Geometric Understanding of Deep Learning

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Thanks for the invitation.
These projects are collaborated with Prof. Shing-Tung Yau, Prof. Dimitris Samaras, Prof. Zhongxuan Luo, Prof. Na Lei and many other mathematicians, computer scientists.
Why does DL work?

Problem

1. What does a DL system really learn?
2. How does a DL system learn? Does it really learn or just memorize?
3. How well does a DL system learn? Does it really learn everything or have to forget something?

Till today, the understanding of deep learning remains primitive.
Why does DL work?

1. What does a DL system really learn?
   
   *Probability distributions on manifolds.*

2. How does a DL system learn? Does it really learn or just memorize?

   *Optimization in the space of all probability distributions on a manifold. A DL system both learns and memorizes.*

3. How well does a DL system learn? Does it really learn everything or have to forget something?

   *Current DL systems have fundamental flaws, mode collapsing.*
Manifold Distribution Principle
Helmholtz Hypothesis

Half of the brain is devoted to vision, Helmholtz hypothesized that vision solves an inverse problem, i.e., inferring the most likely causes of the retina image. In modern language, the brain learns a generative model of visual images, and visual perception is to infer the latent variables of this generative model. The generative model with its multiple layers of latent variables form a representation of our visual world.

About representation learning, the basic idea is that the brain represents a concept by a group of neurons, or latent variables, that form a vector. Sometimes it is also called embedding, i.e., we embed the concept into a multi-dimensional Euclidean space, which is sometimes called latent space.
We believe the great success of deep learning can be partially explained by the well accepted manifold distribution and the clustering distribution principles:

**Manifold Distribution**
A natural data class can be treated as a probability distribution defined on a low dimensional manifold embedded in a high dimensional ambient space.

**Clustering Distribution**
The distances among the probability distributions of subclasses on the manifold are far enough to discriminate them.
LeCun’s MNIST handwritten digits samples on manifold

Each image $28 \times 28$ is treated as a point in the image space $\mathbb{R}^{28 \times 28}$.

The hand-written digits image manifold is only two dimensional;

Each digit corresponds to a distribution on the manifold.
Figure: Each cluster corresponds to a hand written digit. Multiple clusters may correspond to the same digit.
Different embedding result with inferior quality by a Siamese network.
UMap embedding, the samples between modes produce obscure images, which is called mode mixture.
Ambient Space - image space $\mathbb{R}^n$

- manifold - Support of a distribution $\mu$
- parameter domain - latent space $\mathbb{R}^m$
- coordinates map $\varphi_i$ - encoding/decoding maps
- $\varphi_{ij}$ controls the probability measure
Low Dimensional Example

Image space $\mathcal{X}$ is $\mathbb{R}^3$; the data manifold $\Sigma$ is the happy buddha.
The encoding map is $\varphi_i : \Sigma \to \mathcal{L}$; the decoding map is $\varphi_i^{-1} : \mathcal{L} \to \Sigma$. 

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The automorphism of the latent space $\varphi_{ij} : \mathcal{L} \rightarrow \mathcal{L}$ is the chart transition.
Uniform distribution $\zeta$ on the latent space $\mathcal{L}$, non-uniform distribution on $\Sigma$ produced by a decoding map.
Uniform distribution $\zeta$ on the latent space $\mathcal{Z}$, uniform distribution on $\Sigma$ produced by another decoding map.
Central Tasks

1. Learn the manifold structure;
2. Learn the probability distribution.
Generative Model Framework

Training Data | Latent Distribution | Generated Samples
---|---|---
encoder | decoder

Transport Map

white noise

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AE-OT Framework

Training Data → encoder → Latent Distribution → decoder → Generated Samples

OT Mapper

Brenier Potential

white noise
One facial image is determined by a finite number of genes, lighting conditions, camera parameters, therefore all facial images form a manifold.
Given a parametric representation $\varphi : \mathcal{H} \rightarrow \Sigma$, randomly generate a parameter $z \in \mathcal{H}$ (white noise), $\varphi(z) \in \Sigma$ is a human facial image.
Manifold Learning
Lemma (Urysohn’s Lemma)

Let $A, B$ be closed subsets of a normal topological space $X$. There exists a continuous function $f : X \to [0, 1]$ such that $f(A) = 0$ and $f(B) = 1$.

Figure: Urysohn’s lemma provides the theoretic tool for pattern recognition, supervised learning.
Theorem (General Position Theorem)

*Any* $m$-*manifold unknots in* $\mathbb{R}^n$ *provided* $n \geq 2m + 2$.

In deep learning, this means that data is easier to manipulate once it is embedded in higher dimensions.

**Figure:** Increase the dimension of the embedding space to unlink the manifolds.
Theorem (Whitney Embedding)

Any smooth real m-dimensional manifold (required also to be Hausdorff and second-countable) can be smoothly embedded in the real 2m-space ($\mathbb{R}^{2m}$).

1. Construct an atlas, $M \subset \bigcup_{i=1}^{k} U_i$;
2. Build a partition of unity;
3. Embed each open set in $\mathbb{R}^{m}$;
4. Glue the local embeddings to embed $M$ in $\mathbb{R}^{km}$;
5. Random projection to lower dimension.
Related to the Hilbert 13th Problem,

**Theorem (Kolmogorov-Arnold Representation)**

If $f$ is a multivariate continuous function, then $f$ can be written as a finite composition of continuous functions of a single variable and the binary operation of addition.

$$f(x_1, x_2, \ldots, x_n) = \sum_{q=0}^{2n} \Phi_q \left( \sum_{p=1}^{n} \varphi_{p,q}(x_p) \right)$$
Construct a sequence of nested mapping spaces, $\mathcal{F}_{k+1}$ is simpler than $\mathcal{F}_k$,

$$\mathcal{F}_0 \supset \mathcal{F}_1 \supset \mathcal{F}_2 \cdots \supset \mathcal{F}_n,$$

each mapping $f \in \mathcal{F}_k$ can be approximated by a finite composition of mappings $g_1, g_2, \ldots, g_r \in \mathcal{F}_{k+1}$,

$$f = g_1 \circ g_2 \circ g_3 \cdots g_r.$$ $\mathcal{F}_n$ can be computed by deep neural networks.
General $C^2$ diffeomorphisms can be approximated by the followings steps:

1. By finite composition of diffeomorphisms with compact support;
2. By finite composition of flow mappings $\varphi_s$:
   \[
   \frac{d}{dt} \varphi(p, t) = v(\varphi(p, t), t), \quad \varphi(p, 0) = id;
   \]
3. By finite composition of near id maps
   \[|Dg - I| < \delta;\]
4. By deep neural networks, such as affine coupling flows etc, which grantee the mapping is invertible;
**Figure**: Auto-encoder architecture.

Ambient space $\mathcal{X}$, latent space $\mathcal{L}$, encoding map $\varphi_\theta : \mathcal{X} \to \mathcal{L}$, decoding map $\psi_\theta : \mathcal{L} \to \mathcal{X}$. 
Encoding/Decoding

Figure: Auto-encoder pipeline.
ReLU DNN

**Definition (ReLU DNN)**

For any number of hidden layers \( k \in \mathbb{N} \), input and output dimensions \( w_0, w_{k+1} \in \mathbb{N} \), a \( \mathbb{R}^{w_0} \rightarrow \mathbb{R}^{w_{k+1}} \) ReLU DNN is given by specifying a sequence of \( k \) natural numbers \( w_1, w_2, \ldots, w_k \) representing widths of the hidden layers, a set of \( k \) affine transformations \( T_i : \mathbb{R}^{w_{i-1}} \rightarrow \mathbb{R}^{w_i} \) for \( i = 1, \ldots, k \) and a linear transformation \( T_{k+1} : \mathbb{R}^{w_k} \rightarrow \mathbb{R}^{w_{k+1}} \) corresponding to weights of hidden layers.

The mapping \( \varphi_{\theta} : \mathbb{R}^{w_0} \rightarrow \mathbb{R}^{w_{k+1}} \) represented by this ReLU DNN is

\[
\varphi = T_{k+1} \circ \sigma \circ T_k \circ \cdots \circ T_2 \circ \sigma \circ T_1, \tag{1}
\]

where \( \circ \) denotes mapping composition, \( \theta \) represent all the weight and bias parameters.
Fix the encoding map $\varphi_\theta$, let the set of all neurons in the network is denoted as $\mathcal{I}$, all the subsets is denoted as $2^\mathcal{I}$.

**Definition (Activated Path)**

Given a point $x \in \mathcal{X}$, the *activated path* of $x$ consists all the activated neurons when $\varphi_\theta(x)$ is evaluated, and denoted as $\rho(x)$. Then the activated path defines a set-valued function $\rho : \mathcal{X} \rightarrow 2^\mathcal{I}$. 
Fix a encoding map $\varphi_{\theta}$ represented by a ReLU DNN, two data points $x_1, x_2 \in \mathcal{X}$ are *equivalent*, denoted as $x_1 \sim x_2$, if they share the same activated path, $\rho(x_1) = \rho(x_2)$. Then each equivalence relation partitions the ambient space $\mathcal{X}$ into cells,

$$D(\varphi_{\theta}) : \mathcal{X} = \bigcup_{\alpha} U_\alpha,$$

each equivalence class corresponds to a cell: $x_1, x_2 \in U_\alpha$ if and only if $x_1 \sim x_2$. $D(\varphi_{\theta})$ is called the cell decomposition induced by the encoding map $\varphi_{\theta}$.

Furthermore, $\varphi_{\theta}$ maps the cell decomposition in the ambient space $D(\varphi_{\theta})$ to a cell decomposition in the latent space.
Piecewise Linear Mapping

d. cell decomposition $\mathcal{D}(\varphi_\theta)$
e. latent space cell decomposition
f. cell decomposition $\mathcal{D}(\psi_\theta \circ \varphi_\theta)$

Piecewise linear encoding/decoding maps induce cell decompositions of the ambient space and the latent space.
Definition (Learning Capability)

Given a ReLU DNN $N(w_0, \ldots, w_{k+1})$, its rectified linear complexity is the upper bound of the number of pieces of all PL functions $\varphi_\theta$ represented by $N$,

$$N(N) := \max_{\theta} N(\varphi_\theta),$$

where $N(\varphi_\theta)$ is the number of pieces of the PL function $\varphi_\theta$.

This gives a measurement for the representation capability of a neural network.
Lemma

The maximum number of parts one can get when cutting $d$-dimensional space $\mathbb{R}^d$ with $n$ hyperplanes is denoted as $C(d, n)$, then

$$C(d, n) = \binom{n}{0} + \binom{n}{1} + \binom{n}{2} + \cdots + \binom{n}{d}.$$  \hfill (2)

Proof.

Suppose $n$ hyperplanes cut $\mathbb{R}^d$ into $C(d, n)$ cells, each cell is a convex polyhedron. The $(n+1)$-th hyperplane is $\pi$, then the first $n$ hyperplanes intersection $\pi$ and partition $\pi$ into $C(d - 1, n)$ cells, each cell on $\pi$ partitions a polyhedron in $\mathbb{R}^d$ into 2 cells, hence we get the formula

$$C(d, n + 1) = C(d, n) + C(d - 1, n).$$
Theorem (Rectified Linear Complexity of a ReLU DNN)

Given a ReLU DNN \( N(w_0, \ldots, w_{k+1}) \), representing PL mappings 
\[ \varphi_{\theta} : \mathbb{R}^{w_0} \rightarrow \mathbb{R}^{w_{k+1}} \]
with \( k \) hidden layers of widths \( \{w_i\}_{i=1}^{k} \), then the linear rectified complexity of \( N \) has an upper bound,

\[ \mathcal{N}(N) \leq \prod_{i=1}^{k+1} \mathcal{C}(w_{i-1}, w_i). \] (3)
Definition (Linear Rectifiable Manifold)
Suppose $M$ is a $m$-dimensional manifold, embedded in $\mathbb{R}^n$, we say $M$ is linear rectifiable, if there exists an affine map $\varphi : \mathbb{R}^n \to \mathbb{R}^m$, such that the restriction of $\varphi$ on $M$, $\varphi|_M : M \to \varphi(M) \subset \mathbb{R}^m$, is homeomorphic. $\varphi$ is called the corresponding rectified linear map of $M$. 

a. linear rectifiable  
b. non-linear-rectifiable
Definition (Linear Rectifiable Atlas)

Suppose $M$ is a $m$-dimensional manifold, embedded in $\mathbb{R}^n$, $\mathcal{A} = \{(U_\alpha, \varphi_\alpha)\}$ is an atlas of $M$. If each chart $(U_\alpha, \varphi_\alpha)$ is linear rectifiable, $\varphi_\alpha : U_\alpha \to \mathbb{R}^m$ is the rectified linear map of $U_\alpha$, then the atlas is called a linear rectifiable atlas of $M$.

Definition (Rectified Linear Complexity of a Manifold)

Suppose $M$ is a $m$-dimensional manifold embedded in $\mathbb{R}^n$, the rectified linear complexity of $M$ is denoted as $\mathcal{N}(\mathbb{R}^n, M)$ and defined as,

$$\mathcal{N}(\mathbb{R}^n, M) := \min \{|\mathcal{A}| \mid \mathcal{A} \ 	ext{is a linear rectifiable atlas of} \ M\} .$$

(4)
**Encodable Condition**

**Definition (Encoding Map)**

Suppose $M$ is a $m$-dimensional manifold, embedded in $\mathbb{R}^n$, a continuous mapping $\varphi : \mathbb{R}^n \to \mathbb{R}^m$ is called an encoding map of $(\mathbb{R}^n, M)$, if restricted on $M$, $\varphi|_M : M \to \varphi(M) \subset \mathbb{R}^m$ is homeomorphic.

**Theorem (Encodable Condition)**

Suppose a ReLU DNN $N(w_0, \ldots, w_{k+1})$ represents a PL mapping $\varphi_\theta : \mathbb{R}^n \to \mathbb{R}^m$, $M$ is a $m$-dimensional manifold embedded in $\mathbb{R}^n$. If $\varphi_\theta$ is an encoding mapping of $(\mathbb{R}^n, M)$, then the rectified linear complexity of $N$ is no less than the rectified linear complexity of $(\mathbb{R}^n, M)$,

$$\mathcal{N}(\mathbb{R}^n, M) \leq \mathcal{N}(\varphi_\theta) \leq \mathcal{N}(N).$$
Theorem

Given any ReLU deep neural network \( N(w_0, w_1, \ldots, w_k, w_{k+1}) \), there is a manifold \( M \) embedded in \( \mathbb{R}^{w_0} \), such that \( M \) cannot be encoded by \( N \).

Figure: \( \mathcal{N}(\mathbb{R}^2, C_n) \geq 4^{n+1} \)
Probability Measure Learning
A generative model converts a white noise into a facial image.
GAN model

Training Data → encoder → Latent Distribution → decoder → Generated Samples

Discriminator

transporter

Generator

white noise

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GAN Overview

Figure: GAN DNN model.

Figure: GAN learning process.
Wasserstein GAN Model

- $\mathcal{X}$ - image space
- $\Sigma$ - supporting manifold
- $\mathcal{Z}$ - latent space
- $D : W_c(\mu_\theta, \nu), \varphi_\xi$ is the Wasserstein distance.
Wasserstein GAN Model

\[ \Sigma \]
\[ \mathcal{X} \]
\[ G : g_\theta \]
\[ \mu_\theta \]
\[ \zeta \]
\[ \mathcal{Z} \]
\[ \nu \]
\[ D : W_c(\mu_\theta, \nu), \varphi_\xi \]

\( \nu \)-training data distribution; \( \zeta \)-uniform distribution; 
\( \mu_\theta = g_\theta \# \zeta \)-generated distribution; \( G \) - generator computes \( g_\theta \); 
\( D \) - discriminator, measures the Wasserstein distance between \( \nu \) and \( \mu_\theta \), \( W_c(\mu_\theta, \nu) \).
Optimal Transport Framework
Overview

Motivation

- Given a manifold $X$, all the probability distributions on $X$ form an infinite dimensional manifold, Wasserstein Space $\mathcal{P}(X)$;
- Deep Learning tasks are reduced to optimization in $\mathcal{P}(X)$, such as the principle of maximum entropy principle, maximum likely hood estimation, maximum a posterior estimation and so on;
- DL tasks requires variational calculus, Riemannian metric structure defined on $\mathcal{P}(X)$. 

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Solution

- Optimal transport theory discovers a natural Riemannian metric of $\mathcal{P}(X)$, called Wasserstein metric;
- the covariant calculus on $\mathcal{P}(X)$ can be defined accordingly;
- the optimization in $\mathcal{P}(X)$ can be carried out.
The geodesic distance between $d\mu = f(x)dx$ and $d\nu(y) = g(y)dy$ is given by the optimal transport map $T : X \to X$, $T = \nabla u$,

$$\det \left( \frac{\partial^2 u}{\partial x_i \partial x_j} \right) = \frac{f(x)}{g \circ \nabla u(x)}.$$ 

The geodesic between them is McCann’s displacement,

$$\gamma(t) := ((1 - t)I + t\nabla u) \# \mu$$

The tangent vectors of a probability measure is a gradient field on $X$, the Riemannian metric is given by

$$\langle d\varphi_1, d\varphi_2 \rangle = \int_X \langle d\varphi_1, d\varphi_2 \rangle_g f(x)dx.$$
Equivalence to Conventional DL Methods

- Entropy function is convex along the geodesics on $\mathcal{P}(X)$;
- The Hessian of entropy defines another Riemannian metric of $\mathcal{P}(X)$;
- The Wasserstein metric and the Hessian metric are equivalent in general;
- Entropy optimization is the foundation of Deep Learning;
- Therefore Wasserstein-metric driven optimization is equivalent to entropy optimization.
Monge Problem

Problem (Monge)

Find a measure-preserving transportation map $T : (X, \mu) \to (Y, \mu)$ that minimizes the transportation cost,

$$(MP) \quad \min_{T \# \mu = \nu} \mathcal{C}(T) = \min_{T \# \mu = \nu} \int_X c(x, T(x)) d\mu(x).$$

such kind of map is called the optimal mass transportation map.

Definition (Wasserstein distance)

The transportation cost of the optimal transportation map $T : (X, \mu) \to (Y, \nu)$ is called the Wasserstein distance between $\mu$ and $\nu$, denoted as

$$W^2_c(\mu, \nu) := \min_{T \# \mu = \nu} \mathcal{C}(T).$$
Kantorovich relaxed transportation maps to transportation schemes.

Problem (Kantorovich)

Find an optimal transportation scheme, namely a joint probability measure \( \rho \in \mathcal{P}(X \times Y) \), with marginal measures \( \rho_{x\#} = \mu, \rho_{y\#} = \nu \), that minimizes the transportation cost,

\[
(KP) \quad \min_{\rho} \left\{ \int_{X \times Y} c(x, y) \, d\rho(x, y) \bigg| \rho_{x\#} = \mu, \rho_{y\#} = \nu \right\}.
\]

Kantorovich solved this problem by inventing linear programming, and won Nobel’s prize in economics in 1975.
By the duality of linear programming, Kantorovich problem has the dual form:

Problem (Kantorovich Dual)

Find functions $\varphi : X \rightarrow \mathbb{R}$ and $\psi : Y \rightarrow \mathbb{R}$, such that

$$(DP) \quad \max_{\varphi, \psi} \left\{ \int_{X} \varphi(x) du(x) + \int_{Y} \psi(y) dv(y), \varphi(x) + \psi(y) \leq c(x, y) \right\}.$$
Definition (c-transformation)

Given a function \( \varphi : X \to \mathbb{R} \), and \( c(x, y) : X \times Y \to \mathbb{R} \), its c-transform \( \varphi^c : Y \to \mathbb{R} \) is given by

\[
\varphi^c(y) := \inf_{x \in X} \{ c(x, y) - \varphi(x) \}.
\]

Problem (Kantorovich Dual)

The Kantorovich Dual problem can be reformulated as

\[
(DP) \quad \max_{\varphi} \left\{ \int_X \varphi(x) du(x) + \int_Y \varphi^c(y) dv(y) \right\}.
\]

\( \varphi \) is called Kantorovich potential.
Theorem (Brenier)

If $\mu, \nu > 0$ and $X$ is convex, and the cost function is quadratic distance,

$$c(x, y) = \frac{1}{2} |x - y|^2$$

then there exists a convex function $u : X \to \mathbb{R}$ unique up to a constant, such that the unique optimal transportation map is given by the gradient map

$$T : x \mapsto \nabla u(x).$$

Problem (Brenier)

Find a convex function $u : X \to \mathbb{R}$, such that

$$(BP) \quad (\nabla u)_{\#} \mu = \nu,$$

$u$ is called the Brenier potential.
From Jacobian equation, one can get the necessary condition for Brenier potential.

**Problem (Brenier)**

*Find the $C^2$ Brenier potential $u : X \rightarrow \mathbb{R}$ satisfies the Monge-Ampere equation*

\[
(BP) \quad \det \left( \frac{\partial^2 u}{\partial x_i \partial x_j} \right) = \frac{\mu(x)}{v(\nabla f(x))}.
\]
Convex Geometry
Minkowski Problem

Given $k$ unit vectors $\mathbf{n}_1, \ldots, \mathbf{n}_k$ not contained in a half-space in $\mathbb{R}^n$ and $A_1, \ldots, A_k > 0$, such that

$$\sum_i A_i \mathbf{n}_i = 0,$$

find a compact convex polytope $P$ with exactly $k$ codimension-1 faces $F_1, \ldots, F_k$, such that

1. $\text{area}(F_i) = A_i$,
2. $\mathbf{n}_i \perp F_i$. 
Theorem (Minkowski)

$P$ exists and is unique up to translations.
Theorem (Alexandrov 1950)

Given $\Omega$ compact convex domain in $\mathbb{R}^n$, $p_1, \cdots, p_k$ distinct in $\mathbb{R}^n$, $A_1, \cdots, A_k > 0$, such that $\sum A_i = \text{Vol}(\Omega)$, there exists PL convex function

$$f(x) := \max\{\langle x, p_i \rangle + h_i | i = 1, \cdots, k\}$$

unique up to translation such that

$$\text{Vol}(W_i) = \text{Vol}(\{x|\nabla f(x) = p_i\}) = A_i.$$ 

Alexandrov’s proof is topological, not variational. It has been open for years to find a constructive proof.
Variational Proof

Theorem (Gu-Luo-Sun-Yau 2013)

\( \Omega \) is a compact convex domain in \( \mathbb{R}^n \), \( y_1, \cdots, y_k \) distinct in \( \mathbb{R}^n \), \( \mu \) a positive continuous measure on \( \Omega \). For any \( \nu_1, \cdots, \nu_k > 0 \) with \( \sum \nu_i = \mu(\Omega) \), there exists a vector \((h_1, \cdots, h_k)\) so that

\[
 u(x) = \max \{ \langle x, p_i \rangle + h_i \}
\]

satisfies \( \mu(W_i \cap \Omega) = \nu_i \), where \( W_i = \{ x | \nabla f(x) = p_i \} \).

Furthermore, \( h \) is the maximum point of the convex function

\[
 E(h) = \sum_{i=1}^{k} \nu_i h_i - \int_{0}^{h} \sum_{i=1}^{k} w_i(\eta) \, d\eta_i,
\]

where \( w_i(\eta) = \mu(W_i(\eta) \cap \Omega) \) is the \( \mu \)-volume of the cell.

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Computational Algorithm

Figure: Brenier potential and its Legendre dual for the Buddha example.

a. Brenier potential

b. Legendre dual
**Figure:** Optimal transport map between the conformal image and uniform distribution on the disk.
\( \nu \)-training data distribution; \( \zeta \)-uniform distribution; 
\( \mu_\theta = g_\theta \# \zeta \)-generated distribution; \( G \) - generator computes \( g_\theta \); 
\( D \) - discriminator, measures the distance between \( \nu \) and \( \mu_\theta \), 
\( W_c(\mu_\theta, \nu) \).
When \( c(x, y) = |x - y| \), \( \varphi^c = -\varphi \), given \( \varphi \) is 1-Lipsitz, the WGAN model: min-max optimization

\[
\min_{\theta} \max_{\xi} \int_{X} \varphi_{\xi} \circ g_\theta(z) d\zeta(z) - \int_{Y} \varphi_{\xi}(y) d\nu(y).
\]

namely

\[
\min_{\theta} \max_{\xi} \mathbb{E}_{z \sim \zeta} (\varphi_{\xi} \circ g_\theta(z)) - \mathbb{E}_{y \sim \nu} (\varphi_{\xi}(y)).
\]

with the constraint that \( \varphi_{\xi} \) is 1-Lipsitz.
$L^2$ case

The discriminator computes the Kantorovich potential $\varphi$; the generator $G$ computes the optimal transportation map, $T = \nabla u$, where $u$ is the Brenier potential; The Brenier potential equals to

$$u = \frac{1}{2} |x|^2 - \varphi(x),$$

Generator $G$ computes $u$, Discriminator $D$ computes $\varphi$, hence in theory:

- $G$ can be obtained from the optimal $D$ without training;
- Half of the computation is wasted;
- The competition between $D$ and $G$ is unnecessary.
Empirical Distribution

In practice, the target probability measure is approximated by empirical distribution:

$$\nu = \sum_{i=1}^{n} \delta(y - y_i)\nu_i,$$

in general $\nu_i = 1/n$. 
Given a compact convex domain $\Omega$ in $\mathbb{R}^n$ and $p_1, \cdots, p_k$ in $\mathbb{R}^n$ and $A_1, \cdots, A_k > 0$, find a transport map $T : U \to \{p_1, \cdots, p_k\}$ with $\text{vol}(T^{-1}(p_i)) = A_i$, so that $T$ minimizes the transport cost

$$\frac{1}{2} \int_U |x - T(x)|^2 dx.$$
∀y_i ∈ Y, construct a hyper-plane π_i(h) = ⟨x, y_i⟩ − h_i;

2 compute the upper envelope of the planes
u_h(x) = max_i{π_i(h(x))}

3 produce the power diagram of Ω, V(h) = \bigcup_i W_i(h);

4 adjust the heights h, such that µ(W_i(h)) = ν_i.
**Problem**

Since DNNs have large capacities, do they really learn anything or just memorize the training samples?

**Answer**

The DL system learns the Brenier potential implicitly,

\[
\max_i \{\langle x, y_i \rangle - h_i \}
\]

It both learns and memorizes:

1. it memorizes all the training samples \( \{y_i\} \);
2. it learns the probability \( \{h_i\} \).
Complexity of Geometric Optimal Transport
A convex domain $\Omega \subset \mathbb{R}^d$ with a measure $\mu$, $d\mu = f(x)dx$, $f(x)$ is continuous; the range is $Y = \{y_1, y_2, \ldots, y_n\}$ with measure $\mu = \sum_{i=1}^{n} v_i \delta(y - y_i)$. $\mu(\Omega) = \sum_{i=1}^{n} v_i$.

$$u_h := \max_{i=1}^{n} \{ \langle x, y_i \rangle - h_i \}, \quad T = \nabla u_h.$$
Semi-discrete Optimal Transport Map

\[ W_i(h) := \{ x \in \mathbb{R}^d | \nabla u_h(x) = y_i \} \]

\[ \mathcal{D}_h \quad \Omega = \bigcup_{i=1}^n W_i(h), \quad W_i(h) := \{ x \in \mathbb{R}^d | \nabla u_h(x) = y_i \} \]

\[ \mathcal{P}_h \quad \text{Convex Hull}(\{(y_i, h)\}_{i=1}^n), \quad \text{graph of } u^*_h \]
All the triangulations $\mathcal{T} \in \partial \mathcal{P}_Y$ are called regular triangulations.

**Definition (Characteristics)**

Let $\mathcal{T}$ is a triangulation of the convex hull of $Y$, $\text{Conv}(Y)$. The characteristic of $\mathcal{T}$ defined as a vector,

$$c_{\mathcal{T}} = (a_1, a_2, \ldots, a_k)^T,$$

$$a_i = \sum_{v_i \sim \sigma_j} \text{vol}(\sigma_j).$$

**Definition (Secondary Polytope)**

The secondary polytope of $Y$ is the convex hull of all characteristic vectors of all possible triangulations of $\text{Conv}(Y)$, denoted as $\mathcal{P}_Y$. 
Each upper envelope of planes

\[ u_h = \max_{i=1}^{n} \{ \langle x, y_i \rangle - h_i \} \]

induces a closest power diagram \( D_h \). Its dual weighted Delaunay triangulation \( \mathcal{T}_h \) must be on the lower part of the secondary polytope \( P_Y \), and vice versa.
Each lower envelop of planes

\[ u_h = \min_{i=1}^{n} \{ \langle x, y_i \rangle - h_i \} \]

induces a furthest power diagram \( D_h \). Its dual weighted Delaunay triangulation \( T_h \) must be on the upper part of the secondary polytope \( \mathcal{P}_Y \), and vice versa.
The number of regular triangulations of any configuration of $n$ points in dimension $d$ is $O\left( n^{(n-d-2)^2} \right)$.

The diameter of the secondary polytope is bounded by

$$\min \left\{ (d + 2) \left( \left\lfloor \frac{n}{d+1} \right\rfloor \right), \binom{n}{d+2} \right\}$$
Secondary Diagram

Definition (Admissible Height Space)

Fix $\Omega$ and $Y$, the admissible height space is defined as

$$\mathcal{H}_Y = \left\{ h \mid W_i(h) \neq 0, \quad \forall W_i(h) \in \mathcal{D}_h \right\} \cap \left\{ \sum_{i=1}^{n} h_i = 0 \right\}.$$

Theorem (Gu-Luo-Sun-Yau)

The admissible height space $\mathcal{H}_Y$ is a convex non-empty set.

Proof.

By Alexandrov theorem and Brunn-Minkowski inequality.
Definition (Secondary Diagram)

Fix $\Omega$ and $Y$, the admissible height space $\mathcal{H}_Y$ has a cell decomposition:

$$
\mathcal{D}_Y \quad \mathcal{H}_Y := \bigcup_{T \in \mathcal{P}_Y} H_Y(T), \quad H_Y(T) := \{h \mid u_h^* \text{ induces } T\}
$$

Theorem (Gu-Lei-Si)

The secondary diagram $\mathcal{D}_Y$ is a power diagram, induced by lower envelop of hyperplanes

$$
\min \{ \langle h, c_T \rangle \mid T \in \mathcal{P}_Y \}.
$$
Singularity of Geometric Optimal Transport Map
Let $\Omega$ and $\Omega^*$ be bounded domains in $\mathbb{R}^n$, let $f$ and $g$ be mass densities on $\Omega$ and $\Omega^*$ satisfying

1. $0 \leq f \in L^1(\Omega)$, $0 \leq g \in L^1(\Omega^*)$,

$$\int_{\Omega} f = \int_{\Omega^*} g.$$ 

2. $\exists$ constants $f_0, f_1, g_0, g_1 > 0$, such that

$$f_0 \leq f \leq f_1, g_0 \leq g \leq g_1.$$
Let \((u, v)\) be the Kantorovich’s potential functions. The optimal mapping \(T_u\) is given by

\[
Du(x) = D_x c(x, T_u(x))
\]

Differentiate the formula

\[
D^2 u(x) = D^2_x c(x, T_u(x)) + D^2_{xy} c(x, T_u(x)) DT_u.
\]

We obtain the equation

\[
\det[D^2 u(x) - D^2_x c(x, T_u(x))] = \det D^2_{xy} c(x, T_u(x)) \frac{f(x)}{g(T_u(x))},
\]

with the boundary condition \(T_u(\Omega) = \Omega^*\).
Caffarelli obtained the regularity of optimal mappings for the cost function

\[ c(x, y) = |x - y|^2 \]

or equivalently \( c(x, y) = x \cdot y \), then we have the standard Monge-Ampere equation

\[
\det D^2 u = \frac{f(x)}{g(Du(x))},
\]

with boundary condition \( Du(\Omega) = \Omega^* \).

1. If \( f, g > 0, \in C^\alpha \) and \( \Omega^* \) is convex, then \( u \in C^{2,\alpha}(\Omega) \).
2. If \( f, g > 0, \in C^0 \) and \( \Omega^* \) is convex, then \( u \in W^{2,p}_{loc}(\Omega), \forall p > 1 \) (the continuity is needed for large \( p \)).
3. If \( f, g > 0, \in C^\alpha \), both \( \Omega \) and \( \Omega^* \) are uniformly convex and \( C^{2,\alpha} \), then \( u \in C^{2,\alpha}(\bar{\Omega}) \).
Theorem (Ma-Trudinger-Wang)

The potential function $u$ is $C^3$ smooth if the cost function $c$ is smooth, $f, g$ are positive, $f \in C^2(\Omega)$, $g \in C^2(\Omega^*)$, and

- $A1 \ \forall x, \xi \in \mathbb{R}^n, \exists! y \in \mathbb{R}^n$, s.t. $\xi = D_x c(x, y)$ (for existence)
- $A2 \ |D_{xy}^2 c| \neq 0$.
- $A3 \ \exists c_0 > 0$ s.t. $\forall \xi, \eta \in \mathbb{R}^n$, $\xi \perp \eta$

$$\sum (c_{ij,rs} - c^{p,q} c_{ij,p} c_{q,rs}) c^{r,k} c^{s,l} \xi_i \xi_j \eta_k \eta_l \geq c_0 |\xi|^2 |\eta|^2.$$ 

- $B1 \ \Omega^*$ is $c$-convex w.r.t. $\Omega$, namely $\forall x_0 \in \Omega$,

$$\Omega^*_{x_0} := D_x c(x_0, \Omega^*)$$

is convex.
Figure: Optimal transportation map.
Figure: Optimal transportation map.
Figure: Optimal transportation map.
Regularity of Solution to Monge-Ampere Equation

Theorem (Figalli Regularity)

Let $\Omega, \Lambda \subset \mathbb{R}^d$ be two bounded open sets, let $f, g : \mathbb{R}^d \to \mathbb{R}^+$ be two probability densities, that are zero outside $\Omega, \Lambda$ and are bounded away from zero and infinity on $\Omega, \Lambda$, respectively. Denote by $T = \nabla u : \Omega \to \Lambda$ the optimal transport map provided by Brenier theorem. Then there exist two relatively closed sets $\Sigma_\Omega \subset \Omega$ and $\Sigma_\Lambda \subset \Lambda$ with $|\Sigma_\Omega| = |\Sigma_\Lambda| = 0$ such that $T : \Omega \setminus \Sigma_\Omega \to \Lambda \setminus \Sigma_\Lambda$ is a homeomorphism of class $C^{0,\alpha}_{\text{loc}}$ for some $\alpha > 0$. 
Figure: Singularity structure of an optimal transportation map.

We call $\Sigma_\Omega$ as singular set of the optimal transportation map $\nabla u : \Omega \to \Lambda$. 
Medial Axis

Figure: The Brenier potential of the OT map.

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Singularity of OT Map

Figure: The Brenier potential of the optimal transport map.

X. Gu

Geometric Understanding
Given a planar polygonal domain $\Omega$, we densely sample the boundary and the interior, the samples are denoted as $Y = \{y_1, y_2, \cdots, y_n\}$. Given the powers $\{w_1, w_2, \cdots, w_n\}$, or equivalently the height $h = (h_1, h_2, \cdots, h_n)$, the power diagram is denoted as $\mathcal{D}_Y(h)$. For each point $p \in \mathbb{R}^2$, the closest point of $p$ to $Y$ is defined as

$$\text{Cl}_Y(p, h) := \arg\min_i \text{pow}(p, y_i)$$

**Definition (Power Medial Axis)**

Given $(Y, h)$, the power medial axis is defined as

$$\text{MAT}_Y(h) := \{p \in \mathbb{R}^2 \mid |\text{Cl}_Y(p, h)| > 1\}.$$
Singularity Stability

Theorem

Given a convex domain $D \subset \mathbb{R}^n$ and the discrete point set $Y = \{y_1, y_2, \cdots, y_k\}$, then for any two admissible heights $h_1, h_2 \in \mathcal{H}_Y$, their power medial axises are homotopic to each other.

Corollary

The singularity of a semi-discrete optimal transport map is homotopic to the medial axis.
singularity

Figure: Singularity set.

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Geometric Understanding
singularity

X. Gu  Geometric Understanding
Singularity Stability

Geometric Understanding
Singularity Stability

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Geometric Understanding
Singularity Stability

Geometric Understanding
Lemma

Suppose $\partial \Omega$ is a $C^2$ curve, denoted as $\gamma(s)$, where $s$ is the arc length parameter. $\phi : (\Omega, \mu) \to (\mathbb{D}^2, \nu)$ is the optimal transport map, the Brenier potential is $u : \Omega \to \mathbb{R}$, the corresponding power weight is $w : \Omega \to \mathbb{R}$, then

$$\varphi(s) = \gamma(s) - T(s)\dot{w}(s) + h(s)n(s),$$

where $n(s)$ is the normal to $\partial \Omega$ and $h : \partial \Omega \to \mathbb{R}$ is differentiable.
Figure: Discontinuous Optimal transportation map, produced by a GPU implementation of algorithm based on our theorem. The middle line is the singularity set $\Sigma_1$. 
Figure: Discontinuous Optimal transportation map, produced by a GPU implementation of algorithm based on regularity theorem. $\gamma_1$ and $\gamma_2$ are two singularity sets.
Figure: Optimal transportation between a solid ball to the Stanford bunny. The singular sets are the foldings on the boundary surface.
Figure: Optimal transportation between a solid ball to the Stanford bunny. The singular sets are the foldings on the boundary surface.
Figure: Optimal transportation map is discontinuous, but the Brenier potential itself is continuous. The projection of ridges are the discontinuity singular sets.
Figure: Optimal transportation map is discontinuous.
Figure: Optimal transportation map is discontinuous.
Mode Collapse
GANs are difficult to train and sensitive to hyper-parameters;
GANs suffer from mode collapsing, the generated distributions miss some modes;
GANs may generate unrealistic samples;
Mode Collapse

1. The training process is unstable, and doesn’t converge;
2. The searching converges to one of the multiple connected components of $\Lambda$, the mapping converges to one continuous branch of the desired transformation mapping. This means we encounter a mode collapse;
3. The training process leads to a transportation map, which covers all the modes successfully, but also cover the regions outside $\Lambda$. In practice, this will induce the phenomena of generating unrealistic samples.
Intrinsic Conflict

Deep neural networks can only represent continuous mappings, but the transportation maps are discontinuous on singular sets. Namely, the target mappings are outside the functional space of Dnns. This conflict induces mode collapsing.

Avoid Mode Collapse

The optimal transport map is discontinuous, but Brenier potential itself is continuous. The neural network should represent the Brenier potential, instead of its gradient, namely the transportation map.
Avoid Mode Collapsing

Training Data

Latent Distribution

Generated Samples

encoder

decoder

OT Mapper

Brenier Potential

white noise

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Geometric Understanding
Figure: Find a mapping, which transform a source distribution to the data latent code distribution.
Brenier Theorem

Figures: The optimal transportation map is given by a convex function $u$, $T = \nabla u$. 

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Geometric Understanding
Singularity Set Detection

Figure: Singularity set detection.
**Figure:** Curves on facial photo manifold.
Mode Collapse

Figure: Facial images generated by an AE-OT model, the image in the center of (b) shows the transportation map is discontinuous.
Mode Collapse

**Figure:** Facial images with zero probability.
Autoencoder-Optimal Transportation Framework
Use autoencoder to realize encoder and decoder, use OMT in the latent space to realize probability transformation.
### Auntoencoder-OMT

#### Merits

1. Solving Monge-Ampère equation is reduced to a convex optimization, which has unique solution. The optimization won’t be trapped in a local optimum;

2. The Hessian matrix of the energy has explicit formulation. The Newton’s method can be applied with second order convergence; or the quasi-Newton’s method can be used with super-linear convergence. Whereas conventional gradient descend method has linear convergence;

3. The approximation accuracy can be fully controlled by the density of the sampling density by using Monte-Carlo method;

4. The algorithm can be refined to be hierarchical and self-adaptive to further improve the efficiency;

5. The parallel algorithm can be implemented using GPU.

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Geometric Understanding
Experiments - Mode Collapse

Figure: Comparison between conventional models with AE-OT.
Experiments - Mode Collapse

Figure: Comparison between conventional models with AE-OT.
Experiments - mnist

Figure: Comparison between conventional models VAE and WGAN with our model AE-OT (AutoEncoder-OptimalTransportation).
Figure: Failure cases for WGAN-GP and WGAN-div.
Figure: Comparision between CRGAN and our model.
Figure: Human facial images generated by our model.
Figure: Human facial images generated by our model.
Figure: Human facial images generated by our AE-OT model (AutoEncoder-OptimalTransportation).
Figure: Human facial images generated by our model.
Experiments - MNIST Fashion

Figure: Our method has smallest FID score. (Fréchet Inception Distance)

<table>
<thead>
<tr>
<th>Method</th>
<th>FID Score</th>
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<tbody>
<tr>
<td>MM GAN</td>
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<tr>
<td>NSGAN</td>
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<td>LSGAN</td>
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<td>VAE</td>
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<td>GLO</td>
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<td>GLANN</td>
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<td>AE-OMT</td>
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Conclusion

This work introduces a geometric understanding of deep learning:

- The intrinsic pattern of natural data can be represented by manifold distribution principle.
- The deep learning system has two major tasks: manifold learning and probability distribution transformation.
- Optimal transportation assign a Riemannian metric in the space of distributions, so variational optimization can be carried out.
- By Brenier theory, the generator and discriminator should collaborate instead of compete with each other;
- The regularity theory of Monge-Ampere equation explains mode collapse;
- The AE-OT framework can avoid mode collapse, and make half the blackbox transparent.


Thanks

Please email to gu@cmsa.math.harvard.edu, gu@cs.stonybrook.edu.

Thank you!
Autoencoder Framework

Training Data → Latent Distribution → Generated Samples

encoder

decoder
Please email to gu@cs.stonybrook.edu, gu@cmsa.fas.harvard.edu.
Subgradient

Definition (subgradient)

Given an open set $\Omega \subset \mathbb{R}^d$ and $u : \Omega \to \mathbb{R}$ a convex function, for $x \in \Omega$, the subgradient (subdifferential) of $u$ at $x$ is defined as

$$\partial u(x) := \{ p \in \mathbb{R}^n : u(z) \geq u(x) + \langle p, z - x \rangle \ \forall z \in \Omega \}.$$ 

The Brenier potential $u$ is differentiable at $x$ if its subgradient $\partial u(x)$ is a singleton. We classify the points according to the dimensions of their subgradients, and define the sets

$$\Sigma_k(u) := \left\{ x \in \mathbb{R}^d \mid \dim(\partial u(x)) = k \right\}, \quad k = 0, 1, 2, \ldots, d.$$
One can define a cylinder through $\partial \Omega$, the cylinder is truncated by the xy-plane and the convex polyhedron. The energy term $\int^h \sum w_i(\eta) d\eta_i$ equals to the volume of the truncated cylinder.
Definition (Alexandrov Potential)

The concave energy is

\[ E(h_1, h_2, \cdots, h_k) = \sum_{i=1}^{k} v_i h_i - \int_0^{h} \sum_{j=1}^{k} w_j(\eta) d\eta, \]

Geometrically, the energy is the volume beneath the parabola.
The gradient of the Alexanrov potential is the differences between the target measure and the current measure of each cell

\[ \nabla E(h_1, h_2, \cdots, h_k) = (v_1 - w_1, v_2 - w_2, \cdots, v_k - w_k) \]
The Hessian of the energy is the length ratios of edge and dual edges,

$$\frac{\partial w_i}{\partial h_j} = \frac{|e_{ij}|}{|\bar{e}_{ij}|}$$
Figure: Human facial images generated by our AE-OT model (AutoEncoder-OptimalTransportation).