Kantorovich Strikes Back!
Wasserstein GANs are not Optimal Transport?

Alexander Korotin
Skolkovo Institute of Science and Technology
Artificial Intelligence Research Institute
Moscow, Russia
a.korotin@skoltech.ru

Alexander Kolesov*
Skolkovo Institute of Science and Technology
Moscow, Russia
a.kolesov@skoltech.ru

Evgeny Burnaev
Skolkovo Institute of Science and Technology
Artificial Intelligence Research Institute
Moscow, Russia
e.burnaev@skoltech.ru

Abstract
Wasserstein Generative Adversarial Networks (WGANs) are the popular generative models built on the theory of Optimal Transport (OT) and the Kantorovich duality. Despite the success of WGANs, it is still unclear how well the underlying OT dual solvers approximate the OT cost (Wasserstein-1 distance, $W_1$) and the OT gradient needed to update the generator. In this paper, we address these questions. We construct 1-Lipschitz functions and use them to build ray monotone transport plans. This strategy yields pairs of continuous benchmark distributions with the analytically known OT plan, OT cost and OT gradient in high-dimensional spaces such as spaces of images. We thoroughly evaluate popular WGAN dual form solvers (gradient penalty, spectral normalization, entropic regularization, etc.) using these benchmark pairs. Even though these solvers perform well in WGANs, none of them faithfully compute $W_1$ in high dimensions. Nevertheless, many provide a meaningful approximation of the OT gradient. These observations suggest that these solvers should not be treated as good estimators of $W_1$, but to some extent they indeed can be used in variational problems requiring the minimization of $W_1$.

The Wasserstein-1 distance $W_1$ is a popular loss function to learn generative models. It has numerous advantages compared to the vanilla GAN loss $W_2$. For example, $W_1$ is correctly defined if the distributions’ supports differ [2]. Besides, it correlates with the sample quality, provides improved stability of the optimization process and does not suffer from the vanishing gradients issue [3, 84].

Generative models which employ $W_1$ as the loss to update the generator are called the Wasserstein GANs (WGANs). To compute $W_1$, they use its variational approximation based on the Kantorovich duality [20] and the Optimal Transport (OT) theory [52, 47]. Since the introduction of the original WGANs with the weight clipping method [3], a lot of alternative techniques (neural dual OT solvers) to compute $W_1$ have been proposed: gradient penalties [17, 39, 54], entropic regularization [46], architectural constraints [35, 15], batch-based methods [31, 29], maximin methods [38, 23], etc.

Despite the popularity of WGANs, it still remains unclear to what extent their success is connected to OT and $W_1$ rather than, e.g., to a good choice of regularization [49, 57]. Due to the limited amount of pairs of distributions with known $W_1$, it is challenging to evaluate existing dual OT solvers.

Contributions. We develop a generic methodology based on the transport rays ($M_3.1$) to evaluate dual OT solvers for the Wasserstein-1 distance ($W_1$). Our main contributions are as follows:

*Equal contribution.
• We use 1-Lipschitz functions to construct pairs of continuous distributions that we use as a benchmark with analytically-known OT cost, map and gradient for \( W_1 \) transport (§3.2 §3.3).

• We use these benchmark distributions to evaluate (§4) popular WGAN dual OT solvers (§2) in high-dimensional spaces, including the spaces of \( 32 \times 32 \) CIFAR-10 images, \( 64 \times 64 \) CelebA faces.

Related works \[32, 49\] consider discrete distributions and show that some solvers fail to estimate \( W_1 \). In contrast to them, we study how well the solvers compute the gradient in WGANs, not the value of \( W_1 \). We use continuous distributions since in the discrete case the OT gradient may be ill-defined (§1).

Notation. We work in the \( \mathbb{R}^D \) space that is endowed with the Euclidean norm \( \| \cdot \|_2 \). We use \( \mu_L \) to denote the Lebesgue measure on \( \mathbb{R}^D \). For a measurable map \( T : \mathbb{R}^D \rightarrow \mathbb{R}^D \), we denote the associated pushforward operator by \( T_* \). We consider Borel probability distributions \( P, Q \) on \( \mathbb{R}^D \) with finite first moments. We use \( \Pi(P, Q) \) to denote the set of probability distributions on \( \mathbb{R}^D \times \mathbb{R}^D \) with marginals \( P \) and \( Q \) (transport plans). All the integrals are computed over \( \mathbb{R}^D \), if not stated otherwise. We write \( \| f \|_L \leq C \) if \( f : \mathbb{R}^D \rightarrow \mathbb{R} \) is \( C \)-Lipschitz.

1 Background on Optimal Transport

Primal Formulation. For distributions \( P, Q \), the Monge’s formulation of the Wasserstein-1 (\( W_1 \)) distance, i.e., OT with the distance cost function \( \| x - y \|_2 \), is given by (Figure 1a)

\[
W_1(P, Q) \overset{def}{=} \min_{T \in \Pi(P, Q)} \int \| x - T(x) \|_2 dP(x),
\]

where min is taken over measurable functions \( T : \mathbb{R}^D \rightarrow \mathbb{R}^D \) (transport maps) that map \( P \) to \( Q \). The optimal \( T^* \) is called the \emph{optimal transport map} (OT map).

In accordance with \[52, Case 5.16\], dual form \[1\] can be further restricted to 1-Lipschitz functions. In this case, it holds \( f^c(y) = -f(y) \) \[52, Case 5.4\], and the alternative duality formula for \( W_1 \) is

\[
W_1(P, Q) = \max_{\| f \|_L \leq 1} \int f(x) dP(x) - \int f(y) dQ(y).
\]
Optimal transport in GANs. Derivatives of $W_1$ are used implicitly in generative modeling [3, 39, 35, 17, 48, 46, 48, 28] that incorporates $W_1$ loss, in which case $P = P_\alpha$ is a parametric distribution and $Q$ is the data distribution. Typically, $P_\alpha = G_\alpha S$ is the distribution generated from a fixed latent distribution $S$ by a generator network $G_\alpha$. The goal is to find parameters $\alpha$ that minimize $W_1(P_\alpha, Q)$ via gradient descent. The loss function for the generator is:

$$W_1(P_\alpha, Q) = \int_z f^\ast(G_\alpha(z)) dS(z) - \int f^\ast(y) dQ(y),$$

where $f^\ast$ is the optimal potential in [3]. The loss derivative (Figure 2) is given by [13] Eq. 3:

$$\frac{\partial W_1(P_\alpha, Q)}{\partial \alpha} = \int J_\alpha G_\alpha(z)^T \nabla f^\ast(G_\alpha(z)) dS(z),$$

where $J_\alpha G_\alpha(z)^T$ is the transpose of the Jacobian matrix of $G_\alpha(z)$ w.r.t. parameters $\alpha$. This result still holds without assuming the potentials are fixed [3] Theorem 3] by the envelope theorem [33].

In practice, the optimal potential $f^\ast$ is unknown. Therefore, WGANs approximate it with a network $f_1 : \mathbb{R}^D \rightarrow \mathbb{R}$ (potential) by maximizing [3, 17] or [3] via the stochastic gradient ascent (SGA). This is usually associated with evaluating the $W_1$ loss. However, note that the loss value plays no role in generator updates. Only the gradient $\nabla f^\ast$ of the potential is needed. We call it the OT gradient. We use a generic phrase OT solver to refer to any algorithm which is capable of recovering $\nabla f^\ast$.

Quantitative evaluation of OT solvers. Existing solvers are typically tested as the loss in WGANs without evaluating the actual OT performance. The quality of the generated samples is evaluated by $J$-quality or $J$-divergence.

In [41, 42, 49], the authors use discrete $P, Q$ to show that some solvers imprecisely compute $W_1$. Their approach is not applicable to evaluation of the OT gradient, as $\nabla f^\ast$ is ill-defined in the discrete case. For example, when $P = \delta_0, Q = \delta_1$, it holds that $f^\ast = [x]_+$ is an optimal potential, but it is not even differentiable at $x = 0 = \text{Supp}(P)$. The existence of the OT gradient is studied, e.g., in [19].

2 Neural Dual Solvers for the Wasserstein-1 Distance

Our proposed benchmark is useful for testing any OT solver that computes $\nabla f^\ast$ or $W_1$. We evaluate only neural solvers which are based on [5, 41] or [17] and used in WGANs. We provide an overview of these methods below. We group them by the dual formulations which they use.

Most solvers approximate the potential by a network $f_0 : \mathbb{R}^D \rightarrow \mathbb{R}$ and learn it via maximizing [5] with SGA on batches from $P$, $Q$. The main challenge is to enforce the $1$-Lipschitz constraint for $f_0$.

| WC | In [3], the space $\Theta$ of parameters is restricted to a compact, e.g., to a hypercube $[-c, c]^{\dim \theta}$. With mild assumptions on the architecture, $f_0$ is provably Lipschitz continuous with some unknown constant $C$, i.e., $\|f_0\|_L \leq C$. The main practical issue is tuning the boundary $c$ of the set.

| GP | The authors of [17] prove that with mild assumptions on the OT plan $\pi^\ast$, the equation $\|\nabla f^\ast(z)\|_2 = 1$ holds almost surely for $z = tx + (1-t)y$ with $(x, y)$ distributed as the OT plan $\pi^\ast$ and $t \sim \text{Uniform}[0, 1]$. Thus, they softly penalize $f$ for being not $1$-Lipschitz and optimize

$$W_1(P, Q) \approx \max_f \left\{ \int f(x) dP(x) - \int f(y) dQ(y) - \lambda R(f) \right\}, \quad \lambda > 0. \quad (6)$$

The gradient penalty $R_{GP}(f)$ equals $\int (\|\nabla f(r)\|_2 - 1)^2 d\mu(r)$, where $\mu$ is the distribution of a random variable $r = xt + (1-t)y$ with $t \sim \text{Uniform}[0, 1]$ and $(x, y) \sim P \times Q$ (as $\pi^\ast$ is unknown). In [34], it is proved that (6) with $R = R_{GP}$ is a specific OT formulation called congested OT.

| LP | In [39], the authors show that $R_{GP}(f)$ suffers from instabilities and high magnitudes. They introduce the Lipschitz penalty $R_{LP}(f) = \int (\max(0, \|\nabla f(r)\|_2 - 1))^2 d\mu(r)$ resolving the issues.
where the minimization is performed over functions $R$ weight matrices of linear layers of net $f_\theta$ by their spectral norms. This provably makes $f$ globally Lipschitz continuous, which does not hold for \cite{17, 39} which are based on the soft penalization \cite{6}.

[SOL] The authors of \cite{1} claim that spectral normalization negatively affects the expressiveness of the network. They propose to ortho-normalize weight matrices and use GroupSort activations \cite{5}. Such networks $f_\theta$ are $1$-Lipschitz and universally approximate $1$-Lipschitz functions \cite{11} \S 4.

Below we overview methods based on \cite{47} or \cite{4} which do not require enforcing $1$-Lipschitz continuity for the potential. Unlike the above-mentioned methods, they mostly require $2$ neural networks.

[LS] In \cite{46, 48, 12, 6}, the authors optimize the following \textit{unconstrained} regularized form \cite{5}:

\begin{equation}
\mathcal{W}_1(\mathbb{P}, \mathbb{Q}) \approx \max_{f,g} \left\{ \int f(x)d\mathbb{P}(x) + \int g(y)d\mathbb{Q}(y) - \mathcal{R}(f, g) \right\},
\end{equation}

where $\mathcal{R}(f, g)$ is the \textit{entropic} or \textit{quadratic} regularizer \cite{46} Eq.5 which softly penalizes the potentials $f, g$ for disobeying $f \odot g \leq \| \cdot \|_2$. In practice, $f, g$ are neural networks $f_\theta, g_\omega : \mathbb{R}^D \rightarrow \mathbb{R}$.

[MM:B] The authors of \cite{31, 32} expand the dual formulation \cite{4} with the c-transform:

\begin{equation}
\mathcal{W}_1(\mathbb{P}, \mathbb{Q}) = \max_f \left\{ \int f(x)d\mathbb{P}(x) + \int \min_{x \in \mathbb{R}^D} [\|x - y\|_2 - f(y)]d\mathbb{Q}(y) \right\}.
\end{equation}

During optimization, they restrict the inner minimization to the current mini-batch from $\mathbb{P}$. This leads to \textit{overestimation} of the inner problem’s solution since the minimum is taken over a restricted subset. Recently, a more tricky version of this approach appeared \cite{27} \S 3. We call it \[\text{MM:Bv2}].

[MM] In \cite{38}, the authors use a saddle point formulation equivalent to \cite{8}:

\begin{equation}
\mathcal{W}_1(\mathbb{P}, \mathbb{Q}) = \max_f \int f(x)d\mathbb{P}(x) + \min_H \int [\|H(y) - y\|_2 - f(H(y))]d\mathbb{Q}(y),
\end{equation}

where the minimization is performed over functions $H : \mathbb{R}^D \rightarrow \mathbb{R}^D$. The authors use neural networks $f_\theta$ and $H_\omega$ to parametrize the potential and the minimizer of the inner problem (\textit{mover}). To train $\theta, \omega$, the authors apply stochastic gradient ascent/descent (SGAD) over mini-batches from $\mathbb{P}, \mathbb{Q}$.

[MM:R] One may also recover the OT gradient $\nabla f^*$ from the OT map $T^*$. Consider the form

\begin{equation}
\mathcal{W}_1(\mathbb{P}, \mathbb{Q}) = \max_g \min_T \int [\|T(x) - x\|_2 - g(T(x))]d\mathbb{P}(x) + \int g(y)d\mathbb{Q}(y),
\end{equation}

which is a \textit{reversed} \cite{23} version of \cite{8}, i.e., the roles of $\mathbb{P}, \mathbb{Q}$ are swapped and $T : \mathbb{R}^D \rightarrow \mathbb{R}^D$. For \textit{some} optimal saddle points $(g^*, T^*)$ of \cite{10} it holds that mover $T^*$ is an OT map \cite{25} Lemma 4, \cite{11} Lemma 2], \cite{50, 8}. With mild assumptions on $\mathbb{P}, \mathbb{Q}$, one may recover $T^*$ and use the identity $\nabla f^*(x) = \frac{x - T^*(x)}{\|x - T^*(x)\|_2}$ \cite{7} \S 1] to obtain the OT gradient from $T^*$.

3 \ Constructing Benchmark Distributions for Dual Solvers

In this section, we develop a generic methodology to construct pairs $(\mathbb{P}, \mathbb{Q})$ with computable ground truth OT plan, OT cost and OT gradient. Our approach is inspired by the insights about OT plans in \cite{47} \S 3.1, \cite{10], \cite{7} \S 3-7]. In \cite{47} we give the required preliminaries. In \cite{3.2} we provide our method to build benchmark pairs. We construct them in \S 3.3. The proofs are given in Appendix A.

3.1 \ Ray Monotone Transport Plans and 1-Lipschitz Functions

Let $u : \mathbb{R}^D \rightarrow \mathbb{R}$ be a $1$-Lipschitz function. Recall that due to the Rademacher’s theorem, $u$ is differentiable $\mu_L$-almost everywhere. For every $x, y \in \mathbb{R}^D$ satisfying $u(x) - u(y) = \|x - y\|_2$ it holds that $u$ is affine on the segment $[x, y]$, i.e., $u(z) = tu(x) + (1 - t)u(y)$ for $z = tx + (1 - t)y$ with $t \in [0, 1]$ \cite{47} Lemma 3.5. Moreover, $u$ is differentiable at all $z \in (x, y)$ and $\nabla u(z) = \frac{x - y}{\|x - y\|_2}$ \cite{47} Lemma 3.6]. Following \cite{47} Definition 3.7], we call a transport ray any non-trivial (different from a singleton) segment $[x, y]$ such that $u(x) - u(y) = \|x - y\|_2$, which is maximal for the inclusion among segments of this form. The unit vector $\frac{x - y}{\|x - y\|_2}$ is called the direction of a transport ray. Two transport rays can only intersect at their boundary points \cite{46} Corollary 3.8]. In general, not all points
belong to transport rays. For example, for the function \( u(x) = \frac{1}{2}x \) there are no transport rays at all. In Figures 3c and 4, we provide examples of transport rays for 1-Lipschitz functions \( u \) in \( D = 2 \).

For a 1-Lipschitz function \( u : \mathbb{R}^D \to \mathbb{R} \), we say that a transport plan \( \pi \in \Pi(P, Q) \) is \( u \)-ray monotone (decreasing) if \( u(x) - u(y) = \| x - y \|_2 \) holds \( \pi \)-almost surely for \( x, y \in \mathbb{R}^D \). The idea of the definition is that such plans distribute the probability mass of \( x \sim P \) among \( y \in \mathbb{R}^D \) such that \( y = x \) (no mass movement) and/or \( y \) which lie on the same transport ray as \( x \) but below \( x \), i.e., \( u(y) < u(x) \).

**Proposition 1 (Ray monotone transport plans are optimal).** Let \( \pi \in \Pi(P, Q) \) be a \( u \)-ray monotone transport plan for a 1-Lipschitz function \( u \). Then it is an optimal plan between \( P \) and \( Q \). Besides, \( u \) is an optimal potential, i.e., it attains the maximum in dual formulation (4).

For a distribution \( P \), we say that distribution \( Q \) is a \( u \)-ray-forward of \( P \) if there exists a measurable function \( T : \mathbb{R}^D \to \mathbb{R}^D \) satisfying \( T^* P = Q \) and \( u(x) - u(T(x)) = \| x - T(x) \|_2 \) holds \( P \)-almost surely for all \( x \in \mathbb{R}^D \). We say that such a \( T \) is a \( u \)-ray-monotone transport map from \( P \) to \( Q \). Note that the deterministic plan \( \pi = [\text{id}_{\mathbb{R}^D}, T]^* \) is \( u \)-ray monotone. We have the following corollary:

**Corollary 1 (Ray monotone transport maps are optimal).** Let \( T \) be a \( u \)-ray-monotone transport map from \( P \) to \( Q \). Then the plan \( \pi = [\text{id}_{\mathbb{R}^D}, T]^* \) is optimal and \( T \) is an OT map from \( P \) to \( Q \).

In Figures 3b and 4, below, we derive our recipe to construct benchmark pairs \((P, Q)\) such that \( Q \) is a \( u \)-ray-forward of \( P \) with user-defined \( u \) and analytically known \( T \). In such pairs \( P \) is accessible by samples and is also possible to sample from \( Q \) by pushing \( x \sim P \) forward by \( T \). Since \( T \) is an OT map, the ground truth OT cost is \( W_1(P, Q) = \int \| x - T(x) \|_2 dP(x) \). It admits unbiased Monte Carlo estimates from samples \( x \sim P \). Moreover, with mild assumptions (5), \( \nabla u \) is the unique OT gradient. Our benchmark pairs can be used to test how well OT solvers recover \( W_1 \) and the OT gradient.

### 3.2 Method to Construct Benchmark Pairs

Let \( u \) be a known 1-Lipschitz function. We aim to find its transport rays and construct a \( u \)-ray-forward map \( T \) and distribution \( Q = T^* P \) (for a given \( P \)) for testing dual OT solvers. First, we describe the parametric class of 1-Lipschitz functions \( u \) which we employ in our benchmark. Second, we explain how to compute the transport rays of \( u \). Finally, we explain how to define \( u \)-ray monotone maps.

**Part 1. Parameterizing 1-Lipschitz functions.** Inspired by the distance representation of optimal potentials [16], as \( u : \mathbb{R}^D \to \mathbb{R} \), we employ the following 1-Lipschitz MinFunnel functions:

\[
u(x) \overset{\text{def}}{=} \min_n \{ u_n(x) \} = \min_n \{ \| x - a_n \|_2 + b_n \}, \tag{11}\]

where \( a_n \in \mathbb{R}^D \) and \( b_n \in \mathbb{R} \) are the parameters. Each funnel \( u_n(x) = \| x - a_n \|_2 + b_n \) has \( \| \nabla u_n(x) \|_2 = 1 \) when \( x \neq a_n \). Thus, \( u \) is also 1-Lipschitz as it is their minimum. Note that for \( \mu_1 \)-almost every \( x \) it holds that \( u \) is differentiable at \( x \) and \( \| \nabla u(x) \|_2 = 1 \).

**Proposition 2 (MinFunnels are universal approximators of 1-Lipschitz functions on compact sets).** Let \( S \subset \mathbb{R}^D \) be a compact set and \( f^* : S \to \mathbb{R} \) be a 1-Lipschitz function. Then for every \( \epsilon > 0 \) there exists \( N \) and \( \{a_n, b_n\}_{n=1}^N \) such that function (\( f^* \)) satisfies \( \sup_{x \in S} | u(x) - f^*(x) | \leq \epsilon \).
We use our methodology (3.3) to construct high-dimensional (\(D = 2, 3^2, \ldots, 7^2\)) benchmark pairs and benchmark pairs on the space of 64 \times 64 RGB images of celebrity faces (\(D = 12288\)).

For convenience, we use absolutely continuous \(\mathbb{P}\) supported on a hypercube \(\mathcal{S} = [-B, B]^{D} \subset \mathbb{R}^{D}\). In particular, for points \(x \in \mathcal{S}\), we consider transport rays truncated to \(\mathcal{S}\), i.e., \(\text{ray}(x) \cap \mathcal{S}\). We
construct the \( u \)-ray monotone map \( T : \mathbb{R}^D \to \mathbb{R}^D \) by the following principle. Let \([x_0, x_1] \subseteq S\) be the truncated transport ray of \( u \) for \( x \in S\). We pick a parameter \( p > 1 \) and define the map \( T \) as follows:

\[
T(x) \overset{def}{=} \left( \frac{\|x - x_0\|_2}{\|x_0 - x_1\|_2} \right)^p x_0 + \left( 1 - \left( \frac{\|x - x_0\|_2}{\|x_0 - x_1\|_2} \right)^p \right) x_1.
\]

This is a power function, i.e., if a ray is parametrized as \([0, 1]\), it moves the mass along the ray by \( t \mapsto t^p \). Since \( \mathbb{P} \)-almost all the points in \( S \) belong to (truncated) rays, we have \( T(x) \neq x \) on \( S \).

**High-dimensional benchmark pairs.** In dimensions \( D = 2, 2^2, \ldots, 2^7 \), we put \( \mathbb{P} \) to be the standard uniform distribution on \( \mathcal{S} = [-2.5, 2.5]^D \). In each dimension \( D \), we consider \( N = 4, 16, 64, 256 \) funnels and pick random parameters \( a_n \sim \text{Uniform}([-2.5, 2.5]^D) \) and \( b_n \sim \mathcal{N}(0, 1) \). For this initialization of \( a_n, b_n \), the assumptions of Proposition \( \ref{prop:ray_existence} \) hold with probability 1. The random seed is hardcoded. We use \( p = 8 \). For the case \( D = 2, N = 4 \), we visualize the input distribution \( \mathbb{P} \), the function \( u \), the constructed map \( T \) and the output distribution \( \mathbb{Q} = T\mathbb{P} \) in Figure \( \ref{fig:high_dim_benchmark} \). We show examples of constructed \((\mathbb{P}, \mathbb{Q})\) for higher dimensions in Figure \( \ref{fig:high_dim_benchmark} \).

**Images benchmark pairs** for CIFAR-10 and Celeba. As \( \mathbb{P} \) we consider the synthetic distributions of generated \( 32 \times 32 \) RGB images \((D = 3072)\) and \( 64 \times 64 \) RGB images \((D = 12288)\). To generate these images, we use the WGAN-QC \( \cite{28} \) generator model trained on CIFAR-10 \( \cite{26} \) and Celeba \( \cite{30} \) datasets, respectively. For CIFAR-10, we train WGAN-QC by using its publicly available code\( \cite{28} \). For Celeba, we pick a readily available pre-trained generator from the related Wasserstein-2 benchmark\( \cite{23} \) \( \S 4.1 \). To make \( \mathbb{P} \) absolutely continuous, we add the Gaussian noise with axis-wise \( \sigma = 0.01 \). Then we truncate the distribution to \( \mathcal{S} = [-1.1, 1.1]^D \), i.e., we reject samples which are out of \( \mathcal{S} \). We construct two benchmark pairs per each dataset (Figures \( \ref{fig:celeba_benchmark} \)\( \ref{fig:high_dim_benchmark} \)) with \((N, p) = (1, 10), (16, 100)\) and \( a_n \sim \text{Uniform}([-1.1, 1.1]^D) \), \( b_n \sim \mathcal{N}(0, 0.1) \).

In both high-dimensional and images pairs \((\mathbb{P}, \mathbb{Q})\), the input \( \mathbb{P} \) is an absolutely continuous distribution supported on a hypercube \( S \). By the design, the distribution \( \mathbb{P} \) is accessible by random samples. To sample from \( \mathbb{Q} \), we first sample \( x \sim \mathbb{P} \), then compute its transport ray (Proposition \( \ref{prop:ray_existence} \)), truncate it to \( S \), and produce \( y = T(x) \sim \mathbb{Q} \) by \( \overset{def}{=} \left( \frac{\|x - x_0\|_2}{\|x_0 - x_1\|_2} \right)^p x_0 + \left( 1 - \left( \frac{\|x - x_0\|_2}{\|x_0 - x_1\|_2} \right)^p \right) x_1 \). The sampler for \( \mathbb{Q} \) outputs only \( y \), i.e., information about \( u, T, x \) is hidden from the user and employed only when estimating the ground truth \( \mathbb{W}_1(\mathbb{P}, \mathbb{Q}) \) or \( \nabla u \).

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https://github.com/harryliew/WGAN-QC
https://github.com/iamalexkorotin/Wasserstein2Benchmark
Reversed pairs. Doing preliminary tests, we found that for solvers it is more challenging to compute the OT gradient for pair \((Q, P)\) rather than \((P, Q)\). In particular, in our images benchmark, the pair \((Q, P)\) reflects the practical WGAN scenario better. Indeed, in WGANs, the solvers move the generated distribution (bad images, \(Q\) in our construction) to the real distribution (good images, \(P\)). Recall that \(Q = T_\#P\), where \(T\) is a differentiable bijection \((\ref{er:prob})\) along the (truncated) transport rays of a MinFunnel \(u\). As a result, \(Q\) is absolutely continuous and the OT gradient for the reverse \((Q, P)\) is \(Q\)-unique (Proposition \((\ref{er:unique})\)). For this pair, the optimal potential is \(-u\) and its gradient is \(-\nabla u\). To conclude, in all the experiments, we feed the reverse pair \((P, Q) \defeq (Q, P)\) to OT solvers in view.

4 Evaluation of Dual Solvers and Discussion

In this section, we evaluate WGAN dual OT solvers \((\S\ref{er:eval})\) on our constructed benchmark \((\S\ref{er:benchmark})\). Technical details of the implementation are given in Appendix \((\ref{er:implementation})\). The code is written in PyTorch framework and is publicly available together with all the constructed benchmark distributions at https://github.com/justkolesov/Wasserstein1Benchmark.

Metrics. For \(\mathcal{W}_1\), we do not use any specific metric but simply report obtained \(\mathcal{W}_1\) and the ground truth \(\mathcal{W}_1\). To quantify the recovered gradient \(\nabla \hat{f}\), we use \(L^2\) and cosine similarity metrics \((\S\ref{er:cos})\):

\[
L^2(\nabla \hat{f}, \nabla f^*) \defeq \|\nabla \hat{f} - \nabla f^*\|_2^2, \quad \cos(\nabla \hat{f}, \nabla f^*) \defeq \frac{\langle \nabla \hat{f}, \nabla f^* \rangle_{L^2}}{\|\nabla \hat{f}\|_2 \cdot \|\nabla f^*\|_2}, \tag{13}
\]

where \(\langle \nabla f_1, \nabla f_2 \rangle_{L^2} \defeq \int (\nabla f_1(x), \nabla f_2(x))dP(x)\), \(\|\nabla f\|_2^2 \defeq \langle \nabla f_1, \nabla f_2 \rangle_{L^2}\) and \(\nabla f^*\) is the ground truth OT gradient. The \(L^2\) metric compares the gradients \(\nabla \hat{f}, \nabla f^*\) as elements of the space \(L^2(\mathcal{P})\) of quadratically integrable w.r.t. \(\mathcal{P}\) functions. The cosine compares their directions regardless of the magnitude (Figure \((\ref{er:cos})\)). To estimate the metrics, we use 213 samples \(x \sim \mathcal{P}\).

[DOT] For completeness, we add the empirical (batched) OT \((\S\ref{er:eval})\) to evaluation. For batches \(X \sim \mathcal{P}, Y \sim \mathcal{Q}\), we use \(\mathcal{W}_1(X, Y)\) computed by a discrete solver as an estimate of \(\mathcal{W}_1(P, Q)\). The solver can be combined with the automatic differentiation to approximate \(\nabla f^*\) on the batch \(X\).

High-dimensional pairs. We test the solvers and report the estimated \(\mathcal{W}_1\) value and metrics \((\S\ref{er:cos})\) in Tables \((\S\ref{er:eval})\). We use fully-connected nets as potentials \(f_\theta, q_\omega\) and movers \(T_\theta, H_L\) (in the maxmin solvers). In Figure \((\ref{er:W1})\), we show the potentials learned by solvers for \(D = 2, N = 4\).
with GroupSort and orthonormalization. We use DCGAN [42] as potentials θ.

As Table 11 shows, all the solvers randomly over/underestimate W1, typically with notable error. Consequently, none of the solvers can be viewed as precise estimators of the OT cost. Thus, our discussion below primarily focuses on the estimation of the OT gradient needed in WGANs.

Figure 7: Surfaces of potentials fθ learned by OT solvers on the pair with D = 2, N = N.

For [MM:R] we plot (minus) second potential −gω as the solver does not compute the first one. The ground truth optimal potential is in Figure 3b.

As Table[1] shows, all the solvers randomly over/underestimate W1, typically with notable error. Consequently, none of the solvers can be viewed as precise estimators of the OT cost. Thus, our discussion below primarily focuses on the estimation of the OT gradient needed in WGANs.

Original [WC] leads to a pathological value surface of the learned potential (Figure 7a), which is far from the ground truth. This agrees with the claims of [17] §3. Despite this, even in high dimensions the cos metric is positive (Table 9a), i.e., the recovered gradient correlates with the OT gradient. Popular [GP] notably improves upon [WC] and provides higher cos values (Table 9b). According to the results, its modification [LP] does not provide any major improvement (Table 9c).

Surprisingly, [SO] performs worse than [GP] and is comparable to [WC] in cos metric (Table 9d). We presume that this happens since the spectral norm negatively affects the expressive power of the neural net. Even when D = 2 (Figure 7f), [SN] fails to recover the optimal potential. [SO] replaces spectral norm with orthogonalization and uses GroupSort activations which improve performance. The solver scores higher cos values (Table 9e) which are comparable to [GP].

Solvers [LS] recovers biased potential since (7) is the duality formula for regularized OT which yields biased optimal potentials (Table 9f). The bias is huge for large D, N when the benchmark pairs are complex. This is analogous to results for the same solver in the Wasserstein-2 (W2) benchmark [23].

Batch-based [MM:B] suffers from the bias in high dimensions (Table 9g) due to the overestimation of the value of the inner problem in (8). Note that cos metric values are even negative in high dimensions. The same is reported in the W2 benchmark [23]. [MM:Bv2] uses a more tricky optimization scheme and yields high cos values (Table 9h). It captures the direction of the OT gradient but extremely overestimates its magnitude, see high values of L2 in Table 10h.

Maximin solvers [MM], [MM:R] perform comparably to [GP], [SO], [LP], see Tables 9i, 9j. However, their training takes longer and sometimes diverges as it solves a saddle point problem. This agrees with the W2 benchmark [23] §4.3. Using these solvers in GANs is not easy as it yields a challenging min-max-min optimization problem. Importantly, [MM:R] recovers the OT map which can itself be used as a generative model (outside the context of GANs) in computer vision tasks. Here we refer the reader to the recent neural optimal transport (N OT) methods [25] 24 22 21 44 8.

Empirical [DOT] provides precise estimates of W1 (Table 11k) and the OT gradient (Table 9k) only in small dimensions. In high dimensions, it intolerably overestimates W1; its gradient is almost orthogonal to the ground truth (cos ≲ 0). This is due to the exponential (in D) sample complexity of DOT [53]. Thus, (unregularized) DOT is an imprecise estimator of W1 or the OT gradient in high D.

Images pairs. Here we do not consider [SO] as its authors do not provide convolutional architectures with GroupSort and orthonormalization. We use DCGAN [42] as potentials fθ, gω. In [MM] and [MM:R], the movers Tθ, Hω are UNets [43]. The evaluation results on Celeba benchmark pairs are given in Tables 6, 7, 8 and on CIFAR-10 benchmark pairs – in Tables 5, 6, 9, Appendix C.
Table 1: The summary of WGAN dual OT solvers’ performance in $\cos$, $L^2$ and $W_1$ metrics on our high-dimensional (HD) and images (IMG) benchmark pairs. For details, see Appendix C.

| Method | HD $\cos$ | HD $L^2$ | HD $W_1$ | IMG $\cos$ | IMG $L^2$ | IMG $W_1$ |
|--------|-----------|-----------|----------|-------------|-----------|----------|
| WC     | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ |
| GP     | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ |
| LP     | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ |
| SN     | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ |
| SO     | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ |
| LS     | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ |
| MM:B   | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ |
| MM:Bv2 | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ |
| MM:R   | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ |
| DOT    | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ | $\mathbf{\circ}$ |

Surprisingly, our images benchmark pairs turned to be simpler than some high-dimensional benchmark pairs. Although $(P, Q)$ are absolutely continuous and supported on $[-1, 1]$, their actual probability mass is still concentrated around small low-dimensional sub-manifold of data. We suppose that this is one of the causes for the reasonable performance of most solvers. In particular, we see that even [DOT], [LS], [MM:B] score $\cos > 0$ in images benchmark pairs, although they struggled to produce good results on high-dimensional pairs.

Solvers [GP], [LP], [MM:R] provide very high $\cos > 0.9$ (Table 6). However, only [MM:R] provides precise approximation of $\nabla f^*$ in $L^2$ norm (Table 7). Interestingly, maximin [MM] diverges on our images benchmark pairs (tuning the hyper-parameters did not help). Similar to the evaluation in high-dimensional pairs, [WC] and [SN] show moderate $\cos > 0$, but its value is notably smaller than that of the top-performing methods. Solver [MM:Bv2] demonstrates meaningful estimate of $W_1$ (Table 8). Nevertheless, its recovered gradient is almost orthogonal to the ground truth ($\cos \approx 0$, see Table 6), and the values of $L^2$ metric are extremely high (Table 7).

5 Discussion

Our methodology creates pairs of continuous distributions with known ground truth OT cost and gradient, filling the missing gap of benchmarking $W_1$ dual solvers. This development allows us to evaluate the OT performance of WGAN dual methods. The experimental results are summarized in Table 1. Our evaluation shows that these solvers should not be considered as meaningful estimators of $W_1$ as they exhibit large error. However, the OT gradient recovered by these solvers shows positive $\cos$ with ground truth. This suggests that most methods could still be used to minimize $W_1$ in variational problems, e.g., Wasserstein GANs.

Computational complexity. Evaluation of all the OT solvers on our high-dimensional and images benchmark pairs takes less than 50 hours on a single GPU GTX 1080ti (11 GB VRAM).

Potential Impact. Our benchmark distributions can be used to evaluate future dual OT solvers in high-dimensional spaces, a crucial step to improve the transparency and replicability of OT and WGAN-related research. We expect our benchmark to become a standard benchmark for $W_1$ optimal transport as part of the ongoing effort of advancing computational OT.

Limitations (benchmark). We rely on MinFunnels as optimal Kantorovich potentials to generate benchmark pairs. Also, we limit our pairs to be absolutely continuous distributions. It is unclear whether our benchmark sufficiently reflects the real-world scenarios in which the WGAN solvers are used. Nevertheless, our methodology is generic and can be used to construct new benchmark pairs.

Limitations (evaluation). We evaluate how well the OT solvers compute OT cost and gradient but do not assess their performance in GAN settings. Studying this question is a promising future research avenue which could help to develop new OT-based methods for generative modeling.

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   (a) Do the main claims made in the abstract and introduction accurately reflect the paper’s contributions and scope?  
      [Yes]
   
   (b) Did you describe the limitations of your work?  
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