On Deep Generative Models for Approximation and Estimation of Distributions on Manifolds

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Abstract

Deep generative models have experienced great empirical successes in distribution learning. Many existing experiments have demonstrated that deep generative networks can efficiently generate high-dimensional complex data from a low-dimensional easy-to-sample distribution. However, this phenomenon can not be justified by existing theories. The widely held manifold hypothesis speculates that real-world data sets, such a natural images and signals, exhibit low-dimensional geometric structures. In this paper, we take such low-dimensional data structures into consideration by assuming that data distributions are supported on a low-dimensional manifold. We prove approximation and estimation theories of deep generative networks for estimating distributions on a low-dimensional manifold under the Wasserstein-1 loss. We show that the Wasserstein-1 loss converges to zero at a fast rate depending on the intrinsic dimension instead of the ambient data dimension. Our theory leverages the low-dimensional geometric structures in data sets and justifies the practical power of deep generative models. We require no smoothness assumptions on the data distribution which is desirable in practice.

1 Introduction

Deep generative models, such as generative adversarial networks (GANs) [Goodfellow et al., 2014, Arjovsky et al., 2017] and variational autoencoder [Kingma and Welling, 2013, Mohamed and Wierstra, 2014], utilize neural networks to generate new samples which follow the same distribution as the training data. They have been successful in many applications including producing photorealistic images, improving 20 astronomical images, and modding video games [Reed et al., 2016, Ledig et al., 2017, Schawinski et al., 2017, Brock et al., 2018, Volz et al., 2018, Radford et al., 2015, Salimans et al., 2016].

To estimate a data distribution Q, generative models solve the following optimization problem

$$\min_{g_\theta \in \mathcal{G}} \texttt{discrepancy}((g_\theta)_\sharp \rho, Q), \tag{1}$$

where ρ is an easy-to-sample distribution, $\mathcal{G}$ is a class of generating functions, `discrepancy` is some distance function between distributions, and $(g_\theta)_\sharp \rho$ denotes the pushforward measure of ρ under g_θ. In particular, when we obtain a sample z from ρ, we let $g_\theta(z)$ be the generated sample, whose distribution follows $(g_\theta)_\sharp \rho$.

There are many choices of the `discrepancy` function in literature ([**?**], [**?**]) among which Wasserstein distance attracts many attention. The so-called Wasserstein generative models [Arjovsky et al., 2017] consider the Wasserstein-1 distance defined as

$$W_1(\mu, \nu) = \sup_{f \in \mathrm{Lip}_1(\mathbb{R}^D)} \mathbb{E}_{X \sim \mu}[f(X)] - \mathbb{E}_{Y \sim \nu}[f(Y)], \tag{2}$$

where μ, ν are two distributions and $\mathrm{Lip}_1(\mathbb{R}^D)$ consists of 1-Lipschitz functions on $\mathbb{R}^D$. The formulation in (2) is known as the Kantorovich-Rubinstein dual form of Wasserstein-1 distance and can be viewed as an integral probability metric [Müller, 1997].

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In deep generative models, function class $\mathcal{G}$ is often parameterized by a deep neural network class $\mathcal{G}_{\text{NN}}$. Functions in $\mathcal{G}_{\text{NN}}$ can be written in the following compositional form

$$g_\theta(x) = W_L \cdot \sigma(W_{L-1} \ldots \sigma(W_1 x + b_1) + \ldots + b_{L-1}) + b_L, \tag{3}$$

where the W_i's and b_i's are weight matrices and intercepts of corresponding dimensions, respectively, and σ is ReLU activation applied entry-wise: $\sigma(a) = \max(a, 0)$. Here $\theta = \{W_i, b_i\}_{i=1}^L$ denotes the set of parameters.

Solving (1) is prohibitive in practice, as we only have access to a finite collection of samples, $X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} Q$. Replacing Q by its empirical counterpart $\hat{Q}_n = \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$, we end up with

$$\hat{g}_n = \text{argmin}_{g_\theta \in \mathcal{G}_{\text{NN}}} W_1((g_\theta)_\sharp \rho, \hat{Q}_n). \tag{4}$$

Note that (4) is also known as training deep generative models under the Wasserstein loss in existing deep learning literature [Frogner et al., 2015, Genevay et al., 2018]. It has exhibited remarkable ability in learning complex distributions in high dimensions, even though existing theories cannot fully explain such empirical successes. In literature, statistical theories of deep generative models have been studied in Arora et al. [2017], Zhang et al. [2017], Jiang et al. [2018], Bai et al. [2018], Liang [2017, 2018], Uppal et al. [2019], Chen et al. [2020], Lu and Lu [2020], Block et al. [2021], Luise et al. [2020], Schreuder et al. [2021]. Due to the well-known curse of dimensionality, the sample complexity in Liang [2017], Uppal et al. [2019], Chen et al. [2020], Lu and Lu [2020] grows exponentially with respect to the data dimension. For example, the CIFAR-10 dataset consists of 32×32 RGB images. Roughly speaking, to learn this data distribution with accuracy ϵ, the sample size is required to be ϵ^{-D} where $D = 32 \times 32 \times 3 = 3072$ is the data dimension. Setting $\epsilon = 0.1$ requires 10^{3072} samples. However, GANs have been successful with $60,000$ training samples [Goodfellow et al., 2014].

A common belief to explain the aforementioned gap between theory and practice is that practical data sets exhibit low-dimensional intrinsic structures. For example, many image patches are generated from the same pattern by some transformations, such as rotation, translation, and skeleton. Such a generating mechanism induces a small number of intrinsic parameters. It is plausible to model these data as samples near a low dimensional manifold [Tenenbaum et al., 2000, Roweis and Saul, 2000, Peyré, 2009, Coifman et al., 2005].

To justify that deep generative models can adapt to low-dimensional structures in data sets, this paper focuses on the following fundamental questions from a theoretical perspectives of both distribution approximation and estimation :

Q1: *Can deep generative models approximate distributions on a low-dimensional manifold as a pushforward measure of a low-dimensional easy-to-sample distribution?*

Q2: *If the representation in **Q1** can be learned by deep generative models, what is the statistical rate of convergence in terms of the sample size n?*

This paper provides positive answers to these questions. We consider data distributions supported on a d-dimensional compact Riemannian manifold $\mathcal{M}$ isometrically embedded in $\mathbb{R}^D$. The easy-to-sample distribution ρ is uniform on $(0,1)^{d+1}$. To answer **Q1**, our Theorem 1 proves that deep generative models are capable of approximating a transportation map which maps the low-dimensional uniform distribution ρ to a large class of data distributions on $\mathcal{M}$. To answer **Q2**, our Theorem 2 shows that the Wasserstein-1 loss in distribution learning converges to zero *at a fast rate depending on the intrinsic dimension* d instead of the data dimension D. In particular we prove that

$$\mathbb{E} W_1((\hat{g}_n)_\sharp \rho, Q) \leq C n^{-\frac{1}{d+\delta}}$$

for all $\delta > 0$ where C is a constant independent of n and D.

Our proof proceeds by constructing an oracle transportation map g^* such that $g^*_\sharp \rho = Q$. This construction crucially relies on the decomposition of the manifold into geodesic Voronoi cells, such that the data distribution Q is decomposed as the sum of local distributions supported on these Voronoi cells. Each local distribution is then transported onto lower dimensional sets in $\mathbb{R}^d$ from which we can apply optimal transport theory. We then argue that the oracle g^* can be efficiently approximated by deep neural networks.

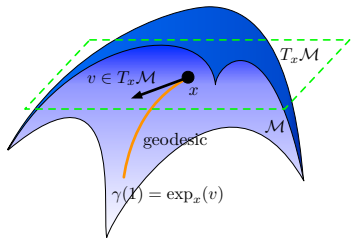

Figure 1: Exponential map on $\mathcal{M}$

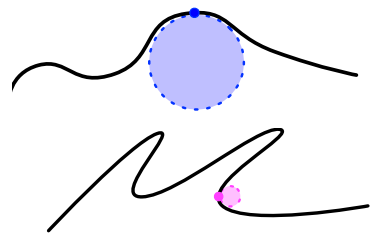

Figure 2: Manifolds with large and small reach.

We make minimal assumptions on the network, only requiring g_θ belong to $\mathcal{G}_{\text{NN}}$ with size depending on some accuracy ϵ. Further we make minimial assumptions on the data distribution Q, only requiring it admit an upper and lower bounded density. Standard technical assumptions are made on the manifold $\mathcal{M}$.

2 Preliminaries

We establish some notation and preliminaries classical differential geometry and optimal transport theory before presenting our proof.

Notation. For $x \in \mathbb{R}^d$, $\|x\|$ is the euclidean norm, unless otherwise specified. $B_X(0, r)$ is the open ball of radius r in metric space X. If unspecified $B(0, r) = B_{\mathbb{R}^d}(0, r)$. $B[0, r]$ is the corresponding closed ball. For $x, y \in \mathbb{R}^d$, $[x : y]$ denotes the line segment between x and y. For a function $f : \mathbb{R}^d \to \mathbb{R}^d$ and $A \subseteq \mathbb{R}^d$, $f^{-1}[A]$ denotes the pre-image of A under f. ∂ denotes the differential operator. For $0 < \alpha \leq 1$, we denote by $C^{0,\alpha}$ the class of Hölder continuous functions with Hölder exponent α. For any positive integer k, C^k denotes the class of functions whose k-th order derivative is continuous. $\|\cdot\|_\infty$ denotes the ∞ norm of a function, vector, or matrix (considered as a vector). $\|\cdot\|_0$ denotes the number of nonzero entries of a vector or matrix.

Classical Geometry. Let $(\mathcal{M}, g)$ be a d-dimensional compact Riemannian manifold isometrically embedded in $\mathbb{R}^D$. Roughly speaking a manifold is a set which is locally Euclidean i.e. there exists a function ϕ continuously mapping a small patch on $\mathcal{M}$ into Euclidean space. This can be formalized with the *open sets* and *charts*. At each point $x \in \mathcal{M}$ we have a *tangent space* $T_x\mathcal{M}$ which, for a manifold embedded in $\mathbb{R}^D$ is the d-dimensional plane tangent to the manifold at x. We say $\mathcal{M}$ is Riemannian because it is equipped with a smooth metric $g_x : T_x\mathcal{M} \times T_x\mathcal{M} \to \mathbb{R}$ which can be thought of as a local inner product. We can define the Riemannian distance $d_{\mathcal{M}} : \mathcal{M} \times \mathcal{M} \to \mathbb{R}$ on $\mathcal{M}$ as

$$d_{\mathcal{M}}(x, y) = \inf\{L(\gamma) | \gamma \text{ is a } C^1(\mathcal{M}) \text{ curve such that } \gamma(0) = x, \gamma(1) = y\}$$

i.e. the length of the shortest path or *geodesic* connecting x and y. An *isometric embedding* of the d-dimensional $\mathcal{M}$ in $\mathbb{R}^D$ preserves the Riemannian distance between points on $\mathcal{M}$ in $\mathbb{R}^D$. For more rigorous statements, see the classic reference Flaherty and do Carmo [2013].

We next define the exponential map at a point $x \in \mathcal{M}$ going from the tangent space onto the manifold.

Definition 1 (Exponential map)**.** *Let $x \in \mathcal{M}$. For all tangent vectors $v \in T_x\mathcal{M}$, there is a unique geodesic γ that starts at x with initial tangent vector v, i.e. $\gamma(0) = x$ and $\gamma'(0) = v$. The exponential map centered at x is given by $\exp_x(v) = \gamma(1)$, for all $v \in T_x\mathcal{M}$.*

The exponential map sends a point on the tangent space to manifold via travelling along a geodesic curve (see Figure 1 for an example).

It is well known that for all $x \in \mathcal{M}$, there exists a radius δ such that the exponential map restricted to $B_{T_x\mathcal{M}}(0, \delta)$ is a diffeomorphism onto its image, i.e. it is a smooth map with smooth inverse. As the sufficiently small δ-ball in the tangent space may vary for each $x \in \mathcal{M}$, we define the injectivity radius of $\mathcal{M}$ as the minimum δ over all $x \in \mathcal{M}$.

Definition 2 (Injectivity radius)**.** *For $x \in \mathcal{M}$ we define the injectivity radius at a point* $\text{inj}_{\mathcal{M}}(x) = \sup\{\delta > 0 | \exp_x : B_{T_x\mathcal{M}}(0, \delta) \subseteq T_x\mathcal{M} \to \mathcal{M} \text{ is a diffeomorphism}\}$. *Then the injectivity radius of $\mathcal{M}$ is*

$$\text{inj}(\mathcal{M}) = \inf\{\text{inj}_{\mathcal{M}}(x) | x \in \mathcal{M}\}$$

The injectivity radius defines the largest balls we can place around the origin in tangent space such that the exponential map is always injective for every base point x. Within the injectivity radius the exponential map is a diffeomorphism between the tangent space and a patch of $\mathcal{M}$, with $\exp^{-1}$ the inverse. Controlling a quantity called reach allows us to lower bound the manifold's injectivity radius.

Definition 3 (Reach[Federer, 1959])**.** *The reach τ of a manifold $\mathcal{M}$ defines the quantity*

$$\tau = \inf\{r > 0 : \exists x \neq y \in \mathcal{M}, v \in \mathbb{R}^D \text{ such that } r = \|x - v\| = \|y - v\| = \inf_{z \in \mathcal{M}} \|z - v\|\}.$$

Intuitively, if the distance of a point x to $\mathcal{M}$ is smaller than the reach, then there is a unique point in $\mathcal{M}$ that is closest to x. However, if the distance between x and $\mathcal{M}$ is larger than the reach, then there will no longer be a unique closest point to x in $\mathcal{M}$. For example, the reach of a sphere is its radius. A manifold with large and small reach is illustrated in Figure 2. The reach gives us control over the injectivity radius $\mathrm{inj}(\mathcal{M})$; in particular, we know $\mathrm{inj}(\mathcal{M}) \geq \pi\tau$ (see Aamari and Levrard [2019] for proof).

Density and Integration on Manifolds. To discuss the notion of a density q for a distribution Q on $\mathcal{M}$ we first define the *volume measure* on a manifold $\mathcal{M}$ and establish integration on $\mathcal{M}$.

Definition 4 (Volume measure)**.** *Let $\mathcal{M}$ be a compact d-dimensional Riemannian manifold. We define the volume measure $\mu_{\mathcal{M}}$ on $\mathcal{M}$ as the restriction of the d-dimensional Hausdorff measure $\mathcal{H}^d$.*

A definition for the restriction of the Hausdorff measure can be found in Federer Federer [1959]. We say that the distribution Q has density q if the Radon–Nikodym derivative of Q with respect to $\mu_{\mathcal{M}}$ is q. According to Evans and Gariepy [1992]), for any continuous function $f : \mathcal{M} \to \mathbb{R}$ supported within the image of the ball $B_{T_x\mathcal{M}}(0, \epsilon)$ under the exponential map for $\epsilon < \mathrm{inj}(\mathcal{M})$, we have

$$\int f \, dQ = \int (fq) \, d\mu_{\mathcal{M}} = \int_{B_{T_x\mathcal{M}}(0,\epsilon)} (fq) \circ \exp_x(v) \sqrt{\det g^x_{ij}(v)} \, dv. \tag{5}$$

Here $g^x_{ij}(v) = \langle \partial \exp_x(v)[e_i], \partial \exp_x(v)[e_j] \rangle$ with $(e_1, ..., e_d)$ an orthonormal basis of $T_x\mathcal{M}$. This is the associated Riemannian metric of $\mathcal{M}$.

Optimal Transport Theory. Let μ, ν be absolutely continuous measures on sets $X, Y \subseteq \mathbb{R}^d$. We say a function $f : X \to Y$ *transports* μ onto ν if $f_\sharp \mu = \nu$. So for all measurable A we have

$$\nu(A) = f_\sharp \mu(A) = \mu\left(f^{-1}(A)\right)$$

where $f^{-1}(A)$ is the pre-image of A under f. Optimal transport studies the maps taking source measures μ on X to target measures ν on Y which also minimize a cost $c : X \times Y \to \mathbb{R}_+$ among all such transport maps. However the results are largely restricted to transport between measures on the same dimensional Euclidean space. In this paper, we will make use of the main theorem in Caffarelli [1992].

Proposition 1. *Let $c(x, y) = \|x - y\|^2$ in $\mathbb{R}^d \times \mathbb{R}^d$ and let Ω_1, Ω_2 be nonempty, connected, bounded, open subsets of $\mathbb{R}^d$. Let f_1, f_2 be probability densities on Ω_1 and Ω_2 respectively, with f_1, g_1 bounded from above and below. Assume further that Ω_2 is convex. Then there exists a unique optimal transport map $T : \Omega_1 \to \Omega_2$ for the associated probability measures $\mu(dx) = f_1(x) \, dx$ and $\nu(dy) = f_2(y) \, dy$, and the cost c. Furthermore, we have that $T \in C^{0,\alpha}(\Omega_1)$ for some $\alpha \in (0, 1)$.*

This proposition allows to produce Hölder transport maps which can be further approximated with neural networks with size depending on a given accuracy.

3 Main Results

We will present our main results in this section, including an approximation theory for a large class of distributions on a regular manifold (Theorem 1), and a statistical estimation theory of deep generative networks for distribution learning (Theorem 2).

We make some regularity assumptions on a manifold $\mathcal{M}$ and assume the target data distribution Q is supported on $\mathcal{M}$. The easy-to-sample distribution ρ is taken to be uniform on $(0, 1)^{d+1}$.

Assumption 1. *$\mathcal{M}$ is a d-dimensional compact Riemannian manifold isometrically embedded in ambient dimension $\mathbb{R}^D$. Via compactness, $\mathcal{M}$ is bounded: there exists $M > 0$ such that $\|x\|_\infty \leq M$, $\forall x \in \mathcal{M}$. Further suppose $\mathcal{M}$ has a positive reach $\tau > 0$.*

Assumption 2. *Q is supported on $\mathcal{M}$ and has a density q with respect to the volume measure on $\mathcal{M}$. Further we assume boundedness of q i.e. there exists some constants $c, C > 0$ such that $c \leq q \leq C$.*

To justify the representation power of feedforward ReLU networks for learning the target distribution Q, we explicitly construct a neural network generator class, such that a neural network function in this generator class can pushfoward ρ to a good approximation of Q.

Consider the following generator class $\mathcal{G}_{\text{NN}}$

$$\begin{aligned}\mathcal{G}_{\text{NN}}(B,\kappa,L,p,K) = \{g = [g_1, ..., g_D] : \mathbb{R}^{d+1} \to \mathbb{R}^D | g_j \text{ in form (3) with at most } L \text{ layers} \\ \text{and max width } p, \text{ while } ||W_i||_\infty \leq \kappa, ||b_i||_\infty \leq \kappa \text{ for } i = 1, \ldots, L, \\ \sum_{i=1}^{L} ||W_i||_0 + ||b_i||_0 \leq K, \text{ and } ||g_j||_\infty \leq B \text{ for } j = 1, \ldots, D\},\end{aligned}$$

where $\|\cdot\|_\infty$ is the maximum magnitude in a matrix or vector, and $\|\cdot\|_0$ is the number of nonzero entries in a matrix or vector.

Theorem 1 (Approximation Power of Deep Generative Models)**.** *Suppose $\mathcal{M}$ and Q satisfy Assumption 1 and 2 respectively. The easy-to-sample distribution ρ is taken to be uniform on $(0,1)^{d+1}$. Then there exists a transport map $g^* \in C^{0,\alpha}((0,1)^{d+1})$ for some $\alpha \in (0,1)$ (independent of D) and Hölder coefficient $C_\alpha$such that*

$$\overset{*}{\sharp}\rho = Q.$$

Furthermore, for any $\epsilon > 0$, there exists a $g_\theta \in \mathcal{G}_{\text{NN}}(B,\kappa,L,p,K)$ with parameters

$$\begin{aligned}L =& O\left(\log\left(1+\frac{1}{\epsilon}\right)\right), \quad p = O\left(D\epsilon^{-\frac{d}{\alpha}}\right), \quad B = M, \\ \kappa =& \max(M, C_\alpha), \quad K = O\left(D\epsilon^{-\frac{d}{\alpha}}\log\left(1+\frac{1}{\epsilon}\right)\right),\end{aligned}$$

such that

$$W_1((g_\theta)_\sharp\rho, Q) < \epsilon.$$

Theorem 1 demonstrates the representation power of deep neural networks for distributions $\mathcal{M}$, which answers Question **Q1**. For a given accuracy ϵ, there exists a neural network g_θ which pushforward a uniform distribution on $(0,1)^{d+1}$ to a good approximation of Q with accuracy ϵ. The network size is exponential in the intrinsic dimension d.

We next present a statistical estimation theory to answer Question **Q2**.

Theorem 2 (Statistical Guarantees of Deep Wasserstein Learning)**.** *Suppose $\mathcal{M}$ and Q satisfy Assumption 1 and 2 respectively. The easy-to-sample distribution ρ is taken to be uniform on $(0,1)^{d+1}$. Let n be the number of samples of Q. Choose any $\delta > 0$. Set $\epsilon = n^{-\frac{1}{d+\delta}}$ in Theorem 1 so that the network class $\mathcal{G}_{\text{NN}}(B,\kappa,L,p,K)$ has parameters*

$$\begin{aligned}L =& O\left(\log\left(1+n^{\frac{1}{d+\delta}}\right)\right), \quad p = O\left(Dn^{\frac{d}{\alpha(d+\delta)}}\right), \quad B = M, \\ \kappa =& \max(M, C_\alpha), \quad K = O\left(Dn^{\frac{d}{\alpha(d+\delta)}}\log\left(1+n^{\frac{1}{d+\delta}}\right)\right).\end{aligned}$$

Then the empirical risk minimizer $\hat{g}_n$ given by (4) *has rate*

$$\mathbb{E}W_1((\hat{g}_n)_\sharp\rho, Q) \leq Cn^{-\frac{1}{d+\delta}}$$

where C is a constant independent of n and D.

Comparison to Related Works. To justify the practical power of generative networks, low-dimensional data structures are considered in Luise et al. [2020], Schreuder et al. [2021], Block et al. [2021], Chae et al. [2021]. These works consider the generative models in (1). They assume that the high-dimensional data are parametrized by low-dimensional latent parameters. Such assumptions

correspond to the manifold model where the manifold is globally homeomorphic to Euclidean space, i.e. the manifold has a single chart.

In Luise et al. [2020], the generative models are assumed to be continuously differentiable up to order s. By jointly training of the generator and the latent distributions, they proved that the Sinkhorn divergence between the generated distribution and data distribution converges, depending on data intrinsic dimension. Schreuder et al. [2021] assumes that the target distribution is a pushforward measure of a latent uniform distribution on a low-dimensional unit cube. Using Lipschitz generator, they proved that the Wasserstein-1 loss converges, depending on the low dimension of the latent space. A similar assumption is made in Chae et al. [2021], corresponding to the special case where the manifold has a single chart. More recently, Block et al. [2021] proposed to estimate the intrinsic dimension of data using the Hölder IPM between some empirical distributions of data. This theory is based on the statistical convergence of the empirical distribution to the data distribution. As an application to GANs, [Block et al., 2021, Theorem 23] gives the statistical error while the approximation error is not studied.

The aforementioned results consider a special case of the manifold which is globally homeomorphic to Euclidean space. A general manifold is locally homeomorphic to Euclidean space. This paper provides a general approximation theory and statistical guarantee for distributions on a manifold. A key ingredient is to explicitly construct an oracle transport map which transforms the low-dimensional easy-to-sample distribution to the data distribution. Our construction is new and novel. In comparison, the single-chart assumption in earlier works is very strong such that the oracle transport naturally exists by the assumption. Our work also provides insights about how distributions on a manifold can be approximated by a neural network pushforward of a low-dimensional easy-to-sample distribution.

4 Proof of Main Results

4.1 Proof Sketch of Approximation Theory in Theorem 1

To prove Theorem 1, we explicitly construct an oracle transport g^* pushing ρ onto Q, i.e. $g^*_\sharp \rho = Q$. Further this oracle will be piecewise α-Hölder continuous for some $\alpha \in (0, 1)$.

Lemma 1. *Suppose $\mathcal{M}$ and Q satisfy Assumption 1 and 2 respectively. The easy-to-sample distribution ρ is taken to be uniform on $(0, 1)^{d+1}$. Then there exists a function $g^* : (0, 1)^{d+1} \to \mathcal{M}$ such that $Q = g^*_\sharp \rho$ where*

$$g^*(x) = \sum_{j=1}^{J} \mathbb{1}_{(\pi_{j-1},\pi_j]}(x_1) g^*_j(x_{2:d+1}) \tag{6}$$

for some α-Hölder continuous functions $g^*_1, \ldots, g^*_J$ and some constants $0 = \pi_0 < \pi_1 < \cdots < \pi_J = 1$.

Proof. We sketch a proof here and attach a full proof in the appendix. The goal is to construct a transport map $g^* : (0, 1)^{d+1} \to \mathcal{M}$ that can be approximated by neural networks. First, we partition the manifold into geodesic Voronoi cells and map local distributions over the cells onto tangent planes. Then we transform the distribution on tangent planes to a distribution on a ball from which we can apply optimal transport theory to produce a map between the source distribution on $(0, 1)^d$ to a ball. Finally we glue together these local maps with indicators and a uniform random sample from $(0, 1)$. We proceed with the first step of partitioning the manifold.

Step 1: Voronoi decomposition. Given $\mathcal{M}$ under Assumption 1, we decompose $\mathcal{M}$ into a partition of finite geodesic Voronoi cells. This is done by first covering $\mathcal{M}$ with Euclidean balls around each point with uniform radius less than the global injectivity radius. Via compactness we can extract a finite subcover $\{U_j\}_{j=1}^J$ with centers $\{c_j\}_{j=1}^J$. We form a Voronoi partition of $\mathcal{M}$ denoted $\{V_j\}$ by taking the c_j as centers, i.e.

$$V_j = \{x \in \mathcal{M} : d_{\mathcal{M}}(x, c_j) = \min_{i\in[J]} d_{\mathcal{M}}(x, c_i)\}.$$

A Voronoi decomposition is illustrated in Figure 3. Given a distribution Q on $\mathcal{M}$ with density q, we can define local distributions Q_j as the conditional distribution of Q on V_j.

Step 2: Defining local lower-dimensional distributions. Next we transform local distribution Q_j on V_j into a distribution $\tilde{Q}_j$ on $\tilde{V}_j = \exp_{c_j}^{-1}(V_j)$ which is inverse of image of the jth Voronoi cell under the exponential map. In particular Q_j is the pushforward of $\tilde{Q}_j$ by the exponential map. The

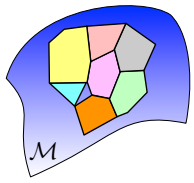

Figure 3: A Voronoi decomposition of $\mathcal{M}$.

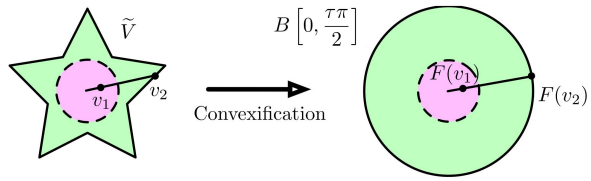

Figure 4: Expansion of star-shaped set into ball via F.

density of $\tilde{Q}_j$ given by

$$\tilde{q}_j(v) = q_j(\exp_{c_j}(v)) \left|\det J_{\exp_{c_j}}(v)\right|$$

via an application of formula (5). For simplicity, we use $\det J_{\exp_{c_j}}(v)$ to denote the Jacobian $\sqrt{\det g^x_{ij}(v)}$. $\tilde{Q}_j$ has two important properties. First, $\tilde{q}_j$ continues to be upper and lower-bounded and so we can still hope to apply optimal transport theory. Second, $\tilde{V}_j \subseteq T_{c_j}\mathcal{M}$ is a d-dimensional set on which $(\exp_{c_j})_\sharp \tilde{Q}_j = Q_j$. Ideally, to apply optimal transport theory, the target domain $\tilde{V}_j$ needs to be convex. However, $\tilde{V}_j$ is not convex here, but it is star-shaped. Recall a set S is star-shaped if $\exists\, x \in S$ such that for all $y \in S$, the set $[x : y] = \{\lambda x + (1-\lambda)y : \lambda \in [0,1]\} \subseteq S$. For an excellent reference on star-shaped sets see Hansen et al. [2020]. This property is crucial and allows us to transform our target domain $\tilde{V}_j$ to a ball via a bi-Lipschitz transformation.

Step 3: Convexifying the Target Domain $\tilde{V}_j$. As we claim above, the target domain $\tilde{V}_j$ is star-shaped and centered at 0. $\tilde{V}_j$ is also bounded and closed and hence compact. Further we know for some $\eta > 0$, $B(0,\eta) \subseteq \tilde{V}_j$. Then we can apply the following lemma to produce a bi-Lipschitz transformation $F : \tilde{V}_j \to B\left(0, \frac{\tau\pi}{2}\right)$, where τ is the reach of $\mathcal{M}$.

Lemma 2. *Let S be a compact star-shaped set centered at 0. Further suppose $\exists \eta > 0$ such that $B(0,\eta) \subseteq S$. Let $L > 0$ be such that $S \subseteq B[0,L]$. Then there exists $F : S \to B[0,L]$ such that F is bi-Lipschitz with constant C dependent on L, η.*

Lemma 2 is proved in the appendix. The main idea is that the bi-Lipschitz map is constructed explicitly by expanding along rays (see Figure 4). Theorem 1 from Toranzos [1967] tells us the radial function on S which computes the radius of $\tilde{V}_j$ in a direction $u \in \mathbb{S}^{d-1}$ is Lipschitz. From this we can construct bi-Lipschitz F_j by fixing points in a ball of radius $\eta/2$ and expanding points at a rate dependent on its distance from $B(0,\eta/2)$ and $R(x)$. Note that we apply Lemma 2 to obtain a map from the closure of $\tilde{V}_j$ to $B\left[0, \frac{\tau\pi}{2}\right]$, which we can then restrict to $\tilde{V}_j$ to obtain a bi-Lipschitz map from $\tilde{V}_j$ to $B(0,L)$. We can define a new distribution $\tilde{\rho}_j$ on $B\left(0, \frac{\tau\pi}{2}\right)$ with density

$$\tilde{p}_j(x) = \tilde{q}(F_j^{-1}(x)) \left|\det J_{F_j^{-1}}(x)\right|.$$

It is important F_j is bi-Lipschitz with constant C as then $\frac{1}{C^d} \leq |\det J_{F_j}(x)| \leq C^d$ and we know $\tilde{p}_j$ is upper and lower-bounded. Further we can write $(F_j^{-1})_\sharp \tilde{\rho}_j = \tilde{Q}_j$ by g_j^*.

Step 4: Constructing the local transport. Now we have a distribution $\tilde{\rho}_j$ with density $\tilde{p}_j$ defined on convex ball $B\left(0, \frac{\tau\pi}{2}\right)$. Further $\tilde{p}_j$ is upper and lower bounded. Set ρ_d to be uniform on $(0,1)^d$. Hence we may apply Proposition 1 to produce a transport map $T_j : (0,1)^d \to B\left(0, \frac{\tau\pi}{2}\right)$ such that $(T_j)_\sharp \rho_d = \tilde{\rho}$. Further T_j is Hölder with Hölder exponent α_j for some $\alpha_j \in (0,1)$. Writing $g_j^* : (0,1)^d \to V_j$ via

$$g_j^*(x) = \exp_{c_j} \circ F_j^{-1} \circ T_j(x) \tag{7}$$

gives rise to $(g_j^*)_\sharp \rho_d = Q_j$. This transport map g_j^* is illustrated in Figure 5. Further g_j^* is the composition of two Lipschitz functions with an α_j-Hölder continuous function and is therefore α_j-Hölder continuous. Thus we can push a uniform distribution on $(0,1)^d$ onto a local patch V_j, as shown in Figure 5.

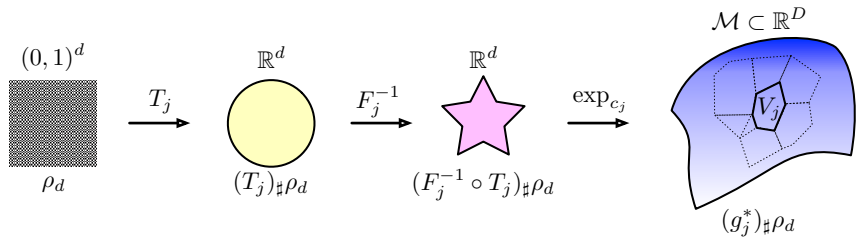

Figure 5: Local transport g_j^* in (7) mapping ρ_d on $(0,1)^d$ to a local distribution $\mathcal{M}$ supported on V_j.

Step 5: Constructing the global transport. Via step 4 we have local transports g_j^* pushing forward ρ_d uniform on $(0,1)^d$ to local distribution Q_j. By setting Set $\pi_j = Q(\bigcup_{i=1}^j V_i)$. Now we define $g^* : (0,1)^{d+1} \to \mathcal{M}$ via (6) where x_1 is the first component of x and $x_{2:d+1}$ are the remaining components.

Set $X \sim \rho$. Then X_1 randomly selects the patch V_j with probability equal to $Q(V_j)$, and g_j^* pushes $X_{2:d+1}$ forward to V_j such that $g_j^*(X_{2:d+1})$ is distributed according to Q_j. Finally note that the overlap of of the Voronoi cells V_i and V_j while $i \neq j$ has measure 0. Hence $g^*(X)$ is distributed on $\mathcal{M}$ according to Q. This constructs the oracle g^*. Furthermore, we note that each of the g_j^* is α_j-Hölder continuous, so by setting $\alpha = \min_j \alpha_j$ we obtain that all of the g_j^* are α-Hölder continuous, which complete the proof of Lemma 1. □

With the oracle g^* we can design a neural network g_θ to approximate this oracle g^*. In order to minimize $W_1((g_\theta)_\sharp\rho, Q) = W_1((g_\theta)_\sharp\rho, g^*_\sharp\rho)$, we show it suffices to have g_θ approximate g^* in $L^1(\rho)$.

Lemma 3. *Let μ be an absolutely continuous probability distribution on a set $Z \subseteq \mathbb{R}^d$, and let $f, g : Z \to R^m$ be transport maps. Then*

$$W_1(f_\sharp\mu, g_\sharp\mu) \leq C\|f - g\|_{L^1(\mu)}$$

for some $C > 0$.

Lemma 3 is proved in the appendix. We next provide a proof sketch of Theorem 1.

Proof of Theorem 1. We sketch a proof here and attach a full proof in the appendix. Note $\|f - g\|_{L^1(\rho)} = \sum_{i=1}^m \|f^i - g^i\|_{L^1(\rho)}$ so we may approximate g^* component wise. To approximate g^* in $L^1(\rho)$ we must approximate indicators $\mathbb{1}_{[\pi_{j-1},\pi_j)}$, multiplication of the indicator $\mathbb{1}_{[\pi_{j-1},\pi_j)}$ and g_j^*, and the α-Hölder function g_j^*. Thus we decompose $\|g^* - g_\theta\|$ into three error terms:

$$\|g^* - g_\theta\|_{L^1(\rho)} \leq J\delta_1 + JM\delta_2 + D\delta_3$$

where δ_1 is the error of the indicator approximation, δ_2 is the error of the multiplication approximation, and δ_3 is the error of the local transport map approximation. Via Shen et al. [2019] we can approximate α-Hölder continuous functions up to ϵ accuracy in $L^1(\rho)$ with $O(log(1+\frac{1}{\epsilon}))$ layers and $O(\epsilon^{-\frac{d}{\alpha}} log(1+\frac{1}{\epsilon}))$ neurons. We can approximate indicators in $L^1(\rho)$ by a shallow network with fixed depth. Finally we can approximate multiplication as in Yarotsky [2017]. This allows us to make $\delta_1, \delta_2, \delta_3$ arbitrarily small with network size depending on the accuracy ϵ. □

4.2 Proof Sketch of Statistical Estimation Theory in Theorem 2

The proof of theorem 2 is facilitated by the common bias-variance inequality, presented here as a lemma.

Lemma 4. *Under the same assumptions of Theorem 2, we have*

$$\mathbb{E}W_1((\hat{g}_n)_\sharp\rho, Q) \leq \inf_{g_\theta \in \mathcal{G}_{\text{NN}}} W_1((g_\theta)_\sharp\rho, Q) + 2\mathbb{E}W_1(\hat{Q}_n, Q) \tag{8}$$

Lemma 4 is proved in the appendix.

In the right hand side of (8), the first term is the approximation error and the second term is the statistical error. This naturally decomposes the problem into two parts: one controlling the approximation error and the other controlling the statistical error. To minimize the bias term we can apply Theorem 1. For the statistical error we leverage existing theory to obtain the following lemma.

Lemma 5. *Under the same assumptions of Theorem 2, for all $\delta > 0$, $\exists C_\delta > 0$ such that*

$$\mathbb{E}\left[W_1(Q, \hat{Q}_n)\right] \leq C_\delta n^{-\frac{1}{d+\delta}}. \tag{9}$$

Proof. Let $\delta > 0$. Consider the manifold $\mathcal{M}$ with the geodesic distance as a metric space. Then by [Weed and Bach, 2019, Theorem 1] applied to $\mathcal{M}$ with the geodesic distance, we have that $\mathbb{E}\left[W_1^{\mathcal{M}}(Q, \hat{Q}_n)\right] \leq C_\delta n^{-\frac{1}{d+\delta}}$ for some constant C_δ independent of n. Here, $W_1^{\mathcal{M}}$ is the 1-Wasserstein distance on $\mathcal{M}$ with the geodesic distance. It suffices to show that $W_1(Q, \hat{Q}_n) \leq W_1^{\mathcal{M}}(Q, \hat{Q}_n)$. Let $\mathrm{Lip}_1(\mathbb{R}^{\mathrm{D}})$ and $\mathrm{Lip}_1(\mathcal{M})$ denote the set of 1-Lipschitz functions defined on $\mathcal{M}$ with respect to the Euclidean distance on $\mathbb{R}^D$ and geodesic distance on $\mathcal{M}$ respectively. But note that $\mathrm{Lip}_1(\mathbb{R}^{\mathrm{D}}) \subseteq \mathrm{Lip}_1(\mathcal{M})$ because for any $f \in \mathrm{Lip}_1(\mathbb{R}^{\mathrm{D}})$ we have

$$\frac{|f(x) - f(y)|}{\|x - y\|_{\mathcal{M}}} \leq \frac{|f(x) - f(y)|}{\|x - y\|_{\mathbb{R}^D}} \leq 1$$

as $\|x - y\|_{\mathcal{M}} \leq \|x - y\|_{\mathbb{R}^D}$ and hence $f \in \mathrm{Lip}_1(\mathcal{M})$. Thus

$$\mathbb{E}\left[W_1(Q, \hat{Q}_n)\right] \leq \mathbb{E}\left[W_1^{\mathcal{M}}(Q, \hat{Q}_n)\right] \leq C_\delta n^{-\frac{1}{d+\delta}}.$$

□

Finally we prove our statistical estimation result in Theorem 2.

Proof of Theorem 2. Choose $\delta > 0$. Recall from Lemma 4 we have

$$W_1((\hat{g}_n)_\sharp \rho, Q) \leq \inf_{g_\theta} W_1((g_\theta)_\sharp \rho, Q) + 2W_1(\hat{Q}_n, Q)$$

The first term is the approximation error which can be controlled within an arbitrarily small accuracy ϵ by Theorem 1. The second term is the statistical error for which we recall from Lemma 5 that $\mathbb{E}\left[W_1(\hat{Q}_n, Q)\right] \leq C_\delta n^{-\frac{1}{d+\delta}}$ for some constant C_δ.

Theorem 1 shows the existence of a neural network function g_θ with $O\left(\log\left(1 + \frac{1}{\epsilon}\right)\right)$ layers and $O(D\epsilon^{-d/\alpha}\log(1 + \frac{1}{\epsilon}))$ neurons such that $W_1((g_\theta)_\sharp \rho, Q) \leq \epsilon$ for any $\epsilon > 0$. We choose $\epsilon = n^{-\frac{1}{d+\delta}}$ to optimally balance the approximation error and the statistical error. Thus we have

$$\mathbb{E}W_1((\hat{g}_n)_\sharp \rho, Q) \leq n^{-\frac{1}{d+\delta}} + 2C_\delta n^{-\frac{1}{d+\delta}} = Cn^{-\frac{1}{d+\delta}},$$

by setting $C = 1 + 2C_\delta$. □

5 Conclusion

We have established approximation and statistical estimation theories of deep generative models for estimating distributions on a low-dimensional manifold. The statistical convergence rate in this paper depends on the intrinsic dimension of data. In light of the manifold hypothesis, which suggests many natural datasets lie on low dimensional manifolds, our theory rigorously explains why deep generative models defy existing theoretical sample complexity estimates and the curse of dimensionality. In fact, deep generative models are able to learn low-dimensional geometric structures of data, and allow for highly efficient sample complexity independent of the ambient dimension. Meanwhile the size of the required network scales exponentially with the intrinsic dimension.

Our theory imposes very little assumption on the target density Q, requiring only that it admit a density q with respect to the volume measure and that q is upper and lower bounded. In particular we make no smoothness assumptions on q. This is practical, as we do not expect existing natural datasets to exhibit high degrees of smoothness.

In this work we assume access to computation of the W_1 distance. However during GAN training a discriminator is trained for this purpose. It would be of interest for future work to investigate the low-dimensional role of such discriminator networks which approximate the W_1 distance in practice.

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Checklist

The checklist follows the references. Please read the checklist guidelines carefully for information on how to answer these questions. For each question, change the default **[TODO]** to [Yes] , [No] , or [N/A] . You are strongly encouraged to include a **justification to your answer**, either by referencing the appropriate section of your paper or providing a brief inline description. For example:

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   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
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