G_\theta \) is Lipschitz continuous with \( \text{Lip}(q) < L + \lambda \), and for any \( x \in \mathbb{R}^d_{\geq 0} \) it holds

\[
\rho_{G_\theta \# \rho_z}(x) \geq \frac{1}{(L + \lambda)^d} \mathcal{N}\left(G_\theta^{-1}(x)|0, I\right).
\]

In other words, \( G_\theta \# \rho_z \) has positive density at any non-negative \( x \in \mathbb{R}^d_{\geq 0} \).

**Proof.** Since the Lipschitz constant of a composition of functions is bounded by the product of the Lipschitz constants of the components, and similarly, the Lipschitz constant of a sum of Lipschitz functions is bounded by the sum of the Lipschitz constants of the components, we have

\[
\text{Lip}(G_\theta) \leq \text{Lip(ReLU)}(L + \lambda) = L + \lambda.
\]

Now, since we are only interested in images \( x \in \mathbb{R}^d_{\geq 0} \), in the following we can without loss of generality assume that \( G_\theta \) is of the form \( G_\theta(z) = \lambda z + \text{net}_\theta(z) \).
From Theorem 1 in (Behrmann et al., 2019), it follows that $G_\theta$ is invertible, and Lemma 2 therein implies

$$\text{Lip}(G_\theta^{-1}) \leq \frac{1}{\lambda - L}.$$  

The Lipschitz continuity of $G_\theta^{-1}$ implies that for any $h, z \in \mathbb{R}^d$ with $h \neq 0$, we have

$$\|\nabla G_\theta(z) h\| = \lim_{t \to 0} \left\| \frac{G_\theta(z + th) - G_\theta(z)}{t} \right\|$$

$$\geq \frac{1}{\text{Lip}(G_\theta^{-1})} \lim_{t \to 0} \left\| \frac{G_\theta^{-1}(G_\theta(z + th)) - G_\theta^{-1}(G_\theta(z))}{t} \right\|$$

$$= \frac{1}{\text{Lip}(G_\theta^{-1})} \|h\| > 0,$$

which shows that $\nabla G_\theta$ is invertible everywhere. Hence, by the inverse function theorem, we get

$$\nabla G_\theta^{-1}(x) = \nabla G_\theta^{-1}(G_\theta(G_\theta^{-1}(x))) = (\nabla G_\theta(G_\theta^{-1}(x)))^{-1}.$$

Furthermore, similar to above, we have

$$\|\nabla G_\theta(z)e_i\| = \lim_{t \to 0} \left\| \frac{G_\theta(z + te_i) - G_\theta(z)}{t} \right\| \leq \text{Lip}(G_\theta) \lim_{t \to 0} \left\| \frac{z + te_i - z}{t} \right\| \leq L + \lambda,$$

where $e_i$ is the $i^{th}$ unit vector. Hence, we get from Hadamard’s inequality that

$$|\det \nabla G_\theta(z)| \leq \Pi_i \|\nabla G_\theta(z)e_i\| \leq \Pi_i (L + \lambda) = (L + \lambda)^d.$$

Putting everything together, by change of variables, we get

$$\rho_{G_{\theta \#}^s}(x) = \rho_z(G_\theta^{-1}(x)) |\det \nabla G_\theta^{-1}(x)|$$

$$= \rho_z(G_\theta^{-1}(x)) |\det \nabla G_\theta(G_\theta^{-1}(x))|^{-1}$$

$$\geq \frac{1}{(L + \lambda)^d} \rho_z(G_\theta^{-1}(x))$$

$$= \frac{1}{(L + \lambda)^d} \mathcal{N}(G_\theta^{-1}(x)|0, I).$$

**Corollary 4.** Let $G_\theta = G_{\theta_1} \circ ... \circ G_{\theta_R}$ be a composition of functions $G_{\theta_i}$, each of which is of the form as in Theorem 3. Let $z \sim \mathcal{N}(0, I)$. Then

$$\rho_{G_{\theta \#}^s}(x) \geq \frac{1}{(L + \lambda)^d} \mathcal{N}(G_\theta^{-1}(x)|0, I).$$

**Proof.** Consider the case where $G_\theta = G_{\theta_1}^x \circ G_{\theta_2}^y$. Then for any $z \sim \mathcal{N}(0, I)$, we get from the proof of Theorem 3 above:

$$\rho_{G_{\theta \#}^s}(x) \geq \frac{1}{(L + \lambda)^d} \rho_{G_{\theta_2}^y \#} \rho_{G_{\theta_1}^x}(G_{\theta_1}^{-1}(x))$$

$$\geq \frac{1}{(L + \lambda)^{2d}} \rho_z \left( (G_{\theta_2}^{-1}) \left( (G_{\theta_1}^{-1})(x) \right) \right)$$

$$\geq \frac{1}{(L + \lambda)^{2d}} \mathcal{N}(G_\theta^{-1}(x)|0, I).$$

The claim now follows by induction over the layers of $G_\theta$. \qed
Next, we prove Proposition 5. The proof is based on the Hilbert projective metric. For two vectors \( u, v \in \mathbb{R}^n_+ \), it is defined as
\[
d_H(u, v) := \max_i [\log(u_i) - \log(v_i)] - \min_i [\log(u_i) - \log(v_i)],
\]
and can be shown to be a distance on the projective cone \( \mathbb{R}^n_+ / \sim \), where \( u \sim u' \) if \( u = ru' \) for some \( r > 0 \) (Peyré & Cuturi, 2019; Franklin & Lorenz, 1989). For \( f = \log(u) \) and \( g = \log(v) \), we thus define the following loss:
\[
L_H(f, g) := \max_i [f_i - g_i] - \min_i [f_i - g_i].
\]

**Lemma B.4.** Let \( f, g \in \mathbb{R}^n \). Then
\[
L_H(f, g) \leq \sqrt{2} \| f - g \|_2.
\]

If, in addition, \( \sum_i f_i = \sum_i g_i = 0 \), then
\[
\| f - g \|_2 \leq \sqrt{n} L_H(f, g).
\]

**Proof.** Let \( h = f - g \). For the first inequality, observe that \( L_H(f, g) = \max_i h_i - \min_i h_i \). Let \( j^* \) and \( k^* \) be the indices achieving \( \max_i h_i \) and \( \min_i h_i \), respectively. Define the vector \( e \) such that \( e_{j^*} = 1, e_{k^*} = -1 \), and \( e_i = 0 \) for all other \( i \). Then:
\[
L_H(f, g) = e \cdot h \leq \| e \|_2 \| h \|_2 = \sqrt{2} \| f - g \|_2.
\]

Now assume that \( \sum_i f_i = \sum_i g_i = 0 \). Set \( M = \max_i h_i \) and \( m = \min_i h_i \). If all \( h_i = 0 \), both statements are trivial. Hence, assume at least one of the \( h_i \) is not zero. Since \( \sum_i h_i = \sum_i f_i - g_i = 0 \), this implies \( M > 0 \) and \( m < 0 \). For any index \( i, h_i \leq M \), and thus
\[
(h_i)^2 \leq M^2 \leq (M - m)^2 = L_H(f, g)^2.
\]

Summing over all indices, we have:
\[
\| f - g \|_2^2 = \| h \|_2^2 = \sum_{i=1}^n (h_i)^2 \leq n \cdot L_H(f, g)^2.
\]

Taking the square root yields:
\[
\| f - g \|_2 \leq \sqrt{n} L_H(f, g).
\]

This finishes the proof.

**Proposition 5.** For two discrete measures \( (\mu, \nu) \) with \( n \) particles, let \( g \) be a potential solving the dual problem, \( g_{\phi} = S_{\phi}(\mu, \nu) \), and \( g_{\tau_k} = \tau_k(\mu, \nu, g_{\phi}) \) the target. Without loss of generality, assume that \( \sum_i g_i = \sum_i g_{\phi i} = \sum_i g_{\tau_k i} = 0 \). Then
\[
L_2(g_{\phi}, g) \leq c(K, k, n) L_2(g_{\phi}, g_{\tau_k})
\]
for some constant \( c(K, k, n) > 1 \) depending only on the Gibbs kernel \( K \), \( k \) and \( n \).

**Proof.** We first show a similar inequality as in Proposition 5 for the Hilbert loss. A well-known fact about the Hilbert metric is that positive matrices (in our case, the Gibb’s kernel \( K \)) act as strict contractions on positive vectors with respect to the Hilbert metric (cf. Theorem 4.1 in (Peyré & Cuturi, 2019)). More precisely, we have
\[
d_H(Kv, Kw') \leq \lambda(K) d_H(v, w')
\]
for any positive vectors \( v, w' \in \mathbb{R}^n \), where
\[
\lambda(K) := \frac{\eta(K) - 1}{\eta(K) + 1}, \quad \eta(K) := \max_{i,j,k,l} \frac{K_{ik}K_{jl}}{K_{jk}K_{il}}.
\]
The same inequality also holds for \( K^T \) in place of \( K \). Note that by definition, \( \eta(K) \geq 1 \), hence \( 0 < \lambda(K) < 1 \). Now consider a starting vector \( v^0 \) to the Sinkhorn algorithm, and let \( v^i \) denote the \( i \)th iterate of the vector. Denote by \( v^* \) the limit
\[ \lim_{l \to \infty} v^l \] of the algorithm. Then (letting \( \prime/\prime \) denote element-wise division):

\[
d_H(v^{l+1}, v^*) = d_H \left( \nu/K^+ u^{l+1}, \nu/K^+ u^* \right)
\]
\[
= d_H \left( K^+ u^{l+1}, K^+ u^* \right)
\]
\[
\leq \lambda(K) d_H(u^{l+1}, u^*)
\]
\[
= \lambda(K) d_H \left( \mu/K v^l, \mu/K v^* \right)
\]
\[
= \lambda(K) d_H \left( K v^l, K v^* \right)
\]
\[
\leq \lambda(K)^2 d_H(v^l, v^*),
\]

where we used the Hilbert metric inequality twice, once on \( K \) and once on \( K^\top \). Iteratively applying this inequality and translating into log-space notation, this gives us

\[
L_H(g_{\tau_k}, g^*) \leq \lambda(K)^{2k} L_H(g, g^*).
\]

Hence, by triangle inequality,

\[
L_H(g, g^*) \leq L_H(g, g_{\tau_k}) + L_H(g_{\tau_k}, g^*) \leq L_H(g, g_{\tau_k}) + \lambda(K)^{2k} L_H(g, g^*),
\]

which gives us

\[
L_H(g, g^*) \leq \frac{1}{1 - \lambda(K)^{2k}} L_H(g_{\tau_k}, g) =: c(K, k) L_H(g_{\tau_k}, g).
\]

Combining this with Lemma B.4 yields

\[
\| g - g^* \|_2 \leq \sqrt{n} L_H(g, g^*) \leq \sqrt{n} c(K, k) L_H(g_{\tau_k}, g) \leq 2\sqrt{n} c(K, k) \| g_{\tau_k} - g \|_2 = c(K, k, n) \| g_{\tau_k} - g \|_2,
\]

from which the claim follows by squaring both sides. 

\[ \Box \]

Remark B.5. Looking at the proof of Proposition 5, one might wonder why we didn’t opt for the Hilbert projective metric as the loss directly. We tried using it instead of L2, and it works quite well, but training with L2 seems to have an edge, probably because the indifference of the Hilbert projective metric to constant shifts is not a helpful inductive bias for deep learning.


C. Training Details

Generator Architecture. Recall that the generator is of the form

\[ G_\theta : \mathbb{R}^d \to \mathcal{P}(X) \times \mathcal{P}(X) \]
\[ z \sim \rho \mapsto R[\sigma(\text{NN}_\theta(z) + \lambda \mathbf{I}_{d,d}(z)) + \delta], \]

where we set \( \lambda = 1.0, \delta = 1e^{-6} \) (note we first normalize, then add \( \delta, \) and then normalize again in practice), and \( z \) is of size \( 2 \times 10^2 \). \( R \) randomly downsizes output distributions to resolutions between \( 28^2 \) and \( 64^2 \) (per distribution). This improves generalization of the FNO \( S_\phi \) across resolutions, which is a known fact for FNOs (Li et al., 2024a). \( \text{NN}_\theta \) is a five-layer fully connected MLP, where all hidden layers are of dimension \( 0.04 \cdot 64^2 \), and the output is of dimension \( 2 \cdot 64^2 \). All layers except the output layer contain Batch Normalization and ELU activations; the last layer has a sigmoid activation only. We note the architecture might seem strange, as the network is relatively deep, while the hidden layers are relatively narrow. However, this architecture worked best amongst an extensive sweep of architectures.

Applying Theorem 3. In the following, we discuss the relation between our generator \( G_\theta \) and Theorem 3 in more detail. Note that Theorem 3 is not directly applicable to our setting for a few reasons: First, we add a small constant \( \eta \) to the generator’s output. This constant ensures that all training samples are positive everywhere, and vastly improves learning speed as it ensures that all inputs are active. However, this is not restrictive of the problem, as the Sinkhorn algorithm requires inputs to be positive anyways. Second, in Theorem 3 both in- and outputs to \( G_\theta \) have the same dimension. This could be achieved in our setting by choosing the input dimension equal to the output dimension, i.e. \( \mathbf{I}_{d,n} \), equal to the identity. However, in practice, using lower-dimensional inputs achieves significantly better results. This can be argued for by the manifold hypothesis (Fefferman et al., 2016), i.e. the fact that typically, datasets live on low-dimensional manifolds embedded in high-dimensional spaces. Depending on the application, i.e. the expected target dataset dimension, the dimension of the input can be adjusted accordingly. Finally, note that the theorem assumes that \( \text{NN}_\theta \) is Lipschitz continuous with Lipschitz constant \( L < \lambda \), where \( \lambda \) is the scaling factor of the skip connection. We do not enforce this constraint, as not doing so yields empirically better results. Still, Theorem 3 goes to show that our algorithm’s performance is not bottlenecked by the generator’s inability to generalizel. We note that a bound on the Lipschitz constant is not necessary for invertibility of ResNets; other approaches have been suggested in the literature, e.g. through the lens of ODEs (Chang et al., 2017) or by partitioning input dimensions (Jacobsen et al., 2018). It is also possible to directly divide by the Lipschitz constant of each layer (Serrurier et al., 2023); these approaches could be studied in future research.

We will now describe how one can bound the Lipschitz constant of the generator. Since \( \lambda = 1.0 \), we need to make sure that the Lipschitz constant of \( \text{net}_\theta \) is smaller than \( 1 \) in order for Theorem 3 to be applicable. Since the Lipschitz constant of a composition of functions is bounded by the product of the Lipschitz constants of each component function, this means we have to bound the product of the Lipschitz constants of components of \( \text{net}_\theta \). ELU is Lipschitz continuous with constant \( 1 \), whereas sigmoid’s Lipschitz constant is \( 0.25 \). Furthermore, for a batch normalization layer \( \text{BN} \), we have

\[ \| \text{BN}(x) - \text{BN}(y) \| = \left\| \frac{x - \mu}{\sigma} - \frac{y - \mu}{\sigma} \right\| = \frac{1}{\sigma} \| x - y \|, \]

where \( \mu \) and \( \sigma \) denote the empirical mean and standard deviation of the batch. Since we draw our data from a standard normal Gaussian, we have \( \mathbb{E}[\sigma] = 1 \), i.e. in expectation, the batch normalization layer is Lipschitz with constant \( 1 \). Hence, all that remains is to bound the product of Lipschitz constants of the three linear layers by (any number smaller than) \( 4 \) (because the constant of sigmoid is \( 0.25 \), this will ensure that the network has a Lipschitz constant smaller than \( 1 \), for which it suffices to bound the operator norms of the weight matrix of each layer. In practice, these can be approximated with the power method as in (Gouk et al., 2020) to find a lower bound on the Lipschitz constant of each linear layer, and these bounds can be used to add a soft constraint to the loss. Empirically, this suffices to bound the Lipschitz constant of the generator. Alternatively, one can use a hard constraint as outlined in (Behrmann et al., 2019). However, empirically, this proved detrimental to training, hence we did not control the Lipschitz constant during our training. Yet, Theorem 3 is still of value, as it goes to show that our algorithm’s performance is not bottlenecked by the generator’s inability to generalize. We leave properly enforcing the Lipschitz constraint for future research.

FNOs and Architecture of \( S_\phi \). The FNO architecture employed in our work follows the general structure outlined in A.5, with modifications to enhance performance. Instead of a fixed weight matrix, we introduce a neural network within the FNO block, allowing for greater expressivity and adaptability. The projection \( Q \), lifting \( P \), and bypass layer \( W \) are implemented as 2D convolutional layers with a kernel size of \( 1 \), ensuring efficient feature transformation. The overall
Universal Neural Optimal Transport

network consists of a standard feedforward architecture, where multiple FNO blocks operate sequentially on the lifted input representation. Each FNO block comprises a spectral convolution layer combined with a bypass convolution, followed by a nonlinear activation function. The final projection step maps the processed features to the desired output space, maintaining the structural integrity of the input.

**Hyperparameters.** In Table 3 we present all hyperparameters used for training UNOT. The most important hyperparameters in this setup include fno_blocks and fno_width, which define the architecture of the Fourier Neural Operator (FNO) and control its expressiveness. The modes_x and modes_y parameters specify the number of Fourier modes used in each spatial dimension, influencing the model’s ability to capture long-range dependencies. gamma_generator and gamma_predictor parameters control the exponential learning rate decay.

| Hyperparameter     | Value       |
|--------------------|-------------|
| batch_size         | 64          |
| \( \delta \)       | 0.000001    |
| fno_blocks         | 4           |
| fno_width          | 64          |
| gamma_generator    | 1           |
| gamma_predictor    | 0.9999      |
| generator          | "MLP"       |
| grid               | false       |
| length             | 64          |
| lr_gen             | 0.001       |
| lr_pred            | 0.0001      |
| model              | "FNO"       |
| modes_x            | 10          |
| modes_y            | 10          |
| n_hidden_spectral_layers | 2     |
| nits               | 40,000      |
| num_layers         | 3           |
| numbr_latent_samples | 5,000      |
| random_shapes      | false       |
| sinkhorn_epsilon   | 0.01        |
| sinkhorn_iterations| 5           |
| spectral_hidden_width | 4          |
| weight_decay_generator | 0     |
| weight_decay_predictor | 0.0001   |
| width_generator    | 0.04        |

*Table 3. Training hyperparameters.*

**Code.** Source code for UNOT, including the weights for the model used in the experiments, can be found at https://github.com/GregorKornhardt/UNOT.
D. Additional Experiments and Materials

D.1. Test Sets

In Figure 9 we show samples from our test datasets. For some of the experiments in the appendix, we included two additional datasets, the "cars" class which is also from the Quick, Draw! dataset, and the Facial Expressions dataset (Hashan, 2022), which consists of 48×48-dimensional greyscale images. The datasets are very diverse, and range in dimensionality from very low (MNIST) to fairly low (BEARS, CARS), medium high (CIFAR) and very high (EXPRESSIONS, LFW).

![MNIST, CIFAR, LFW, BEAR, CAR, EXPRESSIONS samples](image)

*Figure 9. Test dataset samples*

D.2. MLP-UNOT

In applications of fixed-size distributions, one can replace the Neural Operator with a multilayer perception and achieve similar results for a fraction of the training cost. Since the MLP has a fixed discrete space one does need to have equicontinuous samples. In experiments, we found that the MLP approach to also be very reliable for fixed-size inputs, and to vastly outperform the standard initialization of the Sinkhorn algorithm. Notably, it can be trained in just a few minutes to relative errors below 5%.
D.3. Generalization across Resolutions

In this section, we show that UNOT successfully generalizes across resolutions. To this end, we downsample resp. upsample our test datasets to resolutions between $16 \times 16$ and $64 \times 64$. Figure 10 shows the relative errors on the transport distance over this range of resolutions after a single Sinkhorn iteration, compared against the default and the Gaussian initializations. (In Section D.4, we also provide some results on upsampling the dimension of the data beyond $64 \times 64$, i.e. beyond the largest resolution that the network saw during training.) Notably, UNOT not only generalizes well across resolutions that were contained on the training data (between $28 \times 28$ and $64 \times 64$), but also extrapolates very well to dimensions outside this range ($16 \times 16$ to $28 \times 28$).

Figure 10. Relative error on the transport distance over the image resolution, ranging from $16 \times 16$ to $64 \times 64$. 

\[
\begin{array}{ccccccc}
\text{Resolution} & \text{MNIST} & \text{CIFAR} & \text{BEAR} & \text{LFW} & \text{EXPRESSIONS} & \text{CAR} \\
\hline
10 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
20 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
30 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
40 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
50 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
60 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
10 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
20 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
30 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
40 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
50 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
60 & 0.0 & 0.2 & 0.4 & 0.6 & 0.8 \\
\end{array}
\]
D.4. Variable Epsilon

In this section, we provide experimental results on a variant of UNOT that also receives the parameter $\epsilon$ as an input. Instead of the pair of measures $(\mu, \nu)$ encoded as a tensor of size $(B, 2, n, n)$, we use an input size of $(B, 3, n, n)$, where the third channel is equal to $\epsilon$ everywhere. During training, we sample epsilon randomly per sample from a distribution with values between 0.01 and 1. Otherwise, training was identical to the training of UNOT. In Figure 11, we plot the relative errors over $\epsilon$ ranging from 0.01 to 1 on the x-axis, and the resolution of the data ranging from $10 \times 10$ to $70 \times 70$ on the y-axis (where we downsample resp. upsample the data to these dimensions, cf. Section D.3; note that we still only trained on image resolutions between $28 \times 28$ and $64 \times 64$). This variant of UNOT seems to do surprisingly well across different values of $\epsilon$ and across a wide range of resolutions. However, we can see that when the resolution gets smaller than around $15 \times 15$, or close to $70 \times 70$, the error increases.

![Figure 11. Relative error on the transport distance, over the resolution and varying values of $\epsilon$.](image)

27
D.5. Generated Measures

Figure 12 shows images created by the generator (lighter=more mass, darker=less mass). The generator creates very different images over the course of training, including highly structured distributions, large areas of mass, and distributions with mass concentrated in very small areas.

Figure 12. Generated pairs of training samples before and after 20%, 40%, 60%, 80%, and 100% of training, from left to right (lighter=more mass). Top row is actual training images, bottom row is images from training but visualized with a reduced skip constant $\lambda$ in the generator to accentuate the learned features.
D.6. Additional Experiments

We provide material from additional experiments. Figure 13 shows the average relative error on the transport distance over the number of Sinkhorn iterations on a log scale. In Figure 14, we plot the marginal constraint violation, defined as

$$\frac{\|1^T \pi - \nu^T\|_1 + \|\pi 1 - \mu\|_1}{2}$$

for a transport plan $\pi$, which measures how far the transport plan is from the marginals $\mu$ and $\nu$, over the number of Sinkhorn iterations on a log scale. We compute the transport plan from the output of UNOT via equation (4). In Figure 15, we show the relative error on the transport distance w.r.t. computation time when initializing the Sinkhorn algorithm with UNOT, and compare against the default initialization. We see that particularly on higher dimensional data, UNOT is significantly faster than Sinkhorn. However, interestingly, on MNIST the default initialization actually seems to be faster. We note that these results heavily depend on the hardware used, and that we did not optimize our FNO architecture for performance, so a more efficient architecture would probably lead to even more significant speedups. We have not included the initialization from (Thornton & Cuturi, 2022) in the plots, as it was very slow for us, even slower than the standard initialization, despite our best efforts to implement it as efficiently as possible. However, from (Thornton & Cuturi, 2022; Amos et al., 2022) it seems like the speedup should be somewhere between 1.1x and 2x, depending on the dataset, which would make it significantly slower than UNOT on most of our datasets. We mention again that FNOs process complex numbers, but PyTorch is heavily optimized for real number operations. With kernel support for complex numbers, UNOT will likely be much faster.

Figure 13. Relative error on the transport distance over the number of Sinkhorn iterations on a log scale.
Figure 14. Marginal constraint violation over the number of Sinkhorn iterations, on a log scale.

Figure 15. Comparison of relative errors on the transport distance over computation time in seconds.