

Generalized Sliced Wasserstein Distances

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Abstract

The Wasserstein distance and its variations, e.g., the sliced-Wasserstein (SW) distance, have recently drawn attention from the machine learning community. The SW distance, specifically, was shown to have similar properties to the Wasserstein distance, while being much simpler to compute, and is therefore used in various applications including generative modeling and general supervised/unsupervised learning. In this paper, we first clarify the mathematical connection between the SW distance and the Radon transform. We then utilize the generalized Radon transform to define a new family of distances for probability measures, which we call generalized sliced-Wasserstein (GSW) distances. We also show that, similar to the SW distance, the GSW distance can be extended to a maximum GSW (max-GSW) distance. We then provide the conditions under which GSW and max-GSW distances are indeed distances. Finally, we compare the numerical performance of the proposed distances on several generative modeling tasks, including SW flows and SW auto-encoders.

背景：OT理论，评估一个概率分布转换为另一个概率分布的最小代价，计算两个分布之间的相似程度

1. Introduction

The Wasserstein distance has its roots in optimal transport (OT) theory (Villani, 2008) and forms a metric between two probability measures. It has attracted abundant attention in data sciences and machine learning due to its convenient theoretical properties and applications on many domains (Solomon et al., 2014; Frogner et al., 2015; Montavon et al., 2016; Kolouri et al., 2017; Courty et al., 2017; Peyré & Cuturi, 2018; Schmitz et al., 2018), especially in implicit generative modeling such as OT-based generative adversarial networks (GANs) and variational auto-encoders (Arjovsky et al., 2017; Bousquet et al., 2017; Gulrajani et al., 2017; Tolstikhin et al., 2018).

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While OT brings new perspectives and principled ways to formalize problems, the OT-based methods usually suffer from high computational complexity. The Wasserstein distance is often the computational bottleneck and it turns out that evaluating it between multi-dimensional measures is numerically intractable in general. This important computational burden is a major limiting factor in the application of OT distances to large-scale data analysis. Recently, several numerical methods have been proposed to speed-up the evaluation of the Wasserstein distance. For instance, entropic regularization techniques (Cuturi, 2013; Cuturi & Peyré, 2015; Solomon et al., 2015) provide a fast approximation to the Wasserstein distance by regularizing the original OT problem with an entropy term. The linear OT approach, (Wang et al., 2013; Kolouri et al., 2016a) further simplifies this computation for a given dataset by a linear approximation of pairwise distances with a functional defined on distances to a reference measure. Other notable contributions towards computational methods for OT include multi-scale and sparse approximation approaches (Oberman & Ruan, 2015; Schmitz, 2016), and Newton-based schemes for semi-discrete OT (Lévy, 2015; Kitagawa et al., 2016).

There are some special favorable cases where solving the OT problem is easy and reasonably cheap. In particular, the Wasserstein distance for one-dimensional probability densities has a closed-form formula that can be efficiently approximated. This nice property motivates the use of the sliced-Wasserstein distance (Bonneel et al., 2015), an alternative OT distance obtained by computing infinitely many linear projections of the high-dimensional distribution to one-dimensional distributions and then computing the average of the Wasserstein distance between these one-dimensional representations. While having similar theoretical properties (Bonneel, 2013), the sliced-Wasserstein distance has significantly lower computational requirements than the classical Wasserstein distance. Therefore, it has recently attracted ample attention and successfully been applied to a variety of practical tasks (Bonneel et al., 2015; Kolouri et al., 2016b; Carriere et al., 2017; Karras et al., 2017; Şimşekli et al., 2018; Deshpande et al., 2018; Kolouri et al., 2018; 2019).

As we will detail in the next sections, the linear projection process used in the sliced-Wasserstein distance is closely related to the Radon transform, which is widely used in tomography (Radon, 1917; Helgason, 2011). In other words,

the sliced-Wasserstein distance is calculated via linear slicing of the probability distributions. However, the linear nature of these projections does not guarantee an efficient evaluation of the sliced-Wasserstein distance: in high-dimensional settings, the data often lives in a thin manifold and the number of randomly chosen linear projections required to capture the structure of the data distribution grows very quickly (Şimşekli et al., 2018). Reducing the number of required projections would thus result in a significant performance improvement in sliced-Wasserstein computations.

Contributions. In this paper, we address the aforementioned computational issues of the sliced-Wasserstein distance and for the first time, we extend the linear slicing to *non-linear* slicing of probability measures. Our main contributions are summarized as follows:

- Using the mathematics of the generalized Radon transform (Beylkin, 1984) we extend the definition of the sliced-Wasserstein distance to an entire class of distances, which we call the **generalized sliced-Wasserstein (GSW) distance**. We prove that replacing the linear projections with polynomial projections will still yield a valid distance metric and we then **identify general conditions under which the GSW distance is a distance function**.
- We then show that, instead of using infinitely many projections as required by the GSW distance, we can still **capture a valid distance metric by using a single projection**, as long as the **projection gives the maximal distance in the projected space**. We aptly call this distance the max-GSW distance. The max-GSW distance vastly reduces the computational cost induced by the projection operations; however, it comes with an additional cost since it requires optimization over the space of projectors.
- Due to their inherent non-linearity, the GSW and max-GSW distances are expected to **capture the complex structure of high-dimensional distributions by using much less projections**, which will reduce the overall computational burden in a significant amount. We verify this fact in our experiments, where we illustrate the superior performance of the proposed distances in both synthetic and real-data settings.

2. Background

We review in this section the preliminary concepts and formulations needed to develop our framework, namely the p -Wasserstein distance, the Radon transform, the sliced p -Wasserstein distance and the maximum sliced p -Wasserstein distance. In what follows, we denote by $P_p(\Omega)$ the set of Borel probability measures with finite p 'th moment defined on a given metric space (Ω, d) and by $\mu \in P_p(X)$ and $\nu \in P_p(Y)$ probability measures defined on $X, Y \subseteq \Omega$ with corresponding probability density functions I_μ and I_ν , i.e. $d\mu(x) = I_\mu(x)dx$ and $d\nu(y) = I_\nu(y)dy$.

2.1. Wasserstein Distance

The p -Wasserstein distance, $p \in [1, \infty)$, between μ and ν is defined as the solution of the optimal mass transportation problem (Villani, 2008):

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

where $d^p(\cdot, \cdot)$ is the cost function, and $\Gamma(\mu, \nu)$ is the set of all transportation plans $\gamma \in \Gamma(\mu, \nu)$ such that:

就是分布之间的距离吗？

$$\begin{aligned} \gamma(A \times Y) &= \mu(A) && \text{for any Borel subset } A \subseteq X \\ \gamma(X \times B) &= \nu(B) && \text{for any Borel subset } B \subseteq Y \end{aligned}$$

Due to Brenier's theorem (Brenier, 1991), for absolutely continuous probability measures μ and ν (with respect to the Lebesgue measure), the p -Wasserstein distance can be equivalently obtained from

$$W_p(\mu, \nu) = \left(\inf_{f \in MP(\mu, \nu)} \int_X d^p(x, f(x)) d\mu(x) \right)^{\frac{1}{p}} \quad (2)$$

where $MP(\mu, \nu) = \{f : X \rightarrow Y \mid f_\# \mu = \nu\}$ and $f_\# \mu$ represents the pushforward of measure μ , characterized as

$$\int_A df_\# \mu(y) = \int_{f^{-1}(A)} d\mu(x) \text{ for any Borel subset } A \subseteq Y.$$

Note that in most engineering and computer science applications, Ω is a compact subset of \mathbb{R}^d and $d(x, y) = |x - y|$ is the Euclidean distance. By abuse of notation, we will use $W_p(\mu, \nu)$ and $W_p(I_\mu, I_\nu)$ interchangeably.

One-dimensional distributions: The case of one-dimensional continuous probability measures is specifically interesting as the p -Wasserstein distance has a **closed-form solution**. More precisely, for one-dimensional probability measures, there **exists a unique monotonically increasing transport map that pushes one measure to another**. Let $F_\mu(x) = \mu((-\infty, x]) = \int_{-\infty}^x I_\mu(\tau) d\tau$ be the cumulative distribution function (CDF) for I_μ and define F_ν to be the CDF of I_ν . The optimal transport map is then uniquely defined as $f(x) = F_\nu^{-1}(F_\mu(x))$ and, consequently, the p -Wasserstein distance has an analytical form given as follows:

一维分布计算WD：经验上可以将两个分布中的sample进行

$$\begin{aligned} W_p(\mu, \nu) &= \left(\int_X d^p(x, F_\nu^{-1}(F_\mu(x))) d\mu(x) \right)^{\frac{1}{p}} \\ &= \left(\int_0^1 d^p(F_\mu^{-1}(z), F_\nu^{-1}(z)) dz \right)^{\frac{1}{p}} \quad (3) \end{aligned}$$

where Eq. (3) results from the change of variable $F_\mu(x) = z$. Note that for empirical distributions, Eq. (3) is calculated by simply sorting the samples from the two distributions and calculating the average $d^p(\cdot, \cdot)$ between the

疑问1：缺少相关数学基础
对Wasserstein distance的公式无法理解

sorted samples. This requires only $O(M)$ operations at best and $O(M \log M)$ at worst, where M is the number of samples drawn from each distribution (see Kolouri et al. (2019) for more details). The closed-form solution of the p -Wasserstein distance for one-dimensional distributions is an attractive property that gives rise to the sliced-Wasserstein (SW) distance. Next, we review the Radon transform, which enables the definition of the SW distance. We also formulate an alternative OT distance called the maximum sliced-Wasserstein distance.

2.2. Radon Transform

The standard Radon transform, denoted by \mathcal{R} , maps a function $I \in L^1(\mathbb{R}^d)$, where

$$L^1(\mathbb{R}^d) = \{I : \mathbb{R}^d \rightarrow \mathbb{R} / \int_{\mathbb{R}^d} |I(x)| dx < \infty\},$$

to the infinite set of its integrals over the hyperplanes of \mathbb{R}^d and is defined as 将高维平面上的有限点集投射到一个低维的点上

$$\mathcal{R}I(t, \theta) = \int_{\mathbb{R}^d} I(x) \delta(t - \langle x, \theta \rangle) dx, \quad (4)$$

为什么theta可以确定一个投影 for $(t, \theta) \in \mathbb{R} \times \mathbb{S}^{d-1}$, where $\mathbb{S}^{d-1} \subset \mathbb{R}^d$ stands for the d -dimensional unit sphere, $\delta(\cdot)$ the one-dimensional Dirac delta function, and $\langle \cdot, \cdot \rangle$ the Euclidean inner-product. Note that $\mathcal{R} : L^1(\mathbb{R}^d) \rightarrow L^1(\mathbb{R} \times \mathbb{S}^{d-1})$. Each hyperplane can be written as:

$$H(t, \theta) = \{x \in \mathbb{R}^d \mid \langle x, \theta \rangle = t\} \quad (5)$$

which alternatively can be interpreted as a level set of the function $g \in \mathbb{R}^d \times \mathbb{S}^{d-1} \rightarrow \mathbb{R}$ defined as $g(x, \theta) = \langle x, \theta \rangle$. For a fixed θ , the integrals over all hyperplanes orthogonal to θ define a continuous function $\mathcal{R}I(\cdot, \theta) : \mathbb{R} \rightarrow \mathbb{R}$ which is a projection (or a slice) of I .

The Radon transform is a linear bijection (Natterer, 1986; Helgason, 2011) and its inverse \mathcal{R}^{-1} is defined as:

$$\begin{aligned} I(x) &= \mathcal{R}^{-1}(\mathcal{R}I(t, \theta)) \\ &= \int_{\mathbb{S}^{d-1}} (\mathcal{R}I(\langle x, \theta \rangle, \theta) * \eta(\langle x, \theta \rangle)) d\theta \end{aligned} \quad (6)$$

where $\eta(\cdot)$ is a one-dimensional high-pass filter with corresponding Fourier transform $\mathcal{F}\eta(\omega) = c|\omega|^{d-1}$, which appears due to the Fourier slice theorem (Helgason, 2011), and '*' is the convolution operator. The above definition of the inverse Radon transform is also known as the filtered back-projection method, which is extensively used in image reconstruction in the biomedical imaging community. Intuitively each one-dimensional projection (or slice) $\mathcal{R}I(\cdot, \theta)$ is first filtered via a high-pass filter and then smeared back into \mathbb{R}^d along $H(\cdot, \theta)$ to approximate I . The summation of all smeared approximations then reconstructs I . Note that

in practice, acquiring an infinite number of projections is not feasible, therefore the integration in the filtered back-projection formulation is replaced with a finite summation over projections (*i.e.*, a Monte-Carlo approximation).

2.3. Sliced-Wasserstein and Maximum Sliced-Wasserstein Distances

The idea behind the sliced p -Wasserstein distance is to first, obtain a family of one-dimensional representations for a higher-dimensional probability distribution through linear projections (via the Radon transform), and then, calculate the distance between two input distributions as a functional on the p -Wasserstein distance of their one-dimensional representations 此处理论上可以无限微分，实际上通过将其分为多个独立的像素，计算多个patch之间distance的平均值. The sliced p -Wasserstein distance between I_μ and I_ν is then formally defined as

$$SW_p(I_\mu, I_\nu) = \left(\int_{\mathbb{S}^{d-1}} W_p^p(\mathcal{R}I_\mu(\cdot, \theta), \mathcal{R}I_\nu(\cdot, \theta)) d\theta \right)^{\frac{1}{p}} \quad (7)$$

This is indeed a distance function as it satisfies positive-definiteness, symmetry and the triangle inequality (Bonneau, 2013; Kolouri et al., 2016b).

The computation of the SW distance requires an integration over the unit sphere in \mathbb{R}^d . In practice, this integration is approximated by using a simple Monte Carlo scheme that draws samples $\{\theta_l\}$ from the uniform distribution on \mathbb{S}^{d-1} and replaces the integral with a finite-sample average:

$$SW_p(I_\mu, I_\nu) \approx \left(\frac{1}{L} \sum_{l=1}^L W_p^p(\mathcal{R}I_\mu(\cdot, \theta_l), \mathcal{R}I_\nu(\cdot, \theta_l)) \right)^{\frac{1}{p}} \quad (8)$$

The sliced p -Wasserstein distance has important practical implications: provided that $\mathcal{R}I_\mu(\cdot, \theta_l)$ and $\mathcal{R}I_\nu(\cdot, \theta_l)$ can be computed for any sample θ_l , then the SW distance is obtained by solving several one-dimensional optimal transport problems, which have closed-form solutions. It is especially useful when one only has access to samples of a high-dimensional PDF I and kernel density estimation is required to estimate I : one-dimensional kernel density estimation of PDF slices is a much simpler task compared to the direct estimation of I from its samples. The downside is that as the dimensionality grows, one requires a larger number of projections to accurately estimate I from $\mathcal{R}I(\cdot, \theta)$. In short, if a reasonably smooth two-dimensional distribution can be approximated using L projections, then $\mathcal{O}(L^{d-1})$ projections are required to approximate a similarly smooth d -dimensional distribution for $d \geq 2$. grow fast

To further clarify this, let $I_\mu = \mathcal{N}(0, I_d)$ and $I_\nu = \mathcal{N}(x_0, I_d)$, $x_0 \in \mathbb{R}^d$, be two multivariate Gaussian densities with the identity matrix as the covariance ma-

G: 表示一个超平面，将高维分布投射到这个超平面上，所产生的一维分布用于计算SWD，一个随机投影实际上就是一个随机的超平面，同样的高维分布在上面会产生不同的投影结果

rix. Their projected representations are one-dimensional Gaussian distributions of the form $\mathcal{R}I_\mu(\cdot, \theta) = \mathcal{N}(0, 1)$ and $\mathcal{R}I_\mu(\cdot, \theta) = \mathcal{N}(\langle \theta, x_0 \rangle, 1)$. It is therefore clear that $W_2(\mathcal{R}I_\mu(\cdot, \theta), \mathcal{R}I_\nu(\cdot, \theta))$ achieves its maximum value when $\theta = \frac{x_0}{\|x_0\|_2}$ and is zero for θ 's that are orthogonal to x_0 . On the other hand, we know that vectors that are randomly picked from the unit sphere are more likely to be nearly orthogonal in high-dimension. More rigorously, the following inequality holds: $\Pr(|\langle \theta, \frac{x_0}{\|x_0\|_2} \rangle| < \epsilon) > 1 - e^{(-d\epsilon^2)}$, which implies that for a high dimension d , the majority of sampled θ 's would be nearly orthogonal to x_0 and therefore, $W_2(\mathcal{R}I_\mu(\cdot, \theta), \mathcal{R}I_\nu(\cdot, \theta)) \approx 0$ with high probability.

To remedy this issue, one can avoid uniform sampling of the unit sphere, and pick samples θ 's that contain discriminant information between I_μ and I_ν instead. This idea was for instance used in Deshpande et al. (2018), where the authors first calculate a linear discriminant subspace and then measure the empirical SW distance by setting the θ 's to be the discriminant components of the subspace.

A similarly flavored but less heuristic approach is to use the maximum sliced p -Wasserstein (max-SW) distance, which is an alternative OT metric defined as:

$$\text{max-SW}_p(I_\mu, I_\nu) = \max_{\theta \in \mathbb{S}^{d-1}} W_p(\mathcal{R}I_\mu(\cdot, \theta), \mathcal{R}I_\nu(\cdot, \theta)) \quad (9)$$

Given that W_p is a distance, it is easy to show that max-SW _{p} is also a distance: we will prove in Section 3.2 that the metric axioms hold for the maximum generalized sliced-Wasserstein distance, which contains the max-SW distance as a special case.

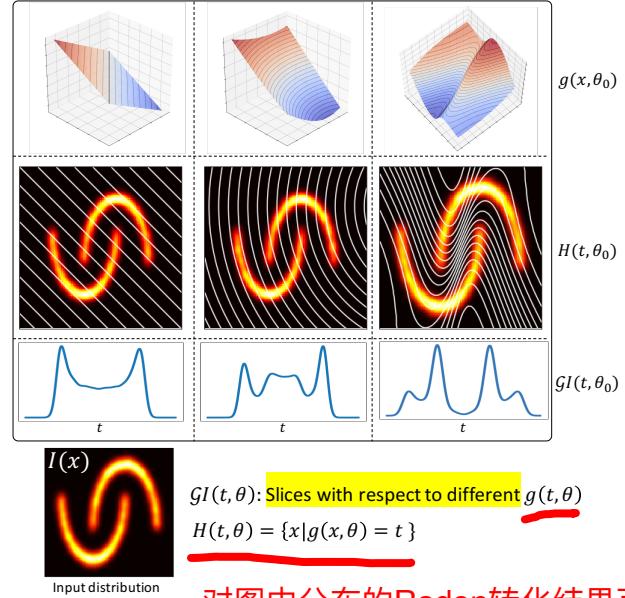
3. Generalized Sliced-Wasserstein Distances

We propose in this paper to extend the definition of the sliced-Wasserstein distance to formulate a new optimal transport metric, which we call the **generalized sliced-Wasserstein (GSW) distance**. The GSW distance is obtained using the same procedure as for the SW distance, except that here, the one-dimensional representations are acquired through nonlinear projections. In this section, we first review the **generalized Radon transform**, which is used to project the high-dimensional distributions, and we then formally define the class of GSW distances. We also extend the concept of max-SW distance to the class of maximum generalized sliced-Wasserstein (max-GSW) distances.

具体工作：generalized Radon transform

3.1. Generalized Radon Transform

The generalized Radon transform (GRT) extends the original idea of the classical Radon transform introduced by Radon (1917) from integration over hyperplanes of \mathbb{R}^d to integration over hypersurfaces, i.e. $(d-1)$ -dimensional manifolds (Beylkin, 1984; Denisyuk, 1994; Ehrenpreis,



对图中分布的Radon转化结果可视化
(可视化为一维曲线)

Figure 1. Visualizing the slicing process for classical and generalized Radon transforms for the Half Moons distribution. The slices $GI(t, \theta)$ follow Equation (10).

2003; Gel'fand et al., 1969; Kuchment, 2006; Homan & Zhou, 2017). The GRT has various applications, including Thermoacoustic Tomography, where the hypersurfaces are spheres, and Electrical Impedance Tomography, which requires integration over hyperbolic surfaces. 在以下四种条件下
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To formally define the GRT, we introduce a function g , defined on $\mathcal{X} \times (\mathbb{R}^n \setminus \{0\})$ with $\mathcal{X} \subset \mathbb{R}^d$. We say that g is a *defining function* when it satisfies the four conditions below:

H1. g is a real-valued C^∞ function on $\mathcal{X} \times (\mathbb{R}^n \setminus \{0\})$

H2. $g(x, \theta)$ is homogeneous of degree one in θ , i.e.,

$$\forall \lambda \in \mathbb{R}, g(x, \lambda\theta) = \lambda g(x, \theta)$$

H3. g is non-degenerate in the sense that

$$\forall (x, \theta) \in \mathcal{X} \times \mathbb{R}^n \setminus \{0\}, \frac{\partial g}{\partial x}(x, \theta) \neq 0$$

H4. The mixed Hessian of g is strictly positive, i.e.

$$\det \left(\left(\frac{\partial^2 g}{\partial x^i \partial \theta^j} \right)_{i,j} \right) > 0$$

Then, the GRT of $I \in L^1(\mathbb{R}^d)$ is the integration of I over hypersurfaces characterized by the level sets of g , which are characterized by $H_{t,\theta} = \{x \in \mathcal{X} \mid g(x, \theta) = t\}$.

Let g be a defining function. The generalized Radon transform of I , denoted by GI , is then formally defined as:

$$GI(t, \theta) = \int_{\mathbb{R}^d} I(x) \delta(t - g(x, \theta)) dx \quad (10)$$

Note that the standard Radon transform is a special case of the GRT with $g(x, \theta) = \langle x, \theta \rangle$. Figure 1 illustrates the slicing process for standard and generalized Radon transforms for the Half Moons dataset as input.

3.2. Generalized Sliced-Wasserstein and Maximum Generalized Sliced-Wasserstein Distances

Following the definition of the SW distance in Equation (7), we define the generalized sliced p -Wasserstein distance using the generalized Radon transform as:

$$GSW_p(I_\mu, I_\nu) = \left(\int_{\Omega_\theta} W_p^p(\mathcal{GI}_\mu(\cdot, \theta), \mathcal{GI}_\nu(\cdot, \theta)) d\theta \right)^{\frac{1}{p}} \quad (11)$$

where Ω_θ is a compact set of feasible parameters for $g(\cdot, \theta)$ (e.g., $\Omega_\theta = \mathbb{S}^{d-1}$ for $g(\cdot, \theta) = \langle \cdot, \theta \rangle$).

The GSW distance can also suffer from the projection complexity issue described in Section 2.3; that is why we formulate the maximum generalized sliced p -Wasserstein distance, which generalizes the max-SW distance as defined in (9):

$$\text{max-GSW}_p(I_\mu, I_\nu) = \max_{\theta \in \Omega_\theta} W_p(\mathcal{GI}_\mu(\cdot, \theta), \mathcal{GI}_\nu(\cdot, \theta)) \quad (12)$$

Proposition 1. *The generalized sliced p -Wasserstein distance and the maximum generalized sliced p -Wasserstein distance are, indeed, distances over $\mathcal{P}_p(\Omega)$ if and only if the generalized Radon transform is injective.*

需要保证Radon transform的单射性
此时MAX-GSW与GSW可以表示测量空间中的距离
Proof. The non-negativity and symmetry are direct consequences of the fact that the Wasserstein distance is a metric (Villani, 2008); see supplementary material.

We prove the triangle inequality for GSW_p and max-GSW_p . Let μ_1, μ_2 and μ_3 in $\mathcal{P}_p(\Omega)$. Since the Wasserstein distance satisfies the triangle inequality, we have, for all $\theta \in \Omega_\theta$,

$$W_p(\mathcal{GI}_{\mu_1}(\cdot, \theta), \mathcal{GI}_{\mu_3}(\cdot, \theta)) \leq W_p(\mathcal{GI}_{\mu_1}(\cdot, \theta), \mathcal{GI}_{\mu_2}(\cdot, \theta)) + W_p(\mathcal{GI}_{\mu_2}(\cdot, \theta), \mathcal{GI}_{\mu_3}(\cdot, \theta))$$

Therefore, we can write:

$$\begin{aligned} GSW_p(I_{\mu_1}, I_{\mu_3}) &= \left(\int_{\Omega_\theta} W_p^p(\mathcal{GI}_{\mu_1}(\cdot, \theta), \mathcal{GI}_{\mu_3}(\cdot, \theta)) d\theta \right)^{\frac{1}{p}} \\ &\leq \left(\int_{\Omega_\theta} (W_p(\mathcal{GI}_{\mu_1}(\cdot, \theta), \mathcal{GI}_{\mu_2}(\cdot, \theta)) + W_p(\mathcal{GI}_{\mu_2}(\cdot, \theta), \mathcal{GI}_{\mu_3}(\cdot, \theta)))^p d\theta \right)^{\frac{1}{p}} \\ &\leq \left(\int_{\Omega_\theta} W_p^p(\mathcal{GI}_{\mu_1}(\cdot, \theta), \mathcal{GI}_{\mu_2}(\cdot, \theta)) d\theta \right)^{\frac{1}{p}} + \left(\int_{\Omega_\theta} W_p^p(\mathcal{GI}_{\mu_2}(\cdot, \theta), \mathcal{GI}_{\mu_3}(\cdot, \theta)) d\theta \right)^{\frac{1}{p}} \end{aligned}$$

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where inequality (13) follows from the application of the Minkowski inequality in $L^p(\Omega_\theta)$. We conclude that GSW_p satisfies the triangle inequality.

Let $\theta^* = \arg \max_{\theta \in \Omega_\theta} W_p(\mathcal{GI}_{\mu_1}(\cdot, \theta), \mathcal{GI}_{\mu_3}(\cdot, \theta))$; then,

$$\begin{aligned} &\text{max-GSW}_p(I_{\mu_1}, I_{\mu_3}) \\ &= \max_{\theta \in \Omega_\theta} W_p(\mathcal{GI}_{\mu_1}(\cdot, \theta), \mathcal{GI}_{\mu_3}(\cdot, \theta)) \\ &= W_p(\mathcal{GI}_{\mu_1}(\cdot, \theta^*), \mathcal{GI}_{\mu_3}(\cdot, \theta^*)) \\ &\leq W_p(\mathcal{GI}_{\mu_1}(\cdot, \theta^*), \mathcal{GI}_{\mu_2}(\cdot, \theta^*)) \\ &\quad + W_p(\mathcal{GI}_{\mu_2}(\cdot, \theta^*), \mathcal{GI}_{\mu_3}(\cdot, \theta^*)) \\ &\leq \max_{\theta \in \Omega_\theta} W_p(\mathcal{GI}_{\mu_1}(\cdot, \theta), \mathcal{GI}_{\mu_2}(\cdot, \theta)) \\ &\quad + \max_{\theta \in \Omega_\theta} W_p(\mathcal{GI}_{\mu_2}(\cdot, \theta), \mathcal{GI}_{\mu_3}(\cdot, \theta)) \\ &\leq \text{max-GSW}_p(I_{\mu_1}, I_{\mu_2}) + \text{max-GSW}_p(I_{\mu_2}, I_{\mu_3}) \end{aligned}$$

So max-GSW_p also satisfies the triangle inequality.

Since $W_p(\mu, \mu) = 0$ for any μ , we have $GSW_p(I_\mu, I_\nu) = 0$ and $\text{max-GSW}_p(I_\mu, I_\nu) = 0$. Now, $GSW_p(I_\mu, I_\nu) = 0$ or $\text{max-GSW}_p(I_\mu, I_\nu) = 0$ is equivalent to $\mathcal{GI}_\mu(\cdot, \theta) = \mathcal{GI}_\nu(\cdot, \theta)$ for almost all $\theta \in \Omega_\theta$. Therefore, GSW and max-GSW are distances if and only if $\mathcal{GI}_\mu(\cdot, \theta) = \mathcal{GI}_\nu(\cdot, \theta)$ for all $\theta \in \Omega_\theta$, i.e. the GRT is injective. \square

Remark 1. *If the chosen generalized Radon transform is not injective, then we can only say that the GSW and max-GSW distances are pseudo-metrics: they still satisfy non-negativity, symmetry, the triangle inequality, and $GSW_p(I_\mu, I_\mu) = 0$ and $\text{max-GSW}_p(I_\mu, I_\mu) = 0$.*

3.3. Injectivity of the Generalized Radon Transform

We have shown that the injectivity of the GRT is crucial for the GSW and max-GSW distances to be, indeed, distances between probability measures. Here, we enumerate some of the known defining functions that lead to injective GRTs.

The investigation of the sufficient and necessary conditions for showing the injectivity of GRTs is a long-standing topic (Beylkin, 1984; Homan & Zhou, 2017; Uhlmann, 2003; Ehrenpreis, 2003). The circular defining function, $g(x, \theta) = \|x - r * \theta\|_2$ with $r \in \mathbb{R}^+$ and $\Omega_\theta = \mathbb{S}^{d-1}$ was shown to provide an injective GRT (Kuchment, 2006). More interestingly, homogeneous polynomials with an odd degree also yield an injective GRT (Rouviere, 2015), i.e.

$$g(x, \theta) = \sum_{|\alpha|=m} \theta_\alpha x^\alpha,$$

where we use the multi-index notation $\alpha = (\alpha_1, \dots, \alpha_{d_\alpha}) \in \mathbb{N}^{d_\alpha}$, $|\alpha| = \sum_{i=1}^{d_\alpha} \alpha_i$, and $x^\alpha = \prod_{i=1}^{d_\alpha} x_i^{\alpha_i}$. Here, the summation iterates over all possible multi-indices α , such that $|\alpha| = m$, where m denotes the degree of the polynomial and $\theta_\alpha \in \mathbb{R}$. The

Algorithm 1 GSW Distance

input $\{x_i \sim I_\mu\}_{i=1}^N, \{y_i \sim I_\nu\}_{i=1}^N$, order p ,
number of slices L , defining function g

Initialize $d = 0$

for $l = 1$ to L **do** **g:** 一个超平面, 一个
 Sample θ_l from Ω_θ uniformly
 Compute $\hat{x}_i = g(x_i, \theta_l)$ and $\hat{y}_i = g(y_i, \theta_l)$ for each i
 Sort \hat{x}_i and \hat{y}_j in ascending order s.t. $\hat{x}_{i[n]} \leq \hat{x}_{i[n+1]}$
 and $\hat{y}_{j[n]} \leq \hat{y}_{j[n+1]}$ 对sample排序
 $d = d + \frac{1}{L} \sum_{n=1}^N |\hat{x}_{i[n]} - \hat{y}_{j[n]}|^p$
end for

output $d^{\frac{1}{p}} \approx GSW_p(I_\mu, I_\nu)$ 计算平均的一维
 distance

Algorithm 2 Max-GSW Distance

input $\{x_i \sim I_\mu\}_{i=1}^N, \{y_j \sim I_\nu\}_{j=1}^N$,
order p , defining function $g(x, \theta)$

Randomly initialize $\theta \in \Omega_\theta$

while θ has not converged **do**

 Compute $\hat{x}_i = g(x_i, \theta_l)$ and $\hat{y}_i = g(y_i, \theta_l)$ for each i
 Sort \hat{x}_i and \hat{y}_j in ascending order s.t. $\hat{x}_{i[n]} \leq \hat{x}_{i[n+1]}$
 and $\hat{y}_{j[n]} \leq \hat{y}_{j[n+1]}$
 $\theta = Proj(ADAM(\nabla_\theta(\frac{1}{N} \sum_{n=1}^N |\hat{x}_{i[n]} - \hat{y}_{j[n]}|^p), \theta))$

end while

Sort \hat{x}_i and \hat{y}_i in ascending order
 $d = \frac{1}{N} \sum_{n=1}^N |\hat{x}_{i[n]} - \hat{y}_{j[n]}|^p$ 梯度下降方法, 求出最佳的
output $d^{\frac{1}{p}} \approx \text{max-GSW}_p(I_\mu, I_\nu)$ projection (由theta唯一确定)

parameter set for homogeneous polynomials is then set to $\Omega_\theta = \mathbb{S}^{d_\alpha-1}$. We can observe that choosing $m = 1$ reduces to the linear case $\langle x, \theta \rangle$, since the set of the multi-indices with $|\alpha| = 1$ becomes $\{(\alpha_1, \dots, \alpha_d); \alpha_i = 1 \text{ for a single } i \in [1, d], \text{ and } \alpha_j = 0, \forall j \neq i\}$ and contains d elements.

4. Numerical Implementation

In this section, we briefly review the numerical methods used to compute the GSW and max-GSW distances.

4.1. Generalized Radon Transforms of Empirical PDFs

In most machine learning applications, we do not have access to the distribution I_μ but to a set of samples $\{x_i\}_{i=1}^N$ drawn from I_μ , for which the empirical density is:

$$I_\mu(x) \approx \frac{1}{N} \sum_{i=1}^N \delta(x - x_i)$$

The GRT of the empirical density is then given by:

$$GI_\mu(t, \theta) \approx \frac{1}{N} \sum_{i=1}^N \delta(t - g(x_i, \theta))$$

Moreover, for high-dimensional problems, estimating I_μ in \mathbb{R}^d requires a large number of samples. However, the projections of I_μ , $GI(\cdot, \theta)$, are one-dimensional and it may not be critical to have a large number of samples to estimate these one-dimensional densities.

4.2. Numerical Implementation of GSW Distances

Let $\{x_i\}_{i=1}^N$ and $\{y_j\}_{j=1}^N$ be samples respectively drawn from I_μ and I_ν , and let $g(\cdot, \theta)$ be a defining function. Following the work of [Kolouri et al. \(2019\)](#), the Wasserstein distance between one-dimensional distributions $GI_\mu(\cdot, \theta)$ and $GI_\nu(\cdot, \theta)$ can be calculated from sorting their samples and calculating the L_p distance between the sorted samples. In other words, the GSW distance between I_μ and I_ν can be approximated from their samples as follows:

$$GSW_p(I_\mu, I_\nu) \approx \left(\frac{1}{L} \sum_{l=1}^L \sum_{n=1}^N |g(x_{i[n]}, \theta_l) - g(y_{j[n]}, \theta_l)|^p \right)^{\frac{1}{p}}$$

where $i[m]$ and $j[n]$ are the indices of sorted $\{g(x_i, \theta)\}_{i=1}^N$ and $\{g(y_j, \theta)\}_{j=1}^N$. The procedure to approximate the GSW distance is summarized in Algorithm 1.

4.3. Numerical Implementation of max-GSW Distances

To compute the max-GSW distance, we perform an EM-like optimization scheme: (a) for a fixed θ , $g(x_i, \theta)$ and $g(y_i, \theta)$ are sorted to compute W_p , (b) θ is updated with:

$$\theta = Proj(ADAM(\nabla_\theta(\frac{1}{N} \sum_{n=1}^N |g(x_{i[n]}, \theta) - g(y_{j[n]}, \theta)|^p), \theta))$$

where *ADAM* refers to the ADAM optimizer ([Kingma & Ba, 2014](#)) and *Proj*(\cdot) is the operator projecting θ onto Ω_θ .

For instance, when $\theta \in \mathbb{S}^{n-1}$, $Proj(\theta) = \frac{\theta}{\|\theta\|}$.

Remark 2. Here, we find the optimal θ by optimizing the actual W_p , as opposed to the heuristic approaches proposed in [Deshpande et al. \(2018\)](#) and [Kolouri et al. \(2019\)](#), where the pseudo-optimal slice is found via perceptrons or penalized linear discriminant analysis ([Wang et al., 2011](#)).

Finally, once convergence is reached, the max-GSW distance is approximated with:

$$\text{max-GSW}_p(I_\mu, I_\nu) \approx \left(\frac{1}{N} \sum_{n=1}^N |g(x_{i[n]}, \theta^*) - g(y_{j[n]}, \theta^*)|^p \right)^{\frac{1}{p}}$$

The whole procedure is summarized in Algorithm 2.

5. Experiments

5.1. Generalized Sliced-Wasserstein Flows

Our first experiment demonstrates the effects of the choice of the GSW distance in its purest form by considering the

实验一：找到GSW中与ν最接近的u（梯度下降），u被初始化为正态

Generalized Sliced Wasserstein Distances

对数越小，说明使用对应投影计算的GSW，梯度下降后可以得到和目标信号更接近的结果

following problem: $\min_{\mu} GSW_p(\mu, \nu)$, where ν is a target distribution and μ is the source distribution, which is initialized to be the normal distribution. The optimization is then solved iteratively via

$$\partial_t \mu_t = -\nabla GSW_p(\mu_t, \nu), \quad \mu_0 = \mathcal{N}(0, 1)$$

We used 5 well-known distributions as the target, namely the **25-Gaussians**, **8-Gaussians**, **Swiss Roll**, **Half Moons** and **Circle distributions**. We compare linear (*i.e.*, SW distance), circular, homogeneous polynomial of degree 3 and homogeneous polynomial of degree 5 as **defining functions**. We used the **exact same optimization scheme** for all methods, with $L = 10$ random projections, and measured the 2-Wasserstein distance between μ_t and ν at each iteration of the optimization (via solving a linear programming at each step). We repeated each experiment 100 times and reported the mean and standard deviation of the 2-Wasserstein distance for all five target datasets in Figure 2. While the **choice of the defining function $g(\cdot, \theta)$** is data-dependent, one can see that the homogeneous polynomial of degree 3 is among the top two performers for all datasets.

For clarity purposes, we chose to not report the max- GSW_p results for the same experiment in Figure 2. These results are included in the supplementary material.

5.2. Generative Modeling via Auto-Encoders

We now demonstrate the application of the GSW and max-GSW distances in generative modeling. We specifically use the recently proposed **Sliced-Wasserstein Auto-Encoder (SWAE)** (Kolouri et al., 2019) framework, which **penalizes the distribution of the encoded data in the latent space of the auto-encoder to follow a prior samplable distribution, p_Z** . More precisely, let $\{x_n \sim p_X\}_{n=1}^n$ be i.i.d. samples from p_X , $\phi(x, \gamma_\phi) : \mathcal{X} \rightarrow \mathcal{Z}$ and $\psi(z, \gamma_\psi) : \mathcal{Z} \rightarrow \mathcal{X}$ be the parametric encoder and decoder (*e.g.*, CNNs) with parameters γ_ϕ and γ_ψ , respectively. Then SWAE's objective function (Kolouri et al., 2019) is defined as:

$$\min_{\gamma_\phi, \gamma_\psi} \mathbb{E}_x [c(x, \psi(\phi(x, \gamma_\phi), \gamma_\psi))] + \lambda SW(p_{\phi(x, \gamma_\phi)}, p_Z) \quad (14)$$

where λ is the regularizer coefficient for matching the encoded distribution to p_Z . Here, we substitute the SW distance in Equation (14) with GSW and max-GSW distances. Specifically, we encode the MNIST dataset (LeCun et al., 1998) into the encoder's latent space and enforce the distribution of the embedded data to **follow a specific prior distribution**, *e.g.* the Swiss Roll distribution as shown in Figure 3, while we simultaneously enforce the encoded features to be decodable to the original input images.

We ran the optimization in Equation (14) with GSW distances, which we denote as GSWAE, with linear, circular, and homogeneous polynomial of degree 3. At each iteration,

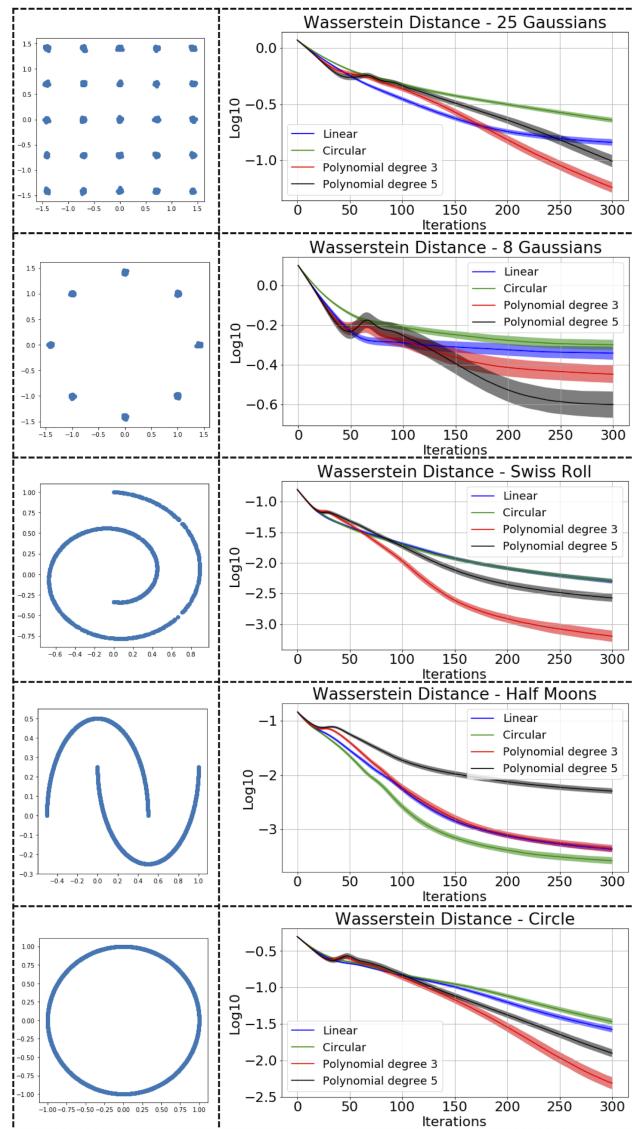


Figure 2. Log 2-Wasserstein distance between the source and target distributions as a function of the number of iterations for 5 classical target distributions.

we measured the 2-Wasserstein distance between the embedded distribution and the prior distribution, $W_2(p_{\phi(x, \gamma_\phi)}, p_Z)$, and also between the input distribution and the distribution of the reconstructed samples, $W_2(p_{\psi(\phi(x, \gamma_\phi), \gamma_\psi)}, p_X)$. Each experiment was repeated 50 times and the average 2-Wasserstein distances are reported in Figure 4. The middle row in Figure 4 shows samples from p_Z and $\phi(x, \gamma_\phi)$ for $x \sim p_X$, and the last row shows decoded random samples, $\psi(z, \gamma_\psi)$ for $z \sim p_Z$. Similar to the previous experiment, we see that the GSWAE with a polynomial defining function, captures the nonlinear geometry of the input samples better.

We also compare the performance of GSWAE and Max-

选用不同的
define
function
相同的
迭代优化器，
迭代相同的次
数

在latent
space
中使
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接近某
种特定
的分布？

SWAE的作用：使embedded的data服从某种分布

Generalized Sliced Wasserstein Distances

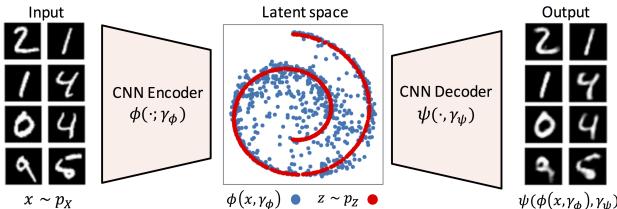


Figure 3. The SWAE architecture. The embedded data in the latent space is enforced to follow a prior samplable distribution p_Z .

GSWAE with those of SWAE and WAE-GAN (Tolstikhin et al., 2018). In particular, we use the improved Wasserstein-GAN (Gulrajani et al., 2017), which is among the state-of-the-art adversarial training methods, in the embedding space of the Wasserstein auto-encoder (Tolstikhin et al., 2018). The adversary was chosen to be a multi-layer perceptron. Similar to the previous experiments, we measured the 2-Wasserstein distance between the input and output distributions as well as the latent and prior distributions. Each experiment was repeated 10 times, and the average 2-Wasserstein distances are reported in Figure 5. It can be seen that, while WAE-GAN provides a better matching of distributions in the latent space, the results of max-GSWAE distances are on par with the WAE-GAN. In addition, by comparing the distance between input and output distributions of the auto-encoder, it seems that max-GSWAE provides a better objective function to train such networks.

6. Conclusion

We introduced a new family of optimal transport metrics for probability measures that generalizes the sliced-Wasserstein distance: while the latter is based on linear slicing of distributions, we propose to perform nonlinear slicing. We provided theoretical conditions that yield the generalized sliced-Wasserstein distance to be, indeed, a distance function, and we empirically demonstrated the superior performance of the GSW and max-GSW distances over the classical sliced-Wasserstein distance in various generative modeling applications. As future work, we plan to study the existing connection between adversarial training and max-GSW distances by showing the defining function for GRTs can be approximated with neural networks.

7. Acknowledgement

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从CNN结果中的采样和z（目标分布）中采样的相似度，说明拟合特定分布的能力更强

x中的采样和decoder输出的feature采样的相似度，越小说明Encode与Decode过程损失的信息最少

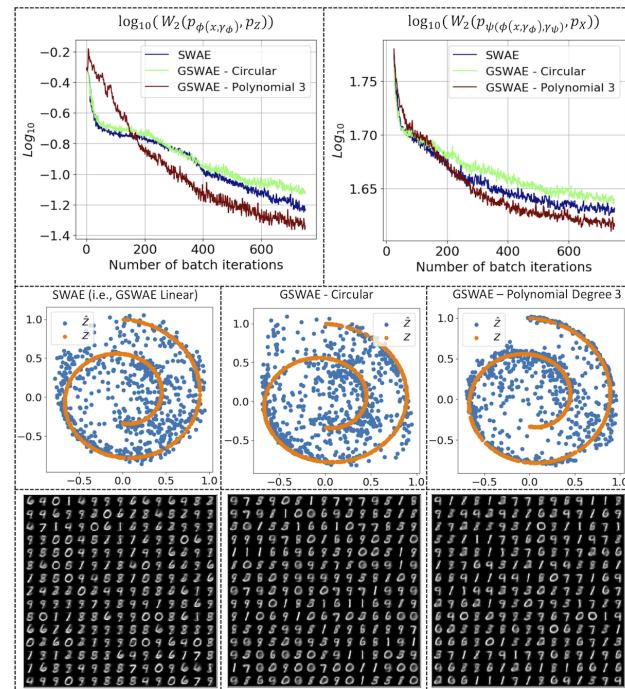


Figure 4. 2-Wasserstein distance between p_Z and $p_{\phi(x, \gamma_\phi)}$ and between p_X and $p_{\psi(\phi(x, \gamma_\phi), \gamma_\psi)}$ at different batch iterations for SWAE and GSWAE with circular and polynomial of degree 3 defining functions.

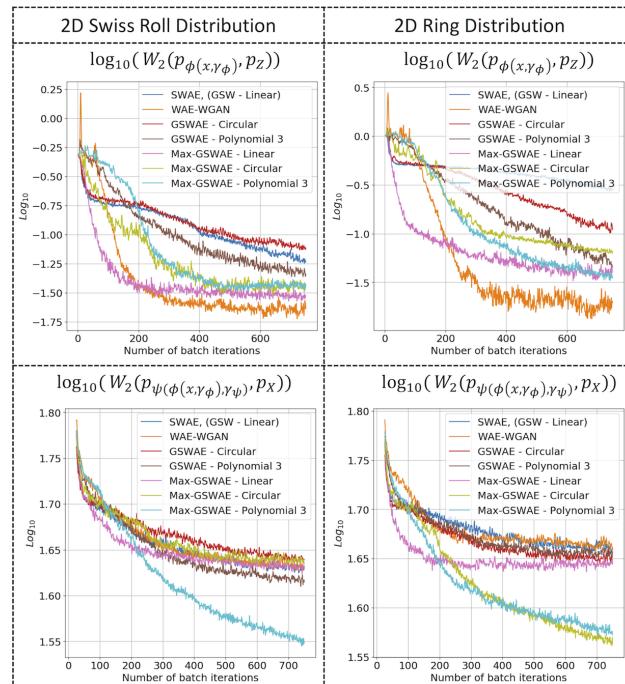


Figure 5. The 2-Wasserstein distance between p_Z and $p_{\phi(x, \gamma_\phi)}$ and between p_X and $p_{\psi(\phi(x, \gamma_\phi), \gamma_\psi)}$ at different batch iterations for SWAE and WAE-GAN compared to GSWAE and Max-GSWAE with circular and polynomial of degree 3 defining functions.

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8. Supplementary material

9. Non-negativity and Symmetry of the GSW and max-GSW Distances

We prove that the GSW and max-GSW distances satisfy non-negativity and symmetry, using the fact that the p -Wasserstein distance is known to be a proper distance function (Villani, 2008). Let μ and ν be in $\mathcal{P}_p(\Omega)$.

9.1. Non-negativity

We use the non-negativity of the p -Wasserstein distance, *i.e.* $W_p(\mu, \nu) \geq 0$ for any μ, ν in $\mathcal{P}_p(\Omega)$, to show that the GSW and max-GSW distances are non-negative as well:

$$\begin{aligned} GSW_p(I_\mu, I_\nu) &= \left(\int_{\Omega_\theta} W_p^p(\mathcal{G}I_\mu(\cdot, \theta), \mathcal{G}I_\nu(\cdot, \theta)) d\theta \right)^{\frac{1}{p}} \\ &\geq \left(\int_{\Omega_\theta} (0)^p d\theta \right)^{\frac{1}{p}} = 0 \end{aligned}$$

$$\begin{aligned} \text{max-GSW}_p(I_\mu, I_\nu) &= \max_{\theta \in \Omega_\theta} W_p(\mathcal{G}I_\mu(\cdot, \theta), \mathcal{G}I_\nu(\cdot, \theta)) \\ &= W_p(\mathcal{G}I_\mu(\cdot, \theta^*), \mathcal{G}I_\nu(\cdot, \theta^*)) \\ &\geq 0 \end{aligned}$$

where $\theta^* = \arg \max_{\theta \in \Omega_\theta} W_p(\mathcal{G}I_\mu(\cdot, \theta), \mathcal{G}I_\nu(\cdot, \theta))$.

9.2. Symmetry

Since the p -Wasserstein distance is symmetric, we have $W_p(\mu, \nu) = W_p(\nu, \mu)$. In particular, we can write for all $\theta \in \Omega_\theta$:

$$W_p(\mathcal{G}I_\mu(\cdot, \theta), \mathcal{G}I_\nu(\cdot, \theta)) = W_p(\mathcal{G}I_\nu(\cdot, \theta), \mathcal{G}I_\mu(\cdot, \theta)) \quad (15)$$

and,

$$\max_{\theta \in \Omega_\theta} W_p(\mathcal{G}I_\mu(\cdot, \theta), \mathcal{G}I_\nu(\cdot, \theta)) = \max_{\theta \in \Omega_\theta} W_p(\mathcal{G}I_\nu(\cdot, \theta), \mathcal{G}I_\mu(\cdot, \theta)) \quad (16)$$

The symmetry of the GSW and max-GSW distances follows from Equations (15) and (16) respectively.

10. Additional Experimental Results

We include the results of maximum generalized sliced-Wasserstein flows on the five datasets used in the main paper, to accompany Figure 4 of our main paper: see Figure 6. It can be seen that the max-GSW distances, in the majority of cases, improve the performance of GSW. Here it should be noted that GSW distances are calculated based on 10 random projections, while max-GSW distances use only one projection by definition.

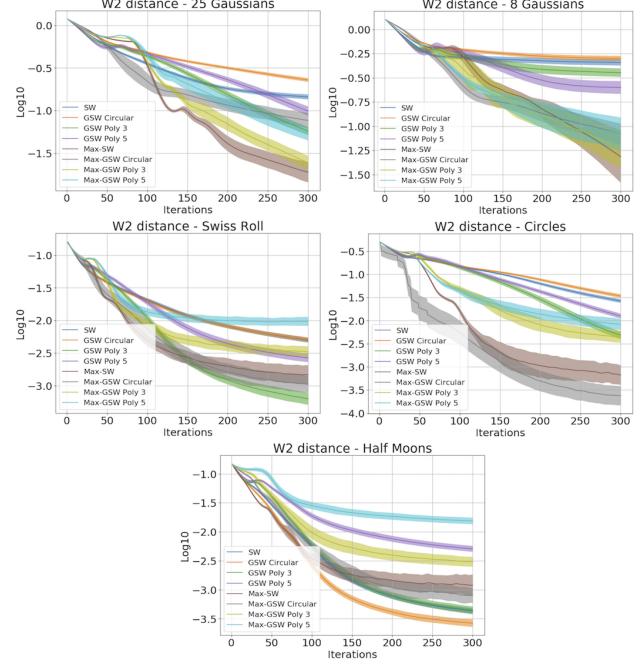


Figure 6. Log 2-Wasserstein distance between the source and target distributions as a function of the number of iterations for 5 classical target distributions using GSW and max-GSW distances.

11. Implementation Details

The PyTorch (Paszke et al., 2017) implementation of our paper will be available here¹. Here we clarify some of the implementation details used in our paper. First, the ‘critic iteration’ for the adversarial training, and the projection maximization for the max-GSW distances, were set to be equal to 50. For all optimizations, we used ADAM (Kingma & Ba, 2014) optimizer with learning rate $lr = 0.001$ and PyTorch’s default momentum parameters.

We used 3×3 convolutional filters in both encoder and

¹<https://github.com/.../GSW/>

decoder architectures. Encoder architecture:

$$\begin{aligned}
 x \in \mathbb{R}^{28 \times 28} &\rightarrow Conv_{16} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow Conv_{16} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow AvgPool_2 \\
 &\rightarrow Conv_{32} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow Conv_{32} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow AvgPool_2 \\
 &\rightarrow Conv_{64} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow Conv_{64} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow AvgPool_2 \rightarrow Flatten \\
 &\rightarrow FC_{128} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow FC_2
 \end{aligned}$$

Decoder architecture:

$$\begin{aligned}
 z \in \mathbb{R}^2 &\rightarrow FC_{128} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow FC_{1024} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow Reshape(4 \times 4 \times 64) \rightarrow Upsample_2 \\
 &\rightarrow Conv_{64} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow Conv_{64} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow Upsample_2 \\
 &\rightarrow Conv_{32} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow Conv_{32} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow Upsample_2 \\
 &\rightarrow Conv_{16} \rightarrow LeakyReLU_{0.2} \\
 &\rightarrow Conv_1
 \end{aligned}$$

The WGAN in WAE-GAN uses an adversary network. Adversary's architecture:

$$\begin{aligned}
 z \in \mathbb{R}^2 &\rightarrow FC_{500} \rightarrow ReLU \\
 &\rightarrow FC_{500} \rightarrow ReLU \\
 &\rightarrow FC_{500} \rightarrow ReLU \\
 &\rightarrow FC_1 \rightarrow ReLU
 \end{aligned}$$