Wasserstein Iterative Networks for Barycenter Estimation

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Abstract

Wasserstein barycenters have become popular due to their ability to represent the average of probability measures in a geometrically meaningful way. In this paper, we present an algorithm to approximate the Wasserstein-2 barycenters of continuous measures via a generative model. Previous approaches rely on regularization (entropic/quadratic) which introduces bias or on input convex neural networks which are not expressive enough for large-scale tasks. In contrast, our algorithm does not introduce bias and allows using arbitrary neural networks. In addition, based on the celebrity faces dataset, we construct Ave, celeba! dataset which can be used for quantitative evaluation of barycenter algorithms by using standard metrics of generative models such as FID.

1. Introduction

Wasserstein barycenters (Agueh & Carlier, 2011) provide a geometrically meaningful notion of the average of probability measures based on optimal transport (OT, see (Villani, 2008)). Methods for computing barycenters have been successfully applied to various practical problems. In geometry processing, shape interpolation can be performed by barycenters (Solomon et al., 2015). In image processing, barycenters are used for color and style translation (Rabin et al., 2014; Mroueh, 2019), texture mixing (Rabin et al., 2011) and image interpolation (Lacombe et al., 2021; Simon & Aberdam, 2020). In language processing, barycenters can be applied to text evaluation (Colombo et al., 2021). In online learning, barycenters are used for aggregating probabilistic forecasts of experts (Korotin et al., 2021d; Paris, 2021). In Bayesian inference, the barycenter of subset posteriors converges to the full data posterior (Srivastava et al., 2015; 2018) allowing efficient computations of full posterior based on barycenters. In reinforcement learning, barycenters are used for uncertainty propagation (Metelli et al., 2019). Other applications include data augmentation (Bezpalov et al., 2021), multivariate density registration (Bigot et al., 2019), distributions alignment (Inouye et al., 2021), domain generalization (Lyu et al., 2021) and adaptation (Montesuma & Mboula, 2021), model ensembling (Dognin et al., 2019).

The bottleneck of obtaining barycenters is the computational complexity. For discrete measures, fast and accurate barycenter algorithms exist for low-dimensional problems; see (Peyré et al., 2019) for a survey. However, discrete methods scale poorly with the number of support points of the barycenter. Consequently, they cannot approximate continuous barycenters well, especially in high dimensions.

For continuous measures, only a few algorithms exist (Li et al., 2020; Fan et al., 2020; Korotin et al., 2021c). Existing continuous barycenter approaches are based on entropic/quadratic regularization, or parametrization of Brenier potentials with input-convex neural networks (ICNNs, see (Amos et al., 2017)). The regularization-based [CRWB] algorithm by (Li et al., 2020) recovers a barycenter biased from the true one. Algorithms [CW2B] by (Korotin et al., 2021c) and [SCW2B] by (Fan et al., 2020) based on ICNNs resolve this issue, see (Korotin et al., 2021c, Tables 1-3).
However, despite the growing popularity of ICNNs in OT applications (Makkuva et al., 2019; Korotin et al., 2021a; Mokrov et al., 2021), they could be suboptimal architectures according to a recent study (Korotin et al., 2021b). According to the authors, more expressive networks without the convexity constraint outperform ICNNs in practical OT problems.

On the other hand, evaluation of barycenter algorithms is challenging due to limited number of continuous measures with explicitly known barycenter. It can be computed in the Gaussian and location-scatter cases (Álvarez-Esteban et al., 2016, §4) and the 1-dimensional case (Bonneel et al., 2015, §2.3). Recent works (Li et al., 2020; Korotin et al., 2021c; Fan et al., 2020) consider the Gaussian case in dimensions ≤ 256 for quantitative evaluation. In higher dimensions, the computation of the ground truth barycenter is hard even for the Gaussian case: it involves matrix inversion and square root extraction (Altschuler et al., 2021, Algorithm 1) with the cubic complexity in the dimension of the ambient space.

Contributions.

- We develop a novel iterative algorithm (§4) for estimating Wasserstein-2 barycenters based on the fixed point approach by (Álvarez-Esteban et al., 2016) combined with a neural solver for optimal transport (Korotin et al., 2021b). Unlike predecessors, our algorithm does not introduce bias and allows arbitrary network architectures.
- We construct the Ave, celeba! (averaging celebrity faces, §5) dataset consisting of 64 × 64 RGB images for large-scale quantitative evaluation of continuous Wasserstein-2 barycenter algorithms. The dataset includes 3 subsets of degraded images of faces. The barycenter of these subsets corresponds to the original clean faces.

Our algorithm is suitable for large-scale Wasserstein-2 barycenters applications. The developed dataset will allow quantitative evaluation of barycenter algorithms at a large scale improving transparency and providing healthy competition in the optimal transport research.

Notation. We work in a Euclidean space $\mathbb{R}^D$ for some $D$. All the integrals are computed over $\mathbb{R}^D$ if not stated otherwise. We denote the set of all Borel probability measures on $\mathbb{R}^D$ with finite second moment by $\mathcal{P}_2(\mathbb{R}^D)$. We use $\mathcal{P}_{2,ac}(\mathbb{R}^D) \subset \mathcal{P}_2(\mathbb{R}^D)$ to denote the subset of absolutely continuous measures. We denote its subset of measures with positive density by $\mathcal{P}_{2,ac}^+(\mathbb{R}^D) \subset \mathcal{P}_{2,ac}(\mathbb{R}^D)$. We denote the set of probability measures on $\mathbb{R}^D \times \mathbb{R}^D$ with marginals $\mathbb{P}$ and $\mathbb{Q}$ by $\Pi(\mathbb{P},\mathbb{Q})$. For a measurable map $T : \mathbb{R}^D \to \mathbb{R}^D$, we denote the associated push-forward operator by $T^*_\#$. For $\phi : \mathbb{R}^D \to \mathbb{R}$, we denote by $\phi$ its Legendre-Fenchel transform (Fenchel, 1949) defined by $(\phi(y) = \max_{x \in \mathbb{R}^D} [\langle x, y \rangle - \phi(x)]$. Recall that $\phi$ is a convex function, even when $\phi$ is not.

2. Preliminaries

Wasserstein-2 distance. For $\mathbb{P}, \mathbb{Q} \in \mathcal{P}_2(\mathbb{R}^D)$, Monge’s primal formulation of the squared Wasserstein-2 distance, i.e., OT with quadratic cost, is

$$W_2^2(\mathbb{P}, \mathbb{Q}) \defeq \min_{T \in \mathcal{P}_2(\mathbb{R}^D \times \mathbb{R}^D)} \int \frac{1}{2} \|x - T(x)\|^2 d\mathbb{P}(x),$$

(1)

where the minimum is taken over measurable functions (transport maps) $T : \mathbb{R}^D \to \mathbb{R}^D$ mapping $\mathbb{P}$ to $\mathbb{Q}$. The optimal $T^*$ is called the optimal transport map. Note that (1) is not symmetric, and this formulation does not allow for mass splitting, i.e., for some $\mathbb{P}, \mathbb{Q} \in \mathcal{P}_2(\mathbb{R}^D)$, there might be no map $T$ that satisfies $T_\#_\mathbb{P} = \mathbb{Q}$. Thus, (Kantorovitch, 1958) proposed the following relaxation:

$$W_2^2(\mathbb{P}, \mathbb{Q}) \defeq \min_{\pi \in \Pi(\mathbb{P}, \mathbb{Q})} \int \frac{1}{2} \|x - y\|^2 d\pi(x, y),$$

(2)

where the minimum is taken over all transport plans $\pi$, i.e., measures on $\mathbb{R}^D \times \mathbb{R}^D$ whose marginals are $\mathbb{P}$ and $\mathbb{Q}$. The optimal $\pi^* \in \Pi(\mathbb{P}, \mathbb{Q})$ is called the optimal transport plan. If $\pi^*$ is of the form $[\text{id}, T^*]_\# \mathbb{P} \in \Pi(\mathbb{P}, \mathbb{Q})$ for some $T^*$, then $T^*$ minimizes (1).

The dual form (Villani, 2003) of $W_2^2$ is:

$$W_2^2(\mathbb{P}, \mathbb{Q}) = \max_{u \in \mathbb{L}^1(\mathbb{P})} \left[ \int u(x) d\mathbb{P}(x) + \int v(y) d\mathbb{Q}(y) \right],$$

(3)

where the maximum is taken over $u \in \mathbb{L}^1(\mathbb{P})$, $v \in \mathbb{L}^1(\mathbb{Q})$ satisfying $u(x) + v(y) \leq \frac{1}{2}\|x - y\|^2$ for all $x, y \in \mathbb{R}^D$. The functions $u$ and $v$ are called potentials.

There exist optimal $u^*, v^*$ satisfying $u^* = (v^*)^*$, where $f^* : \mathbb{R}^D \to \mathbb{R}$ is the c-transform of $f$ defined by $f^*(y) = \min_{x \in \mathbb{R}^D} \left[ \frac{1}{2}\|x - y\|^2 + f(x) \right]$. We can rewrite (3) as

$$W_2^2(\mathbb{P}, \mathbb{Q}) = \max_v \left[ \int v^*(y) d\mathbb{Q}(y) + \int v(y) d\mathbb{Q}(y) \right],$$

(4)

where the maximum is taken over all $v \in \mathbb{L}^1(\mathbb{Q})$.

It is customary (Villani, 2008, Cases 5.3 & 5.17) to define $u(x) = \frac{1}{2}\|x\|^2 - \psi(x)$ and $v(y) = \frac{1}{2}\|y\|^2 - \phi(x)$. There exist convex optimal $\psi^*$ and $\phi^*$ satisfying $\psi^* = \phi^*$ and $\phi^* = \psi^*$.

If $\mathbb{P} \in \mathcal{P}_{2,ac}(\mathbb{R}^D)$, then the optimal $T^*$ of (1) always exists and can be recovered from the dual solution $u^*$ (or $\psi^*$) of (3): $T^*(x) = x - \nabla u^*(x) = -\nabla \psi^*(x)$ (Santambrogio, 2015, Theorem 1.17). Map $T^*$ is a gradient of a convex function, the fact known as the Brenier Theorem (Brenier, 1991).

Wasserstein-2 barycenter. Let $\mathbb{P}_1, \ldots, \mathbb{P}_N \in \mathcal{P}_{2,ac}(\mathbb{R}^D)$ such that at least one of them has bounded density. Their barycenter w.r.t. weights $\alpha_1, \ldots, \alpha_N$ ($\alpha_n > 0; \sum_{n=1}^N \alpha_n = 1$) is given by (Aguué & Carlier, 2011):

$$\mathbb{P}_\mathbb{B} \defeq \arg \min_{\mathbb{P} \in \mathcal{P}_2(\mathbb{R}^D)} \sum_{n=1}^N \alpha_n W_2^2(\mathbb{P}_n, \mathbb{P}).$$

(5)
We use the phrase OT solver to denote any method capable of recovering the OT map \( T^* \) or the potential \( v^* \) (or \( \psi^* \)).

**Primal-form** solvers based on (1) or (2), e.g., (Xie et al., 2019; Lu et al., 2020), parameterize \( T^* \) using complicated generative modeling techniques with adversarial losses to handle the pushforward constraint \( T^* P = \hat{Q} \) in the primal form (1). They depend on careful hyperparameter search and complex optimization (Lucic et al., 2018).

**Dual-form** continuous solvers (Genevay et al., 2016; Seguy et al., 2017; Nhan Dam et al., 2019; Taghvaei & Jalali, 2019; Korotin et al., 2021a) based on (3) or (4) have straightforward optimization procedures and can be adapted to various tasks without extensive hyperparameter search.

A comprehensive overview and a benchmark of dual-form solvers are given in (Korotin et al., 2021b). According to the evaluation, the best performing OT solver is reversed maximin solver [MM:R], a modification of the idea proposed by (Nhan Dam et al., 2019) in the context of Wasserstein-1 GANs (Arjovsky et al., 2017). In this paper, we employ this solver as a part of our algorithm. We review it below.

### 3.1. Continuous OT Solvers for \( W_2 \)

**Reversed Maximin Solver.** In (4), \( v^*(x) \) can be expanded through \( v \) via the definition of \( c \)-transform:

\[
\max_v \int \min_{y \in \mathbb{R}^D} \left[ \frac{||x - y||_2^2}{2} - v(y) \right] d\mathbb{P}(x) + \int v(y) d\mathbb{Q}(y) =
\]

\[
\max_v \min_T \int \left[ \frac{||x - T(x)||_2^2}{2} - v(T(x)) \right] d\mathbb{P}(x) + \int v(y) d\mathbb{Q}(y). \tag{7}
\]

In the derivations above, the optimization over \( y \in \mathbb{R}^D \) is replaced by the equivalent optimization over functions \( T : \mathbb{R}^D \rightarrow \mathbb{R}^D \). This is done by the interchanging of integral and minimum, see (Rockafellar, 1976, Theorem 3A).

The key point of this reformulation is that the optimal solution of this maximin problem is given by \( (v^*, T^*) \), where \( T^* \) is the OT map from \( P \) to \( Q \). See discussion in (Korotin et al., 2021b, §2) or (Rout et al., 2021, §4.1).

In practice, the potential \( v : \mathbb{R}^D \rightarrow \mathbb{R} \) and the map \( T : \mathbb{R}^D \rightarrow \mathbb{R}^D \) are parametrized by neural networks \( v_{\theta}, T_\phi \).

To train \( \theta \) and \( \omega \), stochastic gradient ascent/descent (SGAD) over mini-batches from \( P, Q \) is used.

### 3.2. Algorithms for Continuous \( W_2 \) Barycenters

**Variational optimization.** Problem (5) is optimization over probability measures. To estimate \( \mathbb{P} \), one may employ a generator network \( G_{\xi} : \mathbb{R}^D \rightarrow \mathbb{R}^D \) with a latent measure \( \mathbb{S} \) on \( \mathbb{R}^D \) and train \( \xi \) by minimizing

\[
\sum_{n=1}^N \alpha_n W^2_2(G_{\xi}\mathbb{P}_n, \mathbb{P}_n) \rightarrow \min. \tag{8}
\]

Optimization (8) can be performed by using SGD on random mini-batches from the measure \( \mathbb{S} \) and measures \( \mathbb{P}_n \).

The difference between possible variational algorithms lies in the particular estimation method for \( W^2_2 \) terms. To our knowledge, only ICNN-based minimax solver (Makkuva et al., 2019) has been used to compute \( W^2_2 \) in (8) yielding \( [SCW_2B] \) algorithm (Fan et al., 2020).

**Potential-based optimization.** (Li et al., 2020; Korotin et al., 2021c) recover the optimal potentials \( \{\psi^*_n, \phi^*_n\} \) for each pair \((\mathbb{P}, \mathbb{P}_n) \) via a non-minimax regularized dual formulation. No generative model is needed: the barycenter is recovered by pushing forward measures using gradients of potentials or by barycentric projection. However, the non-trivial choice of the prior barycenter distribution is required. Algorithm \([CRWB]\) by (Li et al., 2020) uses entropic or quadratic regularization and \([CW_2B]\) algorithm by (Korotin et al., 2021c) uses ICNNs, congruence and cycle-consistency (Korotin et al., 2021a) regularization.

### 4. Iterative \( W_2 \)-Barycenter Algorithm

Our proposed algorithm is based on the fixed point approach by (Álvarez-Esteban et al., 2016) which we recall in §4.1. In §4.2, we formulate our algorithm for computing Wasserstein-2 barycenters. In §4.3, we show that our algorithm generalizes the variational barycenter approach.

#### 4.1. Theoretical Fixed Point Approach

Following (Álvarez-Esteban et al., 2016), we define an operator \( \mathcal{H} : \mathcal{P}_{2,ac}(\mathbb{R}^D) \rightarrow \mathcal{P}_{2,ac}(\mathbb{R}^D) \) by

\[
\mathcal{H}(\mathbb{P}) = \left[ \sum_{n=1}^N \alpha_n T_{\mathbb{P} \rightarrow \mathbb{P}_n} \right] \mathbb{P}, \tag{9}
\]
Algorithm 1: Wasserstein Iterative Networks

**Input**: latent $S$ and input $\mathbb{P}_1, \ldots, \mathbb{P}_N$ measures; weights $\alpha_1, \ldots, \alpha_N > 0$ ($\sum_{n=1}^N \alpha_n = 1$); number of iter per network: $K_{G'}, K_{T'}, K_v$; generator $G_\xi: \mathbb{R}^H \rightarrow \mathbb{R}^D$; mapping networks $T_{\theta_1}, \ldots, T_{\theta_K}: \mathbb{R}^D \rightarrow \mathbb{R}^D$; potentials $\omega_1, \ldots, \omega_N: \mathbb{R}^D \rightarrow \mathbb{R}$; regression loss $\ell: \mathbb{R}^D \times \mathbb{R}^D \rightarrow \mathbb{R}^+$.

**Output**: generator satisfying $G_\xi \sharp \mathbb{P} \approx \mathbb{P}$; OT maps satisfying $T_{\theta_n}(G_\xi \sharp \mathbb{P}) \approx \mathbb{P}_n$.

**repeat**

1. **# OT solvers update**
   **for** $n = 1, 2, \ldots, N$ **do**
   ```
   for $k_v = 1, 2, \ldots, K_v$ **do**
   Sample batches $Z \sim S, Y \sim \mathbb{P}_n$; $X \leftarrow G_\xi(Z)$;
   $\mathcal{L}_v \leftarrow \frac{1}{|X|} \sum_{x \in X} v_{\omega_n}(T_{\theta_n}(x)) - \frac{1}{|Y|} \sum_{y \in Y} v_{\omega_n}(y)$;
   Update $\omega_n$ by using $\frac{\partial \mathcal{L}_v}{\partial \omega_n}$;
   for $k_T = 1, 2, \ldots, K_T$ **do**
   Sample batch $Z \sim S$; $X \leftarrow G_\xi(Z)$;
   $\mathcal{L}_T = \frac{1}{|X|} \sum_{x \in X} \left( \frac{1}{2} \| x - T_{\theta_n}(x) \|^2 - v_{\omega_n}(T_{\theta_n}(x)) \right)$;
   Update $\theta_n$ by using $\frac{\partial \mathcal{L}_T}{\partial \theta_n}$;
   ```

2. **# Generator update (regression)**
   **for** $k_G = 1, 2, \ldots, K_G$ **do**
   ```
   Sample batch $Z \sim S$;
   $\mathcal{L}_G \leftarrow \frac{1}{|Z|} \sum_{z \in Z} \ell(G_\xi(z), \sum_{n=1}^N \alpha_n T_{\theta_n}(G_\xi(z)))$;
   Update $\xi$ by using $\frac{\partial \mathcal{L}_G}{\partial \xi}$;
   ```

**until not converged**;

and $Q \leftarrow \mathbb{P}_n$. For each $n = 1, 2, \ldots, N$, we perform SGAD by using batches from $G_\xi \sharp \mathbb{S}$ and $\mathbb{P}_n$ and get $T_{\theta_n} \approx T_{\theta_n} \rightarrow \mathbb{P}_n$.

Second, we update $G_\xi$ to represent $\mathbb{H}(P_\xi)$ instead of $\mathbb{P}_n$. We do this via regression, the approach inspired by (Chen et al., 2019). We introduce $G_{\xi_0}$, a fixed copy of $G_\xi$. Next, we regress generator $G_\xi(\cdot)$ onto $\sum_{n=1}^N \alpha_n T_{\theta_n}(G_{\xi_0}(\cdot))$.

\[
\int \ell \left( G_\xi(z), \sum_{n=1}^N \alpha_n T_{\theta_n}(G_{\xi_0}(z)) \right) dS(z) \rightarrow \min_{\xi}
\]

by performing SGD on random batches from $S$, e.g., by using squared error $\ell(x, x') \overset{\text{def}}{=} \frac{1}{2} \| x - x' \|^2$. As a result, generator $G_\xi(\cdot)$ becomes close to $\sum_{n=1}^N \alpha_n T_{\theta_n}(G_{\xi_0}(\cdot))$ as a function $\mathbb{R}^H \rightarrow \mathbb{R}^D$. Consequently, we get

\[
\mathbb{P}_\xi = G_\xi \sharp \mathbb{S} \approx \left( \sum_{n=1}^N \alpha_n T_{\theta_n} \right) \sharp [G_{\xi_0} \sharp \mathbb{S}]
\]
We prove the lemma in Appendix A. In practice, we choose $K_G = 50$ as we found it empirically works better.

Figure 2: Our proposed two-step implementation of the fixed-point operator $\mathcal{H}(\cdot)$ that we use to compute the barycenter.

\[
\int_{n=1}^{N} \alpha_n T_{\theta_n} \|P_\xi \|_{Fro} \approx \int_{n=1}^{N} \alpha_n T_{\theta_n} \|P_\xi \|_{Fro} = \mathcal{H}(P_{\xi_0}),
\]
i.e. new generated $G_\xi \# S$ measures approximate $\mathcal{H}(P_{\xi_0})$.

**Summary.** Our two-step approach iteratively recomputes OT maps $T_{\theta_n} \rightarrow P_n$ (Figure 2a) and then updates regression (Figure 2b). The optimization procedure is detailed in Algorithm 1. Note that when fitting OT maps $T_{\theta_n} \rightarrow P_n$, we start from previously used $\{T_{\theta_n}, v_{\omega_n}\}$ rather than re-initialize them. Empirically, this works better.

### 4.3. Relation to Variational Barycenter Algorithms

We show that our Algorithm 1 reduces to variational approach (§3.2) when the number of generator updates, $K_G$, is equal to 1. More specifically, we show the equivalence of the gradient update w.r.t. parameters $\xi$ of the generator in our iterative Algorithm 1 and that of (8). We assume that $\mathbb{W}_2^2$ terms are computed exactly in (8) regardless of the particular OT solver. Similarly, in Algorithm 1, we assume that maps $G_{\xi_0} \# S \rightarrow P_n$ before the generator update are always exact, i.e., $T_{\theta_n} = T_{\theta_n} \rightarrow P_n$.

**Lemma 1.** Assume that $P_\xi = G_\xi \# \mathbb{S} \in \mathcal{P}_{2,ac}(\mathbb{R}^D)$. Consider $K_G = 1$ for the iterative Algorithm 1, i.e., we do a single gradient step regression update per OT solvers’ update. Assume that $\ell(x, x') = \frac{1}{2} \|x - x'\|^2$, i.e., the squared loss is used for regression. Then the generator’s gradient update in Algorithm 1 is the same as the variational algorithm:

\[
\frac{\partial}{\partial \xi} \int \frac{1}{2} \|G_\xi(z) - \sum_{n=1}^{N} \alpha_n T_{\theta_n} \cdot P_n(\xi) \|^2 d\mathcal{S}(z) = \frac{\partial}{\partial \xi} \sum_{n=1}^{N} \alpha_n \mathbb{W}_2^2(G_\xi \# S, P_n),
\]

where the derivatives are evaluated at $\xi = \xi_0$.

We prove the lemma in Appendix A. In practice, we choose $K_G = 50$ as we found it empirically works better.

### 5. Ave, celeba! Images Dataset

In this section, we develop a generic methodology for building probability measures with known $\mathbb{W}_2$ barycenter. We then use the methodology to construct Ave, celeba! dataset for quantitative evaluation of barycenter algorithms.

**Key idea.** Consider $\alpha_1, \ldots, \alpha_N > 0$ with $\sum_{n=1}^{N} \alpha_n = 1$, congruent convex functions $\psi_1, \ldots, \psi_N : \mathbb{R}^D \rightarrow \mathbb{R}$ and a measure $P \in \mathcal{P}_{2,ac}(\mathbb{R}^D)$ with positive density. Define $P_n = \nabla \psi_n \# P$. Thanks to the Brenier’s theorem (Brenier, 1991), $\nabla \psi_n$ is the unique OT map from $P$ to $P_n$. Since the support of $P$ is $\mathbb{R}^D$, $\psi_n$ is the unique (up to a constant) dual potential for $(P, \nabla \psi_n)$, see (Staudt et al., 2022). Since potentials $\psi_n$ are congruent, the barycenter $P$ of $P_n$ w.r.t. weights $\alpha_1, \ldots, \alpha_N$ is $P$ itself (Chewi et al., 2020, C.2).

If $\psi_n$ are such that all $P_n$ are absolutely continuous, then $P = P$ that is the unique barycenter (§2).

If one obtains $N$ congruent $\psi_n$, then for any $P \in \mathcal{P}_{2,ac}(\mathbb{R}^D)$, pushforward measures $P_n = \nabla \psi_n \# P$ can be used as the input measures for the barycenter task. For $P$ accessible by samples, $P_n$ are also accessible by samples: one may sample $x \sim P$ and push samples forward by $\nabla \psi_n$.

The challenging part is to construct non-trivial congruent convex functions $\psi_n$. First, we provide a novel method to transform a single convex function $\psi$ into a pair $(\psi', \psi'')$ of convex functions satisfying $\alpha \psi'(x) + (1 - \alpha) \psi''(x) = x$ for all $x \in \mathbb{R}^D$ (Lemma 2). Next, we extend the method to generate congruent $N$-tuples (Lemma 3).

**Lemma 2** (Constructing congruent pairs). Let $\psi$ be a strongly convex and $L$-smooth (for some $L > 0$) function. Let $\beta \in (0, 1)$. Define $\beta$-left and $\beta$-right functions of $\psi$ by

\[
\psi' \overset{def}{=} \frac{\beta}{2} \| \cdot \|^2 + (1 - \beta) \psi; \quad \psi'' \overset{def}{=} (1 - \beta) \| \cdot \|^2 + \beta \psi.
\]

Then $\beta \psi'(x) + (1 - \beta) \psi''(x) = \frac{\|x\|^2}{2}$ for $x \in \mathbb{R}^D$, i.e., convex functions $\psi', \psi''$ are congruent w.r.t. weights $(\beta, 1 - \beta)$. 

\[
\beta \psi'(x) + (1 - \beta) \psi''(x) \overset{def}{=} \frac{\|x\|^2}{2}.
\]
We prove Lemma 3 in Appendix A. We visualize the idea of generating our Lemma 3 in Figure 7b. The lemma provides an elegant way to create $N$ congruent functions from convex linear combinations of functions in given congruent pairs $(\psi_1^l, \psi_1^r)$, $\ldots$, $(\psi_N^l, \psi_N^r)$. Gradients $\nabla_1 \psi_n$ of these functions are respective linear combinations of gradients $\nabla_1^l \psi_m$ and $\nabla_1^r \psi_m$.

Besides, for all $x \in \mathbb{R}^D$ the gradient $y^l \equiv \nabla_1^l(x)$ can be computed via solving $\beta$-strongly concave optimization:

$$y^l = \arg \max_{y \in \mathbb{R}} \left( (x, y) - \frac{\beta \|y\|^2}{2} - (1 - \beta) \psi(y) \right). \quad (12)$$

In turn, the value $y^r \equiv \nabla_1^r(x)$ is given by $y^r = \nabla(y^l)$.

The proof is given in Appendix A. We visualize the idea of our Lemma 2 in Figure 7a. Thanks to Lemma 2, any analytically known convex function $\psi$, e.g., an ICNN, can be used to produce a congruent pair $\psi_1^l$, $\psi_1^r$. To compute the gradient maps, optimization (12) can be solved by convex optimization tools with $\nabla \psi$ computed by automatic differentiation.

**Lemma 3 (Constructing $N$ congruent functions).** Let $\psi_1^l, \ldots, \psi_M^l$ be convex functions, $\beta_1, \ldots, \beta_M \in (0, 1)$ and $\psi_1^r, \ldots, \psi_M^r$ be $\beta_m$-$\text{left}$, $\beta_m$-$\text{right}$ functions for $\psi_m^0$ respectively. Let $\gamma^l, \gamma^r \in \mathbb{R}^{N \times M}$ be two rectangular matrices with non-negative elements and the sum of elements in each column equals to 1. Let $w_1, \ldots, w_M > 0$ satisfy $\sum_{m=1}^M w_m = 1$.

For $n = 1, \ldots, N$ define

$$\psi_n(x) \equiv \frac{\sum_{m=1}^M w_m \beta_m \gamma^l_{nm} \psi_m^l(x) + (1 - \beta_m) \gamma^r_{nm} \psi_m^r(x)}{\sum_{m=1}^M w_m [\beta_m \gamma^l_{nm} + (1 - \beta_m) \gamma^r_{nm}]} \quad (13)$$

Then $\psi_1, \ldots, \psi_N$ are congruent w.r.t. weights

$$\alpha_n \equiv \sum_{m=1}^M w_m [\beta_m \gamma^l_{nm} + (1 - \beta_m) \gamma^r_{nm}].$$

We prove Lemma 3 in Appendix A. We visualize the idea of our Lemma 3 in Figure 7b. The lemma provides an elegant way to create $N \geq 2$ congruent functions from convex linear combinations of functions in given congruent pairs $(\psi_1^l, \psi_1^r)$, $\ldots$, $(\psi_N^l, \psi_N^r)$. Gradients $\nabla_1 \psi_n$ of these functions are respective linear combinations of gradients $\nabla_1^l \psi_m$ and $\nabla_1^r \psi_m$.

6. Evaluation

**Dataset creation.** We use CelebA $64 \times 64$ faces dataset (Liu et al., 2015) as the basis for our Ave, celeba! dataset. We assume that CelebA dataset is an empirical sample from the continuous measure $\mathbb{P}_{\text{Celeba}} \in \mathbb{P}^{+}_{2,ac}(\mathbb{R}^{64 \times 64})$ which we put to be the barycenter in our design, i.e., $\mathbb{P} = \mathbb{P}_{\text{Celeba}}$. We construct differentiable congruent pairs by bijection functions that produce $\mathbb{P}_n = \nabla_1 \psi_n^l \mathbb{P}_{\text{Celeba}} \in \mathbb{P}^{+}_{2,ac}(\mathbb{R}^{64 \times 64})$ whose unique barycenter is $\mathbb{P}_{\text{Celeba}}$. In Lemma 3, we set $N = 3$, $M = 2$, $\beta_1 = \beta_2 = \frac{1}{2}$, $w_1 = w_2 = \frac{1}{2}$ and

$$(\alpha^l)^\top = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (\gamma^r)^\top = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

which yields weights $(\alpha_1, \alpha_2, \alpha_3) = \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right)$. We choose the constants above mainly to make sure the final produced measures $\mathbb{P}_n$ are visually distinguishable. We use $\psi_m^0(x) = \text{ICNN}_m(s_m(\sigma_m(d_m(x)))) + \lambda \frac{\|x\|^2}{2}$ as convex functions, where ICNNs have ConvICNN64 architecture (Korotin et al., 2021b, Appendix B.1), $\sigma_1, \sigma_2$ are random permutations of pixels and channels, $s_1, s_2$ are axis-wise random reflections, $\lambda = \frac{1}{1000}$. In both functions, $d_m$ is a de-colorization transform which sets R, G, B channels of each pixel to $\frac{7}{10}R + \frac{1}{5}G + \frac{1}{2}B$ for $\psi_1^l$ and $\frac{3}{2}(R+G+B)$ for $\psi_1^r$. The weights of ICNNs are initialized by the pre-trained potentials of $\mathcal{W}_2$ “Early” transport benchmark which map blurry faces to the clean ones (Korotin et al., 2021b, §4.1). All the implementation details are given in Appendix B.1.

Finally, to create Ave, celeba! dataset, we randomly split the images dataset into 3 equal parts containing $\approx 67$K samples, and map each part to respective measure $\mathbb{P}_n = \nabla_1 \psi_n^l \mathbb{P}_{\text{Celeba}}$ by $\nabla_1 \psi_n^r$. Resulting $3 \times 67$K samples form the dataset consisting of 3 parts. We show the samples in Figure 3. The samples from the respective parts are in green boxes.

Figure 3: The production of Ave, celeba! dataset. The 1st line shows images $x \sim \mathbb{P}_{\text{Celeba}}$. Each of 3 next lines shows OT maps $\nabla \psi_n(x) \sim \nabla \psi_n^l \mathbb{P}_{\text{Celeba}} = \mathbb{P}_n$ to constructed measures $\mathbb{P}_n$. Their barycenter w.r.t. $(\alpha_1, \alpha_2, \alpha_3) = \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right)$ is $\mathbb{P}_{\text{Celeba}}$. The last line shows congruence of $\psi_n$, i.e., $\sum_{n=1}^N \alpha_n \nabla \psi_n(x) \equiv x$. Samples in green boxes are included to dataset.
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Figure 4: The barycenter and maps to input measures estimated by barycenter algorithms. The 1st line shows generated samples $P_{\xi} = G_{\xi} \sharp S \approx P_{\text{Celeba}}$. Lines 2-4 show maps $\hat{T}_{P_{\xi} \rightarrow P_{n}}$. The last line shows the average map $\sum_{n=1}^{N} \alpha_{n} \hat{T}_{P_{\xi} \rightarrow P_{n}}$.

(a) Our Algorithm 1.
(b) Competitive [SCW2B] algorithm.

Figure 5: Maps from input measures $P_{n}$ ($n = 1, 2, 3$) to the barycenter $P$ estimated by the barycenter algorithms in view. For comparison with the original barycenter images, the faces are the same as in Figure 3.

(a) Maps from $P_{1}$ to the barycenter.
(b) Maps from $P_{2}$ to the barycenter.
(c) Maps from $P_{3}$ to the barycenter.

The code is written on the PyTorch and includes the script for producing Ave, celeba’ dataset. The experiments are conducted on 4×GPU GTX 1080ti. Implementation details, architectures and hyperparameters are given in Appendix B.

6.1. Evaluation on Ave, celeba’ Dataset

We evaluate our iterative algorithm 1 and a recent variational [SCW2B] by (Fan et al., 2020) on Ave, celeba’ dataset. Both algorithms use a generative model $P_{\xi} = G_{\xi} \sharp S$ for the barycenter and yield approximate maps $\hat{T}_{P_{\xi} \rightarrow P_{n}}$ to input measures. In our case, the maps are neural networks $T_{\theta_{n}}$, while in [SCW2B] they are gradients of ICNNs.

The barycenters of Ave, celeba’ fitted by our algorithm and [SCW2B] are shown in Figures 4a and 4b respectively. Recall the ground truth barycenter is $P_{\text{Celeba}}$. Thus, for quantitative evaluation we use FID score (Heusel et al., 2017) computed on 200K generated samples w.r.t. the original CelebA dataset, see Table 1. Our method drastically outperforms [SCW2B]. Presumably, this is due to the latter using ICNNs which do not provide sufficient performance.

Additionally, we evaluate to which extent the algorithms allow to recover the inverse OT maps $\hat{T}_{P_{n} \rightarrow P_{\xi}}$ from inputs $P_{n}$ to the barycenter $P_{\xi}$ in [SCW2B], these maps are computed during training. Our algorithm does not compute them. Thus, we separately fit the inverse maps after main training by using [MM:R] solver between each input $P_{n}$ and learned $P_{\xi}$ (Algorithm 2 of Appendix 2). The inverse maps are given in Figure 5; their FID scores – in Table 2. Here we add an additional constant shift [CS] baseline which simply shifts the mean of input $P_{n}$ to the mean $\mu$ of $P$. The vector $\mu$ is given by $\sum_{n=1}^{N} \alpha_{n} \mu_{n}$, where $\mu_{n}$ is the mean of $P_{n}$ ($\text{Álvarez-Esteban et al.}, 2016$). We empirically estimate $\mu$ from input samples $y \sim P_{n}$.

6.2. Additional Experimental Results

Different domains. To stress-test our algorithm 1, we compute the barycenters w.r.t. $(\alpha_{1}, \alpha_{2}, \alpha_{3}) = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ of notably different datasets: 50K Shoes (Yu & Grauman, 2019), 300K COCO (Lin et al., 2014), 50K PQS (Prezioso et al., 2016) and 50K SHOE (Yu & Grauman, 2019).
We provide more examples in Figure 12 of Appendix C.4. All the images are rescaled to 64 × 64, similar to (Fan et al., 2020), we compute barycenters through $T_{\hat{\xi}} = \mathcal{H}(\hat{\xi})$. In Appendix C.1, we provide Extra results. We present a scalable barycenter algorithm based on fixed-point iterations with many application prospects. For instance, in medical imaging, MRI is often acquired at multiple sites where the overlap of information (imaging, genetic, diagnosis) between any two sites is limited. Consequently, the data on each site may be biased and can cause generalizability and robustness issues when training models. The developed algorithm could help to aggregate data from multiple sites and overcome the distributional shift issue across sites.

We expect our Ave, celeba! to become a standard dataset for evaluating continuous barycenter algorithms. In addition, we describe a generic recipe (§5) to produce new datasets.

**Limitations.** During our fixed-point iterations, the barycenter objective (5) decreases. However, there is no guarantee that the sequence of measures converges to a fixed point or the fixed point is the barycenter. Identifying the precise conditions on the input measures and the initial point is an important future direction. Besides, our algorithm does not recover reverse OT maps $T_{\hat{\xi}} = \mathcal{H}(\hat{\xi})$; we compute them with an OT solver as a follow-up. To avoid this second step, one may consider using invertible neural networks (Etmann et al., 2020) to parametrize maps $T_{\hat{\xi}}$ in our Algorithm 1.

To create Ave, celeba! dataset (§5), we compose ICNNs with decolorization, random reflections and permutations to simulate degraded images. It is unclear how to produce other practically interesting effects via ICNNs. Studying how to generate more realistic barycenter benchmark is an interesting direction for the future work that will provide insights for benchmarking other OT problems.

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A. Proofs

First, we recall basic properties of convex conjugate functions that we rely on in our proofs. Let \( \psi : \mathbb{R}^D \to \mathbb{R} \) be a convex function and \( \overline{\psi} \) be its convex conjugate. From the definition of \( \overline{\psi} \), we obtain

\[
\psi(x) + \overline{\psi}(y) \geq \langle x, y \rangle
\]

for all \( x, y \in \mathbb{R}^D \). Assume that \( \psi \) is differentiable and has an invertible gradient \( \nabla \psi : \mathbb{R}^D \to \mathbb{R}^D \). The latter condition holds, e.g., for strongly convex functions. From the convexity of \( \psi \), we derive

\[
x = \arg \max_{x \in \mathbb{R}^D} [(x, y) - \psi(x)] \iff y = \nabla \psi(x) \iff x = (\nabla \psi)^{-1}(y),
\]

which yields

\[
\overline{\psi}(y) = \langle (\nabla \psi)^{-1}(x), x \rangle - \psi((\nabla \psi)^{-1}(x)).
\]

In particular, the strict equality \( \psi(x) + \overline{\psi}(y) = \langle x, y \rangle \) holds if and only if \( y = \nabla \psi(x) \). By applying the same logic to \( \overline{\psi} \), we obtain \( (\overline{\nabla \psi})^{-1} = \nabla \psi \) and \( (\nabla \psi)^{-1} = \overline{\nabla \psi} \), i.e., the gradients of conjugate functions are mutually inverse.

### A.1. Proof of Lemma 1

**Proof.** For each \( n = 1, 2, \ldots, N \) we perform the following evaluation:

\[
\frac{\partial}{\partial \xi} \mathbb{W}^2_2(G_{\xi} \mathbb{S}, \mathbb{P}_n) = \int_{z} J_{\xi} G_{\xi}(z)^T \nabla u^*_n(G_{\xi}(z)) d\mathbb{S}(z) = \int_{z} J_{\xi} G_{\xi}(z)^T (G_{\xi}(z) - T_{\mathbb{P}_\xi \to \mathbb{P}_n}(G_{\xi}(z))) d\mathbb{S}(z),
\]

(14)

where \( u^*_n \) is the optimal dual potential for \( \mathbb{P}_\xi = G_{\xi} \mathbb{S} \) and \( \mathbb{P}_n \). The first equation in (14) follows from (Genevay et al., 2017, Equation 3). The second equation in (14) follows from the property \( \nabla u^*_n(x) = x - T_{\mathbb{P}_\xi \to \mathbb{P}_n}(x) \) connecting dual potentials and OT maps.

We sum (14) for \( n = 1, \ldots, N \) w.r.t. weights \( \alpha_n \) with \( \xi = \xi_0 \) and obtain

\[
\frac{\partial}{\partial \xi} \sum_{n=1}^{N} \alpha_n \mathbb{W}^2_2(G_{\xi} \mathbb{S}, \mathbb{P}_n) = \int_{z} J_{\xi} G_{\xi}(z)^T (G_{\xi}(z) - \sum_{n=1}^{N} \alpha_n T_{\mathbb{P}_\xi \to \mathbb{P}_n}(G_{\xi}(z))) d\mathbb{S}(z).
\]

(15)

The last step is to note that (15) exactly matches the derivative of the left-hand side of (10) evaluated at \( \xi = \xi_0 \). \( \square \)

### A.2. Proof of Lemma 2

**Proof.** First, we prove the congruence, i.e., \( \beta \psi^l(x) + (1 - \beta) \psi^r(x) = \frac{\|x\|^2}{2} \) for all \( x \in \mathbb{R}^D \).

\[
\beta \max_{y_1 \in \mathbb{R}^D} [(x, y_1) - \overline{\psi}(y_1)] + (1 - \beta) \max_{y_2 \in \mathbb{R}^D} [(x, y_2) - \overline{\psi}(y_2)] = \frac{\|x\|^2}{2} - (1 - \beta) \psi(x)
\]

(16)

\[
\max_{y_1, y_2 \in \mathbb{R}^D} [(x, y_1 + (1 - \beta)y_2) - \beta \frac{\|y_1\|^2}{2} - (1 - \beta)^2 \frac{\|y_2\|^2}{2} - \beta(1 - \beta)(\psi(y_1) + \overline{\psi}(y_2))] \leq \frac{\|x\|^2}{2} - (1 - \beta)^2 \frac{\|y_2\|^2}{2} - \beta(1 - \beta)(y_1, y_2)
\]

(17)

\[
\max_{y_1, y_2 \in \mathbb{R}^D} [(x, y_1 + (1 - \beta)y_2) - \beta \frac{\|y_1\|^2}{2} - (1 - \beta)^2 \frac{\|y_2\|^2}{2} - \beta(1 - \beta)(y_1, y_2)] = \frac{\|x\|^2}{2} - \frac{1}{2} \|x - (\beta y_1 + (1 - \beta)y_2)\|^2 \leq \frac{\|x\|^2}{2}.
\]

(18)

First, we substitute \( (y_1, y_2) = (y', \nabla \psi(y')) \). For this pair, \( x = \nabla \overline{\psi}(y') = \beta y' + (1 - \beta) \nabla \psi(y') \), which results in \( x = \beta y_1 + (1 - \beta)y_2 \). Moreover, since \( y_2 = \nabla \psi(y_1) \), we have \( \psi(y_1) + \overline{\psi}(y_2) = (y_1, y_2) \). As the consequence, both inequalities (17) and (18) turn to strict equalities yielding congruence of \( \psi^l, \psi^r \).
From (11), the smoothness and strong convexity of \( \psi \) imply that \( \psi^l \) and \( \psi^r \) are smooth. Consequently, \( \overline{\psi}^l \) and \( \overline{\psi}^r \) are strongly convex. Thus, the maximizer of (16) is unique. We know the maximum of (16) is attained at \((y_1, y_2) = (\nabla \psi^l(x), \nabla \psi^r(x)) = (y^l, y^r)\). We conclude \((y^l, y^r) = (y^l, \nabla \psi(y^l))\), i.e., \(y^r = \nabla \psi(y^l)\). Finally, \(y^l = \nabla \psi^l(x) \Leftrightarrow x = \nabla \overline{\psi}^l(y^l) \Leftrightarrow y^l = \max_{y \in \mathbb{R}^D} \left[ (x, y) - \overline{\psi}^r(y) \right] \), which matches (12).

A.3. Proof of Lemma 3

**Proof.** First, we check that \( \sum_{n=1}^{N} \alpha_n \) indeed equals 1:

\[
\sum_{n=1}^{N} \alpha_n = \sum_{n=1}^{N} \sum_{m=1}^{M} w_m \left[ \beta_m \gamma_{nm}^l + (1 - \beta_m) \gamma_{nm}^r \right] = \sum_{m=1}^{M} \left[ w_m \beta_m \sum_{n=1}^{N} \gamma_{nm}^l \right] + \sum_{m=1}^{M} \left[ w_m (1 - \beta_m) \sum_{n=1}^{N} \gamma_{nm}^r \right] = \sum_{m=1}^{M} w_m \beta_m + \sum_{m=1}^{M} w_m (1 - \beta_m) = \sum_{m=1}^{M} w_m (\beta_m + (1 - \beta_m)) = \sum_{m=1}^{M} w_m = 1. \tag{19}
\]

Next, we check that \( \psi_1, \ldots, \psi_N \) are congruent w.r.t. weights \( \alpha_1, \ldots, \alpha_N \):

\[
\sum_{n=1}^{N} \alpha_n \psi_n(x) = \sum_{n=1}^{N} \sum_{m=1}^{M} w_m \left[ \beta_m \gamma_{nm}^l \psi_m(x) + (1 - \beta_m) \gamma_{nm}^r \psi_m(x) \right] = \sum_{m=1}^{M} \left[ w_m \beta_m \psi_m(x) \sum_{n=1}^{N} \gamma_{nm}^l \right] + \sum_{m=1}^{M} \left[ w_m (1 - \beta_m) \psi_m(x) \sum_{n=1}^{N} \gamma_{nm}^r \right] = \sum_{m=1}^{M} \left[ w_m \left( \beta_m \psi_m(x) + (1 - \beta_m) \psi_m(x) \right) \right] = \sum_{m=1}^{M} w_m \left\| x \right\|^2 = \frac{\left\| x \right\|^2}{2}.
\]

\[\square\]

B. Experimental Details

B.1. Ave, celeba! Dataset Creation

The initialization of random permutations \( \sigma_m \) and reflections \( s_m \) (for \( m = 1, 2 \)) as well as the random split of CelebA dataset into 3 parts (each containing \( \approx 67 \) \( K \) images) are hardcoded in our provided script for producing Ave, celeba! dataset. To initialize ICNN\(_N\) (for \( m = 1, 2 \)), we use ConvICNN\(_{64}\) (Korotin et al., 2021b, Appendix B.1) checkpoints Early.v1_conj.pt, Early.v2_conj.pt from the official Wasserstein-2 benchmark repository\(^1\).

We rescale CelebA images to 64 \( \times \) 64 by using imresize from scipy.misc. To create empirical samples from input distributions \( \mathbb{P}_n \) by using the rescaled CelebA dataset, we compute the gradient maps \( \nabla \psi_n(x) \) \( (n = 1, 2, 3) \) in Lemma 3 for images \( x \) in the CelebA dataset. This computation implies computing gradient maps \( \nabla \psi_m^l(x) \) and \( \nabla \psi_m^r(x) \) for each base function \( \psi_m^0 \) \( (m = 1, 2) \) and summing them with respective coefficients \( (13) \). Following our Lemma 2, we compute \( y_m^l \overset{\text{def}}{=} \nabla \psi_m^l(x) \) by solving a concave optimization problem \( (12) \) over the space of images. We solve this problem with the gradient descent. We use Adam optimizer (Kingma & Ba, 2014) with default betas, \( \ell r = 2 \cdot 10^{-2} \) and do 1000 gradient steps. To speed up the computation, we simultaneously solve the problem for a batch of 256 images \( x \) from CelebA dataset. After the optimization, we compute \( y^r \overset{\text{def}}{=} \nabla \psi_m^r(x) \) as \( y^r = \nabla \psi_m(y^l) \) (Lemma 2).

**Computational complexity.** The process of producing Ave, celeba! dataset takes about 1, 5 days on a GPU GTX 1080 ti.

B.2. Hyperparameters (Algorithm 1, Main Training)

We provide the hyperparameters of all the experiments with algorithm 1 in Table 3. The column total iters shows the sum of gradient steps over generator \( G_\xi \) and each of \( N \) potentials \( v_{\omega_n} \) in OT solvers.

\[\text{https://github.com/iamalexkorotin/Wasserstein2Benchmark}\]
(a) Construction of a pair of congruent functions \( \psi',\psi^* \) from a convex \( \psi \), see Lemma 2. 

(b) Construction of \( N \) congruent \( \psi_n \), as convex combinations of \( M \) congruent pairs \( (\psi_n^*,\psi_n^{**}) \), see Lemma 3.

Figure 7: Construction of tuples of congruent functions and production of measures with known \( \mathcal{W}_2 \) barycenter (§5).

**Optimization.** We use Adam optimizer with the default betas. During training, we decrease the learning rates of the generator \( G \) and each potential \( v_w \) every 10K steps of their optimizers. In the Gaussian case, we use a single GPU GTX 1080ti. In all other cases we split the batch over 4 GPUs. Other experiments converge faster.

**Neural Network Architectures.** In the Gaussian case, we use In the evaluation in the Gaussian case, we use sequential fully-connected neural networks with ReLU activations for the generator \( G \) and transport maps \( T_{\theta_n} : \mathbb{R}^D \to \mathbb{R}^D \). For all the networks the sizes of hidden layers are:

\[
\text{[max(100, 2D), max(100, 2D), max(100, 2D)]}.
\]

In the experiments with images, we use the ResNet\(^2\) generator and discriminator architectures of WGAN-QC (Liu et al., 2019) for our generator \( G \) and potentials \( v_{\omega_n} \) respectively. As the maps \( T_{\theta_n} \), we use U-Net\(^3\) (Ronneberger et al., 2015).

**Generator regression loss.** In the Gaussian case and experiments with grayscale images (MNIST, FashionMNIST), we use mean squared loss for generator regression. In other experiments, we use the perceptual mean squared loss based on the features of the pre-trained VGG-16 network (Simonyan & Zisserman, 2014). The loss is hardcoded in the implementation.

**Data pre-processing.** In all experiments with images we normalize them to \([-1, 1]\). We rescale MNIST and FashionMNIST images to 32 × 32. In all other cases, we rescale images to 64 × 64. Note that Fruit360 dataset originally contains 114 × 114 images; before rescaling, we add white color padding to make the images have the size 128 × 128. Working with Ave, celeba! dataset, we additionally shift each subset \( P_n \) by \( \vec{\mu}_n \), i.e., we train the models on the \([\text{CS}]\) baseline. This helps the models to avoid learning the shift.

**Computational complexity.** The most challenging experiments (Ave, celeba! and Handbags, Shoes, Fruit barycenters) take about 2-3 days to converge on 4×GPU GTX 1080 ti. Other experiments converge faster.

| Experiment       | D   | H   | N   | \( G_\xi \) | \( v_{w_n} \) | \( T_{\theta_n} \) | \( k_G \) | \( k_v \) | \( t_{\hat{G}} \) | \( t_{\hat{v}} \) | \( t_{\ell T} \) | \( \ell \) | Total iters | Batch size |
|------------------|-----|-----|-----|-------------|---------------|---------------|--------|--------|----------------|----------------|----------------|--------|------------|------------|
| Gaussians        | 2-128 | 2-128 | 4   | MLP         | MLP           | 10            | 1      | 10^{-3} | 10^{-3}        | 10^{-4}        | 10^{-4}        | MSE    | 12K        | 1024       |
| MNIST 0/1        | 1024 | 16  | 2   | 10          | ResNet        | 50            | 50     | 10^{-4} | 10^{-4}        | 10^{-4}        | 10^{-4}        |          |            |            |
| FashionMNIST     | 12288 | 128 | 3   | 1           | UNet         | 15            | 15     | 10^{-4} | 10^{-4}        | 10^{-4}        | 10^{-4}        | VGG    | 60K        | 36K        |
| Bags, Shoes, Fruit | 12288 | 128 | 3   | 1           | UNet         | 15            | 15     | 10^{-4} | 10^{-4}        | 10^{-4}        | 10^{-4}        | VGG    | 60K        | 80K        |
| Ave, celeba!     | 12288 | 128 | 3   | 1           | UNet         | 15            | 15     | 10^{-4} | 10^{-4}        | 10^{-4}        | 10^{-4}        | VGG    | 60K        | 80K        |
| Celeba (fixed \( G \)) | 12288 | 128 | 3   | 1           | UNet         | 15            | 15     | 10^{-4} | 10^{-4}        | 10^{-4}        | 10^{-4}        | VGG    | 60K        | 80K        |

Table 3: Hyperparameters that we use in the experiments with our algorithm 1.

\(^2\)https://github.com/harryliew/WGAN-QC

\(^3\)https://github.com/milesial/Pytorch-UNet
Algorithm 2: Learning maps from input measures to the learned barycenter \( P_\xi \approx P \) with [MM:R] OT solver.

**Input**: latent \( S \) and input \( P_1, \ldots, P_n \) measures; pretrained generator \( G_\xi : \mathbb{R}^H \rightarrow \mathbb{R}^D \) satisfying \( G_\xi \sharp S \approx P \); mapping networks \( T^\text{inv}_{\theta_1}, \ldots, T^\text{inv}_{\theta_K} : \mathbb{R}^D \rightarrow \mathbb{R}^D \); potentials \( v^\text{inv}_{\omega_1}, \ldots, v^\text{inv}_{\omega_K} : \mathbb{R} \rightarrow \mathbb{R} \); number of inner iterations for training transport maps: \( K_T \).

**Output**: OT maps satisfying \( \sum_{n} P_n \approx P_\xi = (G_\xi \sharp S) \approx P \);

\[\text{repeat}\]

\[\begin{array}{l}
\text{for } n = 1, 2, \ldots, N \\
\text{Sample batches } Z \sim S, Y \sim P_n; X \leftarrow G_\xi(Z); \\
\mathcal{L}_v \leftarrow \frac{1}{|Y|} \sum_{y \in Y} \sum_{n} v^\text{inv}_{\omega_n}(T^\text{inv}_{\theta_n}(y)) - \frac{1}{|X|} \sum_{x \in X} v^\text{inv}_{\omega_n}(x); \\
\text{Update } \omega_n \text{ by using } \frac{\partial \mathcal{L}_v}{\partial \omega_n}; \\
\text{for } k_T = 1, 2, \ldots, K_T \text{ do} \\
\text{Sample batch } Y \sim P_n; \\
\mathcal{L}_T = \frac{1}{|Y|} \sum_{y \in Y} \frac{1}{2} \|y - T^\text{inv}_{\theta_n}(y)\|^2 - v^\text{inv}_{\omega_n}(T^\text{inv}_{\theta_n}(y)); \\
\text{Update } \theta_n \text{ by using } \frac{\partial \mathcal{L}_T}{\partial \theta_n}; \\
\end{array}\]

until not converged;

**B.3. Hyperparameters (Algorithm 2, Learning Maps to the Barycenter)**

After using the main algorithm 1 to train \( G_\xi \), we use algorithm 2 to extract the inverse optimal maps \( P_n \rightarrow P_\xi \). We detail the hyperparameters in Table 4 below. In all the cases we use Adam optimizer with the default betas. The column **total iters** show the number of update steps for each potential \( v^\text{inv}_{\omega_n} \).

| Experiment      | D     | N   | \( v^\text{inv}_{\omega_n} \) | \( T^\theta_n \) | \( k_T \) | \( l_{\mathcal{L}_v} \) | \( l_{\mathcal{L}_T} \) | Total iters | Batch size |
|-----------------|-------|-----|-----------------------------|-----------------|---------|-----------------|-----------------|-------------|------------|
| MNIST 0/1       | 1024  | 2   | ResNet                      | UNet            | 10      | 1 \cdot 10^{-4} | 1 \cdot 10^{-4} | 4k          | 4k         |
| FashionMNIST    | 12288 | 3   |                             |                 |         |                 |                 | 20k         | 12K        |
| Bags, Shoes, Fruit, Ave, celeba! |       | 3   |                             | ResNet          | 10      | 1 \cdot 10^{-4} | 1 \cdot 10^{-4} | 4k          | 4k         |

Table 4: Hyperparameters that we use in the experiments with algorithm 2

**B.4. Hyperparameters of competitive [SC\( \mathcal{W}_2 \)B] algorithm**

On Ave, celeba! we use (Fan et al., 2020, Algorithm 1) with \( k_3 = 50000, k_2 = k_1 = 10 \). The optimizer, the learning rates and the generator network are the same as in our algorithm. However, for the potentials (OT solver), we use ICNN architecture as it is required by their method. We use ConvICNN64 (Korotin et al., 2021b, Appendix B.1) architecture.

**C. Additional Experimental Results**

**C.1. Gaussian Case**

Similar to (Korotin et al., 2021c; Fan et al., 2020), we consider toy Gaussian case for which the true barycenter can be computed (Álvarez- Esteban et al., 2016, §4). We use \( N = 4 \) measures with weights \( (\alpha_1, \ldots, \alpha_4) = (\frac{1}{10}, \frac{2}{10}, \frac{3}{10}, \frac{4}{10}) \). By using the publicly available code of (Korotin et al., 2021c), we initialize \( P_n = \mathcal{N}(0, S_n^2 \Lambda S_n) \), where \( S_n \) is a random rotation matrix and \( \Lambda \) is diagonal with entries \( \frac{1}{2} b^0, \frac{1}{2} b^1, \ldots, \frac{1}{2} b^2 \), where \( b = \sqrt{\frac{\mu}{4}} \). We quantify the generated \( \mathcal{W}_2 \) barycenter \( G_\xi \sharp S \) with the Bures-Wasserstein Unexplained Variance Percentage (Korotin et al., 2021c, §5) metric:

\[\text{B}^2 \mathcal{W}_2\text{-UVP}(G_\xi \sharp S, P) = 100 \cdot \text{B}^2 \mathcal{W}_2(G_\xi \sharp S, P)/\left[ \frac{1}{2} \text{Var}(P) \right] \%,
\]

where \( \text{B}^2 \mathcal{W}_2(P, Q) = \mathcal{W}_2^2(\mathcal{N}(\mu_P, \Sigma_P), \mathcal{N}(\mu_Q, \Sigma_Q)) \) is the Bures-Wasserstein metric and \( \mu_P, \Sigma_P \) denote mean and co-variance of the measure \( P \). The metric admits the closed form (Chewi et al., 2020). For the trivial baseline prediction \( G_\xi(\cdot) \equiv \mu_P \equiv \sum_{n=1}^N \alpha_n \mu_{P_n} \) the metric value is 100%. We denote this baseline as \([C]\).
Table 5: Comparison of $\mathbb{W}_2^2$-UVP$_{1}$ (%) in the Gaussian case.

| Method          | 128 | 64 | 32 | 16 | 8  | 4  | 10 |
|-----------------|-----|----|----|----|----|----|-----|
| $[\text{SCW}_2 B]$ | 0.01 | 0.03 | 0.01 | 0.08 | 0.11 | 0.23 | 0.38 |
| $\text{Ours}$   | 0.01 | 0.02 | 0.01 | 0.08 | 0.11 | 0.23 | 0.38 |

The results of our algorithm 1 and $[\text{SCW}_2 B]$ adapted from (Korotin et al., 2021c, Table 1) are given in Table 5. Both algorithms work well in the Gaussian case and provide $\mathbb{W}_2^2$-UVP < 2% in dimension 128.

C.2. Generative Modeling

Analogously to (Fan et al., 2020), we evaluate our algorithm when $N = 1$. In this case, the minimizer of (5) is the measure $P_1$ itself, i.e., $P = P_1$. As the result, our algorithm 1 works as a usual generative model, i.e., it fits data $P_1$ by a generator $G_\xi$. For experiments, we use CelebA $64 \times 64$ dataset. Generated images $G_\xi(z)$ and $\hat{T}_{P_\xi \rightarrow P_1}(G_\xi(z))$ are shown in Figure 8a.

![Image](image1.png)

(a) Generator $G_\xi$ training enabled ($K_G > 0$).

![Image](image2.png)

(b) Generator $G_\xi$ training disabled ($K_G = 0$).

Figure 8: Images generated by our algorithm 1 serving as a generative model. The 1st line shows samples from $G_\xi\sharp S \approx P_1$, the 2nd line shows estimated OT map $\hat{T}_{P_\xi \rightarrow P_1}$ from $G_\xi\sharp S$ to $P_1$ which further improves generated images.

In Table 6, we provide FID for generated images. For comparison, we include FID for ICNN-based $[\text{SCW}_2 B]$, and WGAN-QC (Liu et al., 2019). FID scores are adapted from (Korotin et al., 2021b, §4.5). Note that for $N = 1$, $[\text{SCW}_2 B]$ is reduced to the OT solver by (Makkiva et al., 2019) used as the loss for generative models, a setup tested in (Korotin et al., 2021b, Figure 3a). Serving as a generative model when $N = 1$, our algorithm 1 performs comparably to WGAN-QC and drastically outperforms ICNN-based $[\text{SCW}_2 B]$.

| Method          | FID$_{\downarrow}$ |
|-----------------|--------------------|
| $[\text{SCW}_2 B]$ | $G_\xi(z)$ 90.2  |
| $\hat{T}_{P_\xi \rightarrow P_1}(G_\xi(z))$ | 89.8 |
| WGAN-QC         | $G_\xi(z)$ 14.4  |
| $\text{Ours}$   | $G_\xi(z)$ 46.6   |
| $\text{Ours}$ (fixed $G_\xi$) | $G_\xi(z)$ N/A |
| $\hat{T}_{P_\xi \rightarrow P_1}(G_\xi(z))$ | 15.7 |

Table 6: FID scores of generated faces.

Fixed generator. For $N = 1$, the fixed point approach §4.1 converges in only one step since operator $H$ immediately maps $G_\xi\sharp S$ to $P_1$. As a result, in our algorithm 1, exclusively when $N = 1$, we can fix generator $G_\xi$ and train only OT map $T_{P_\xi}$ from $G_\xi\sharp S$ to data measure $P_1$ and related potential $w_\omega$. As a sanity check, we conduct such an experiment with randomly initialized generator network $G_\xi$. The results are given in Figure 8b, the FID is included in Table 6. Our algorithm performs well even without generator training at all.

C.3. Barycenters of MNIST Digits and FashionMNIST Classes

Similar to (Fan et al., 2020, Figure 6), we provide qualitative results of our algorithm applied to computing the barycenter of two MNIST classes of digits 0, 1. The barycenter w.r.t. weights $(\frac{1}{2}, \frac{1}{2})$ computed by our algorithm is shown in Figure 9. We also consider a more complex FashionMNIST (Xiao et al., 2017) dataset. Here we compute the barycenter of 10 classes w.r.t. weights $(\frac{1}{10}, \ldots, \frac{1}{10})$. The results are given in Figures 10 and Figure 11.

Due to (6), each barycenter images are an average (in pixel space) of certain images from the input measure. In all
the Figures, the produced barycenter images satisfy this property. The maps to input measures are visually good. The approximate fixed point operator $H(P_\xi)$ is almost the identity as expected (the method converged).

C.4. Additional Results

In Figure 13, we visualize maps between Ave, Celeba! subsets through the learned barycenter. In Figure 12, we provide additional qualitative results for computing barycenters of Handbags, Shoes, Fruit360 datasets.

Figure 9: The barycenter of MNIST digit classes 0/1 learned by Algorithm 1.
Figure 10: The barycenter and maps to input measures estimated by our method on 10 FashionMNIST classes (32 × 32). The 1st line shows generated samples from $\mathbb{P}_\xi = G_\xi \sharp \mathbb{S} \approx \mathbb{P}$. Each of 10 next lines shows estimated optimal maps $\hat{T}_{\mathbb{P}_\xi \rightarrow \mathbb{P}_n}$ to measures $\mathbb{P}_n$. The last line shows average $\left[ \sum_{n=1}^{N} \alpha_n \hat{T}_{\mathbb{P}_\xi \rightarrow \mathbb{P}_n} \right] \sharp \mathbb{P}_\xi$. 
Figure 11: Maps between FashionMNIST classes through the learned barycenter. The 1st images in each $n$-th column shows a sample from $P_n$. The 2nd columns maps these samples to the barycenter. Each next column shows how the maps from the barycenter to the input classes $P_n$. 
Figure 12: The barycenter of Handbags, Shoes, Fruit (64 × 64) datasets fitted by our algorithm 1.
Wasserstein Iterative Networks for Barycenter Estimation

Figure 13: Maps between subsets of Ave, celeba! dataset through the barycenter learned by our algorithm 1.