Optimal Transportation

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Motivation

Why dose 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

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

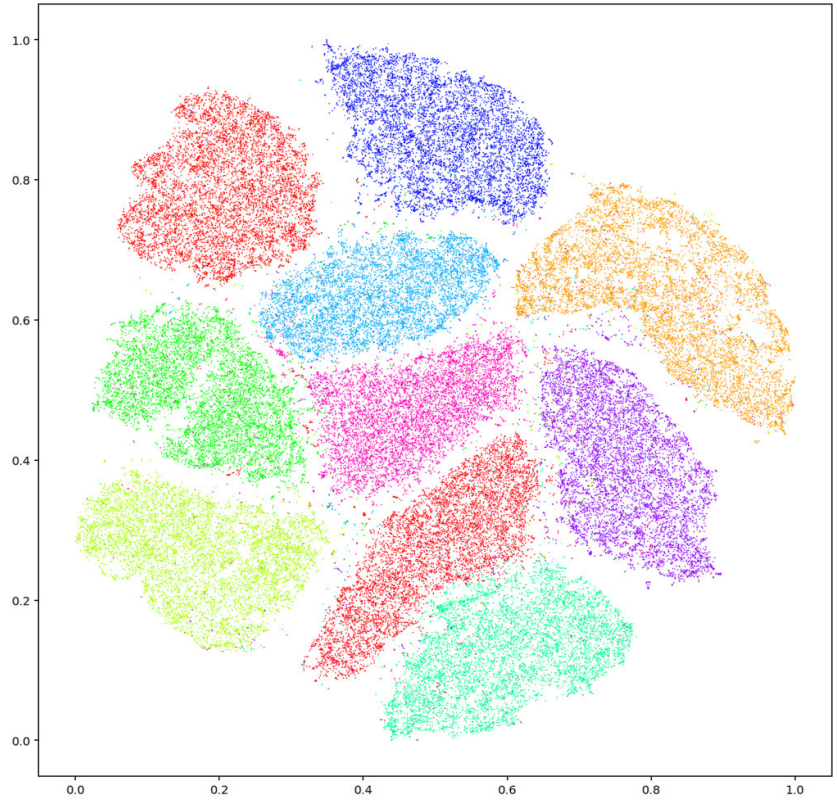
A natural data class can be treated as a probability distribution defined on a low dimensional manifold embedded in a high dimensional ambient space.

Clustering Distribution

The distances among the probability distributions of subclasses on the manifold are far enough to discriminate them.

MNIST tSNE Embedding

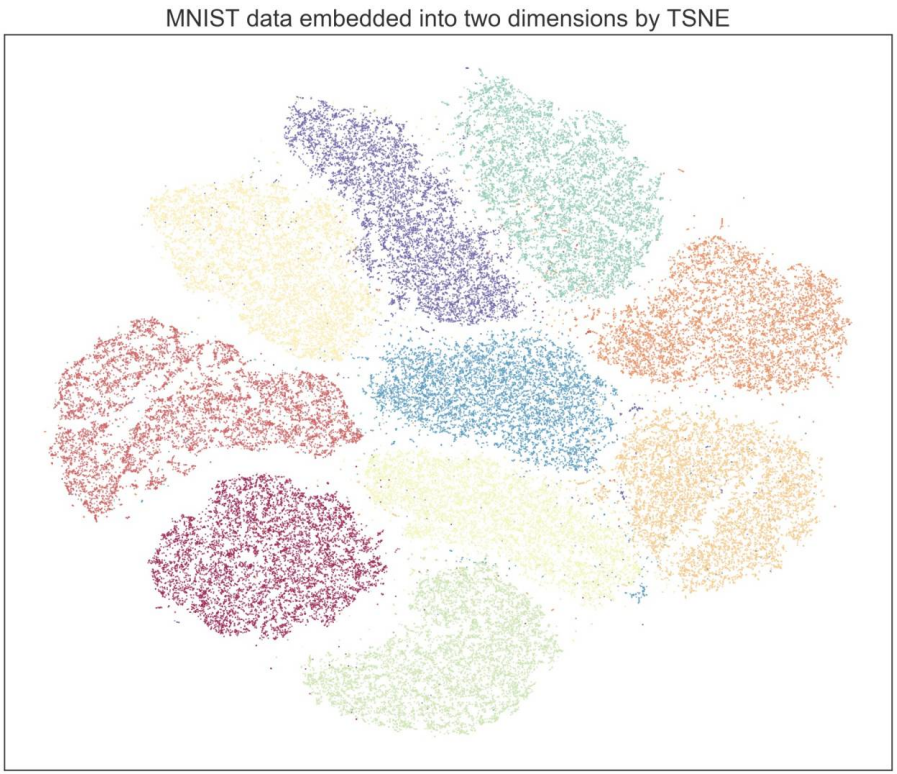
a. LeCunn's MNIST



b. Hinton's t-SNE embemdding

- Each image 28×28 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.

Manifold Learning



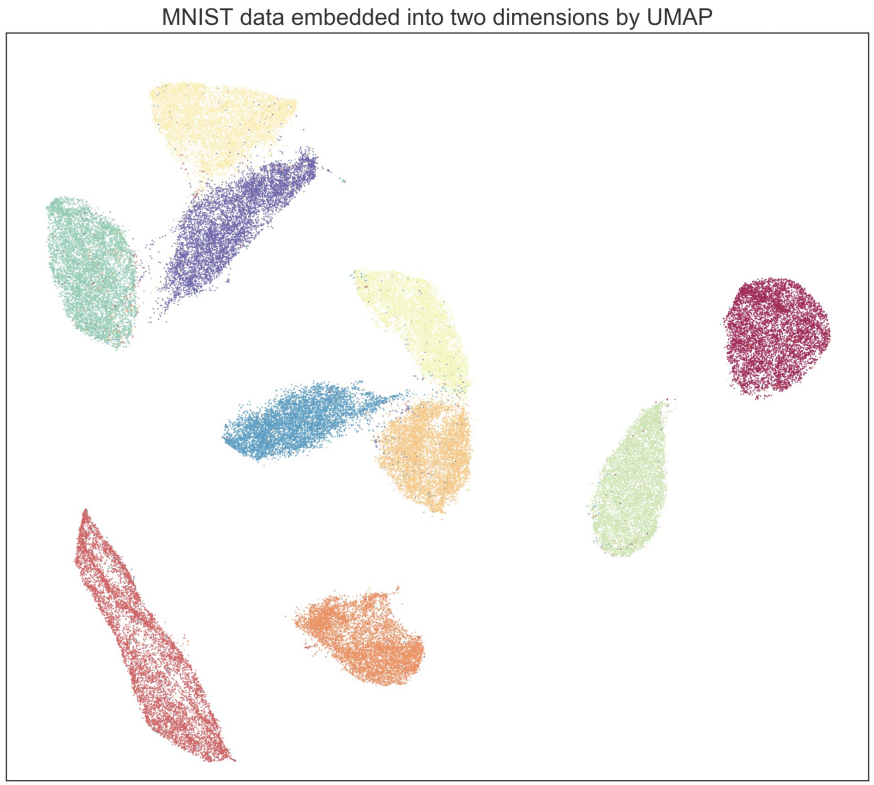


Figure: t-SNE embedding and UMap embedding.

How does a DL system learn ?

Optimization

- 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 $\mathcal{P}(X)$.

Optimal Transportation

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.

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.

Optimal Transportation

- 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,

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

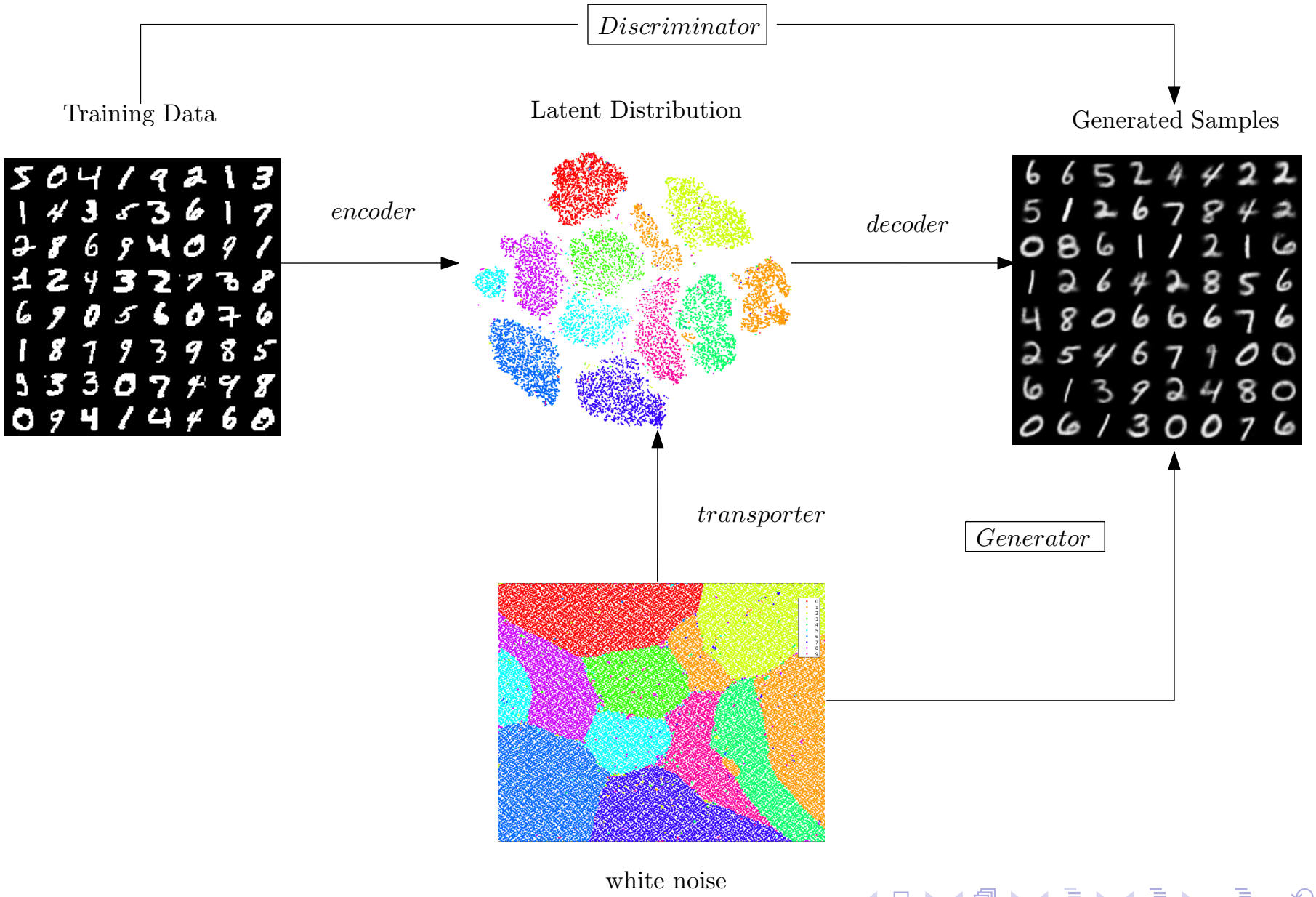
- The tangent vectors of a probability measure is a gradient field on X, the Riemannian metric is given by

$$\langle d\varphi_1, d\varphi_2 \rangle = \int_X \langle d\varphi_1, d\varphi_2 \rangle_{\mathbf{g}} f(x)dx.$$

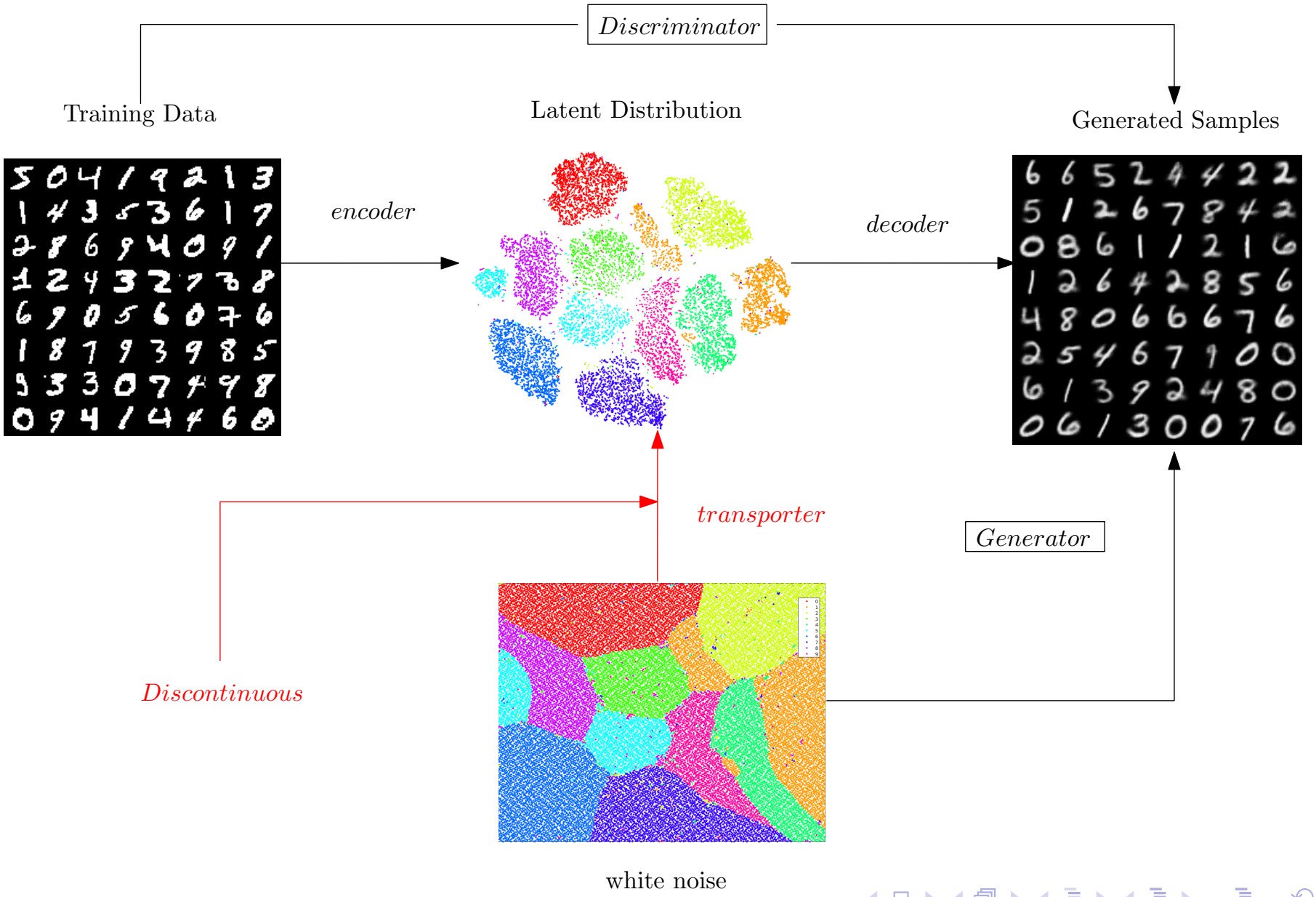
How well does a DL system learn ?

Fundamental flaws: mode collapsing and mode mixture.

GAN model


Discriminator
Training Data
Latent Distribution
Generated Samples
encoder
decoder
transporter
Generator
white noise

GAN model - Mode Collapse Reason



Mode Collapse Reason

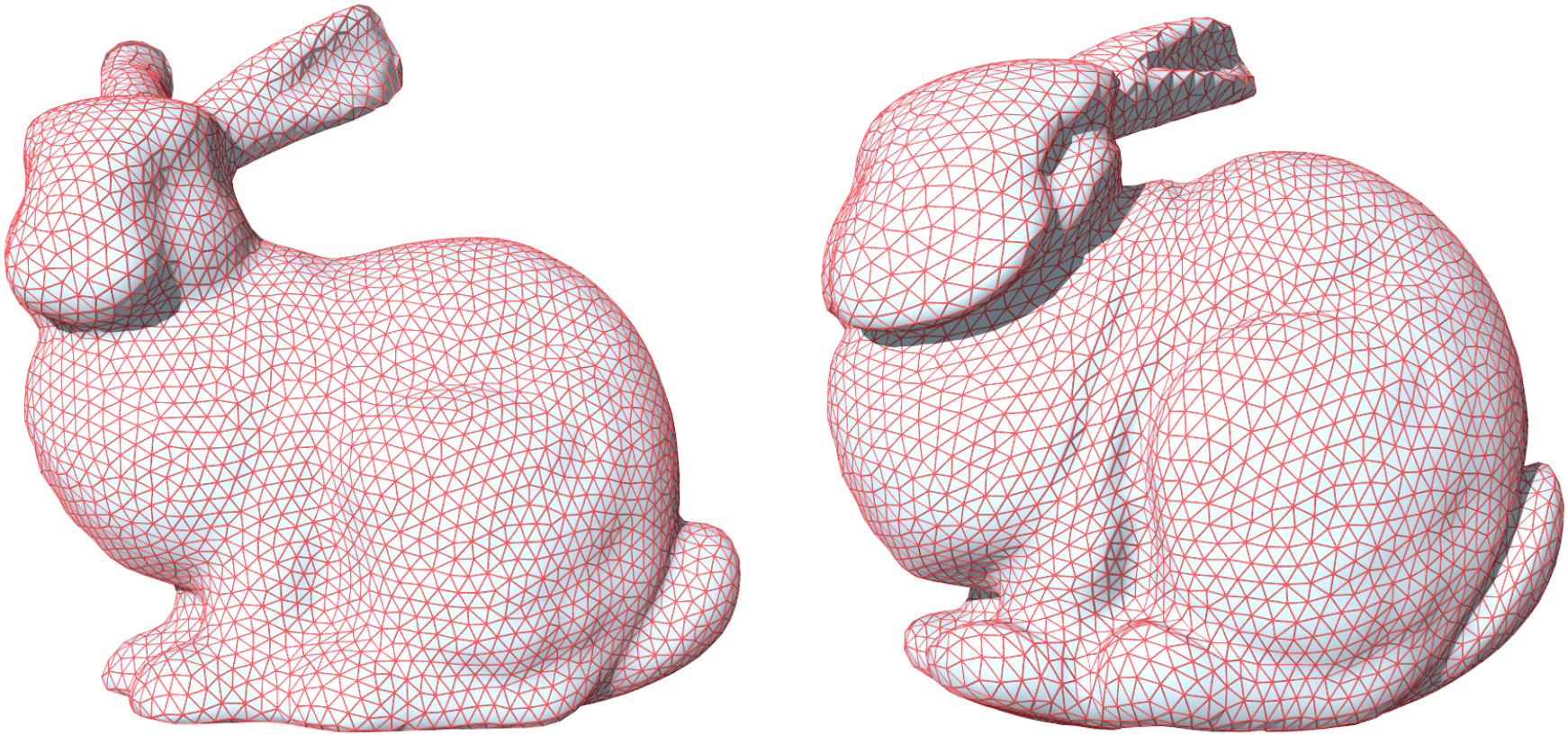


Figure: Singularities of an OT map.

Mode Collapse Reason

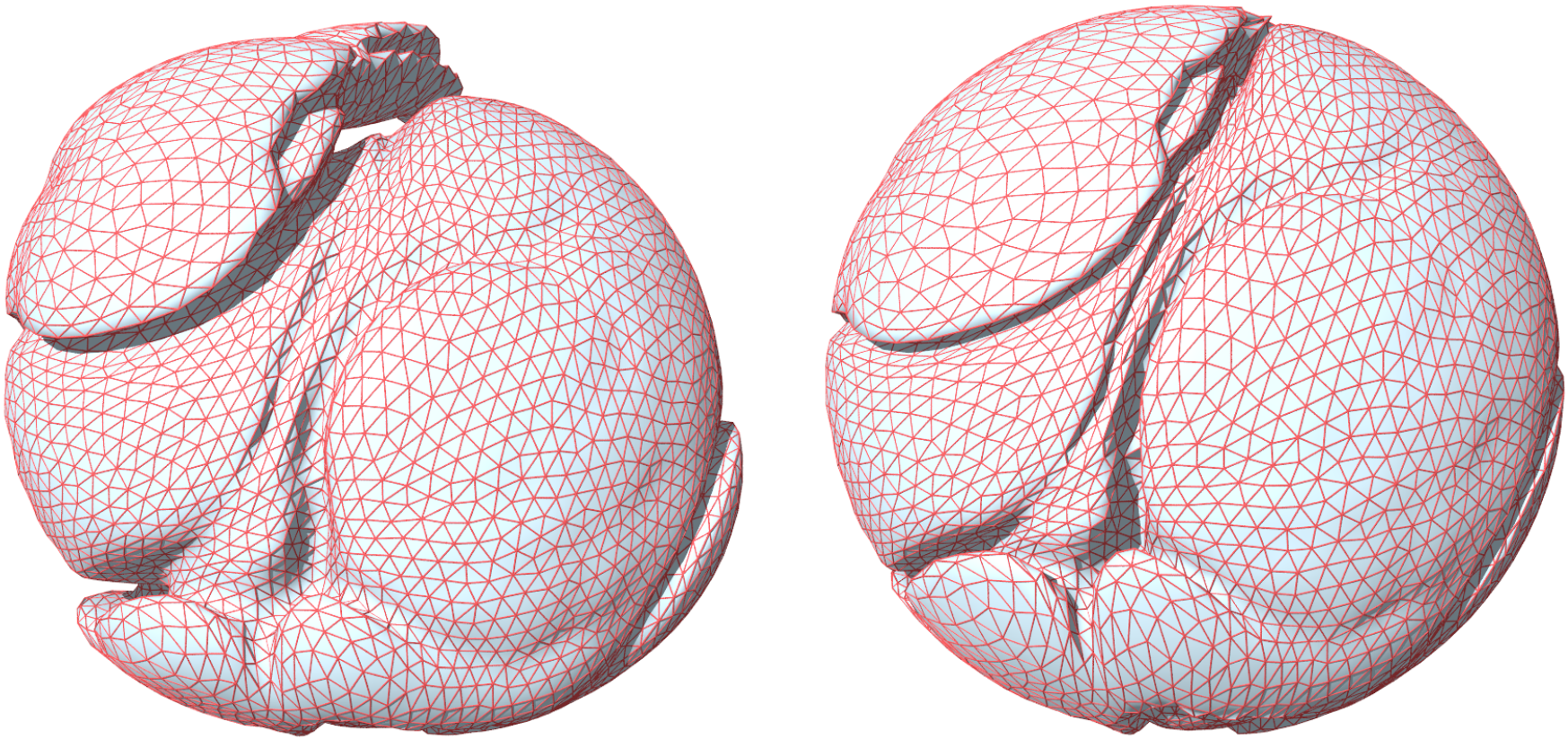


Figure: Singularities of an OT map.

How to eliminate mode collapse?

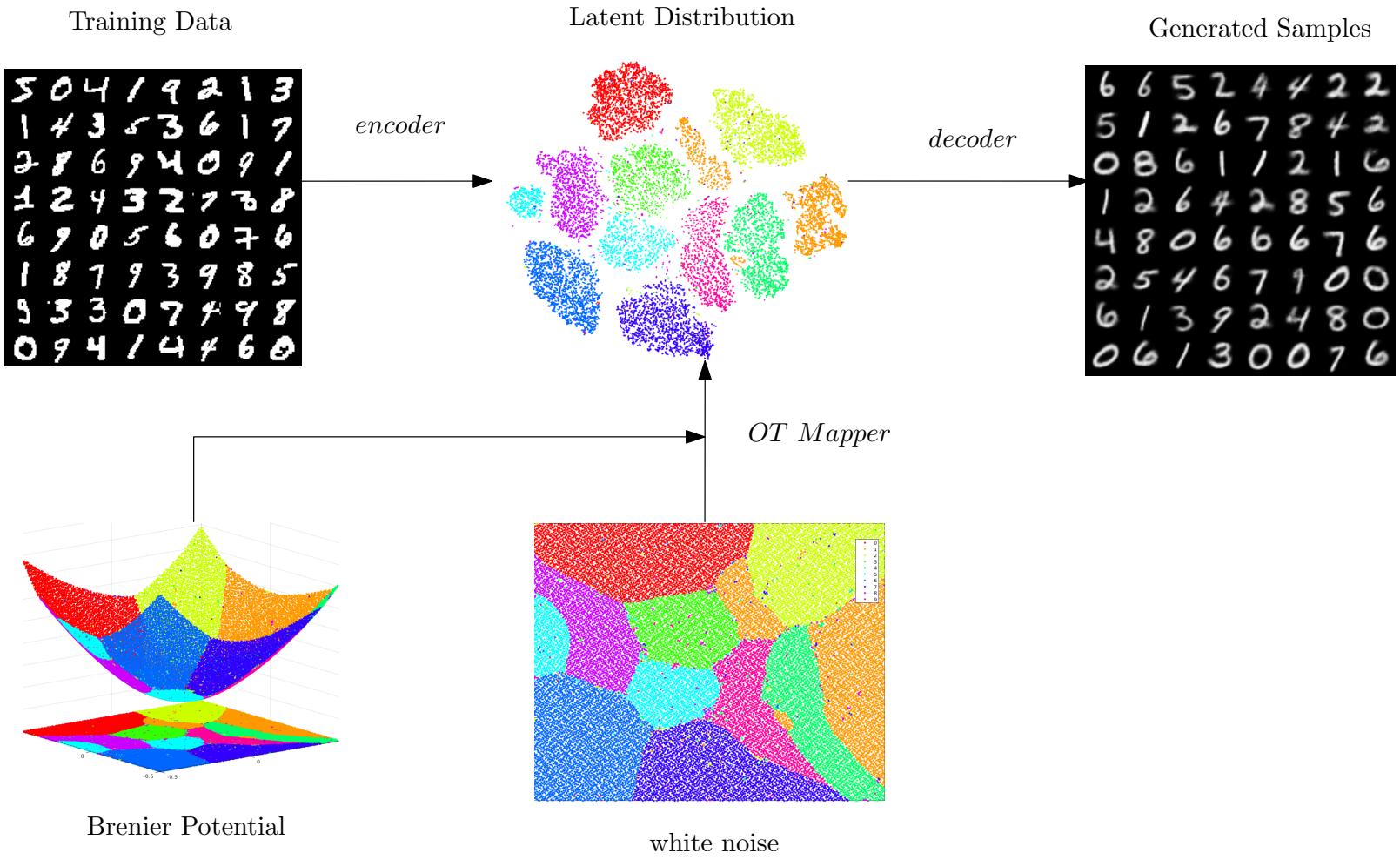


Figure: Geometric Generative Model.

Generative and Adverse rial Networks

A generative model converts a white noise into a facial image.

Generative and Adverse rial Networks

A GAN model based on OT theory.

Overview

There are three views of optimal transportation theory:

1. Duality view
2. Fluid dynamics view
3. Differential geometric view

Different views give different insights and induce different computational methods; but all three theories are coherent and consistent.

Optimal Transportation Map

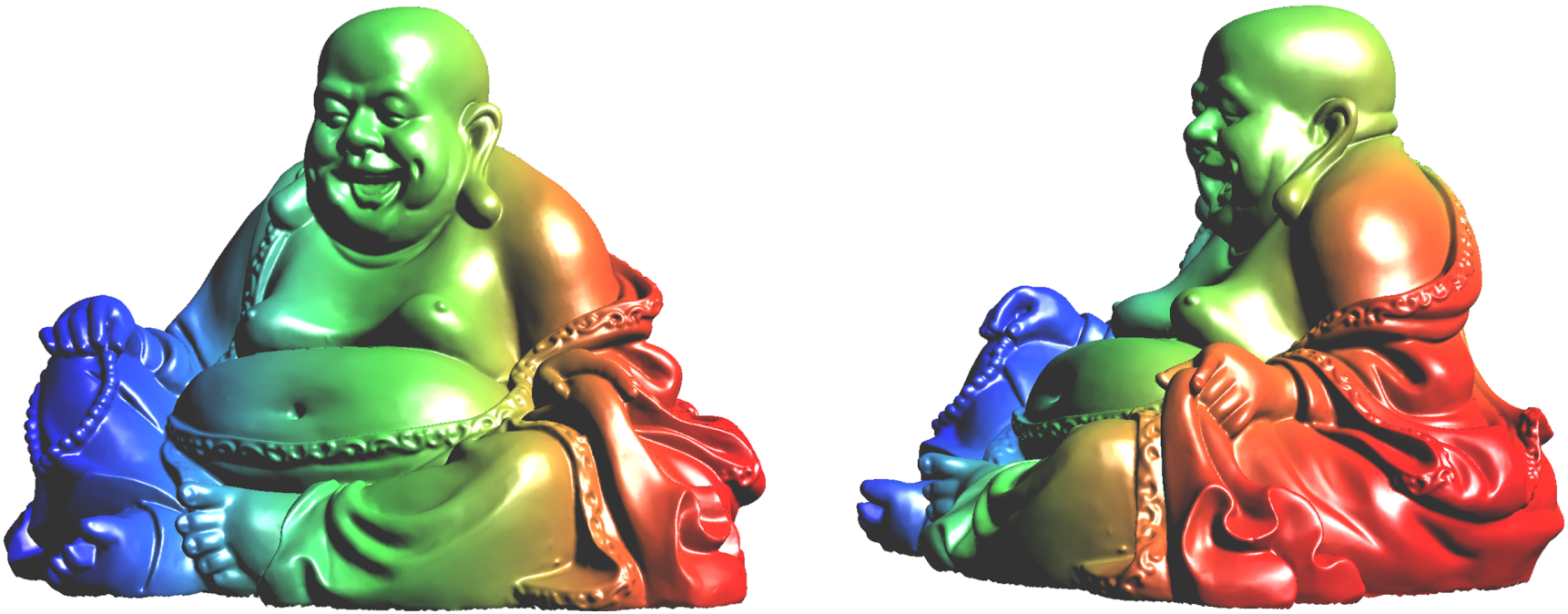


Figure: Buddha surface.

Optimal Transportation Map

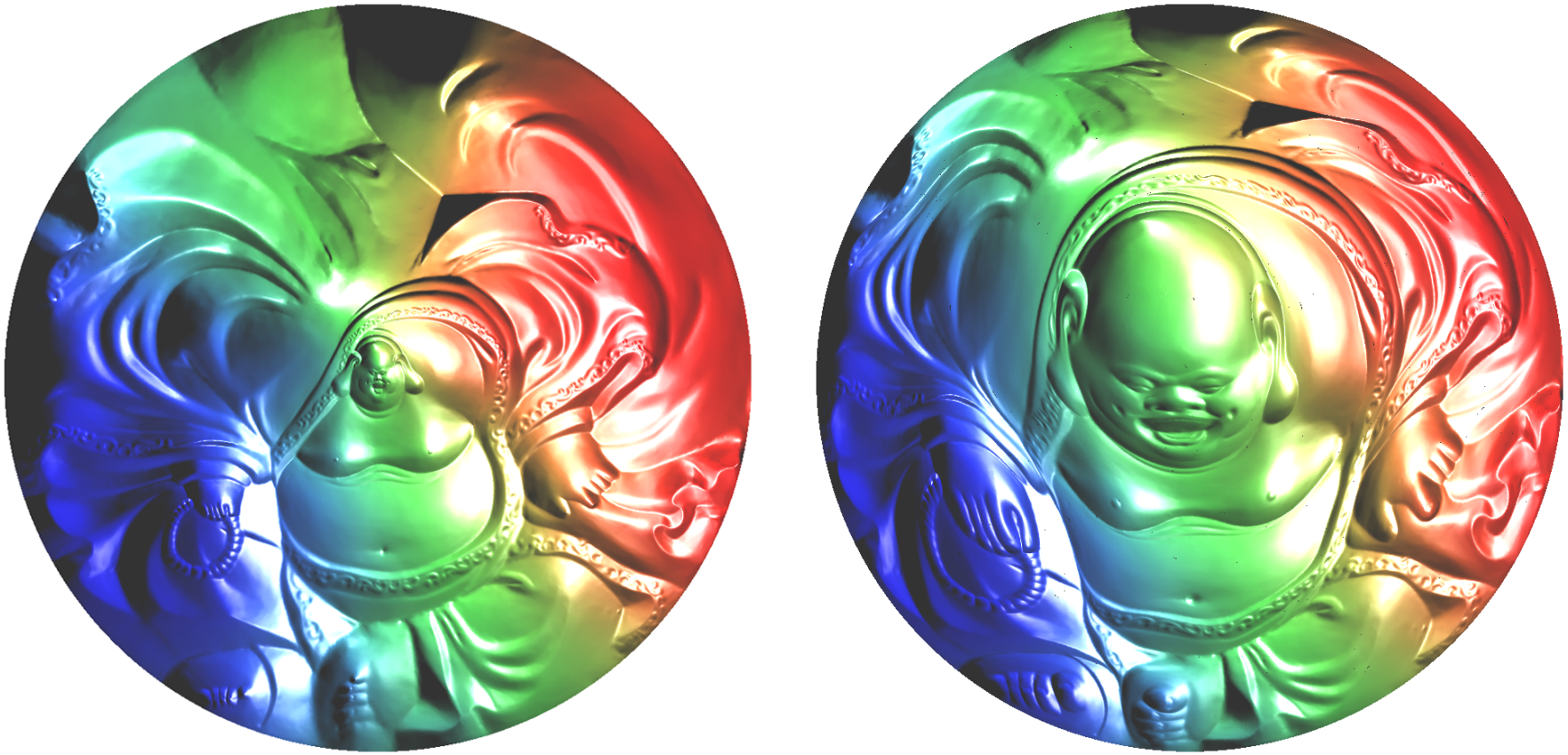


Figure: Optimal transportation map.

Optimal Transportation Map

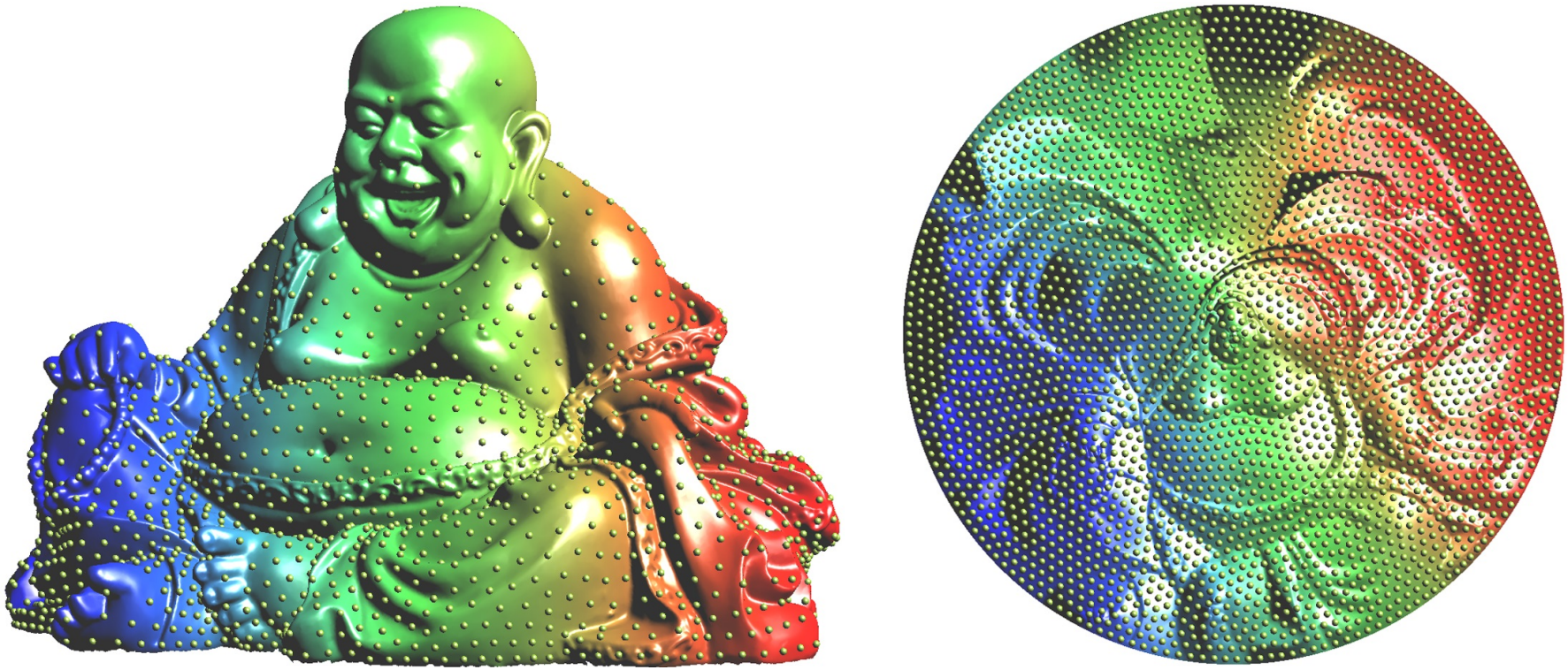


Figure: Brenier potential.

Optimal Transportation Map

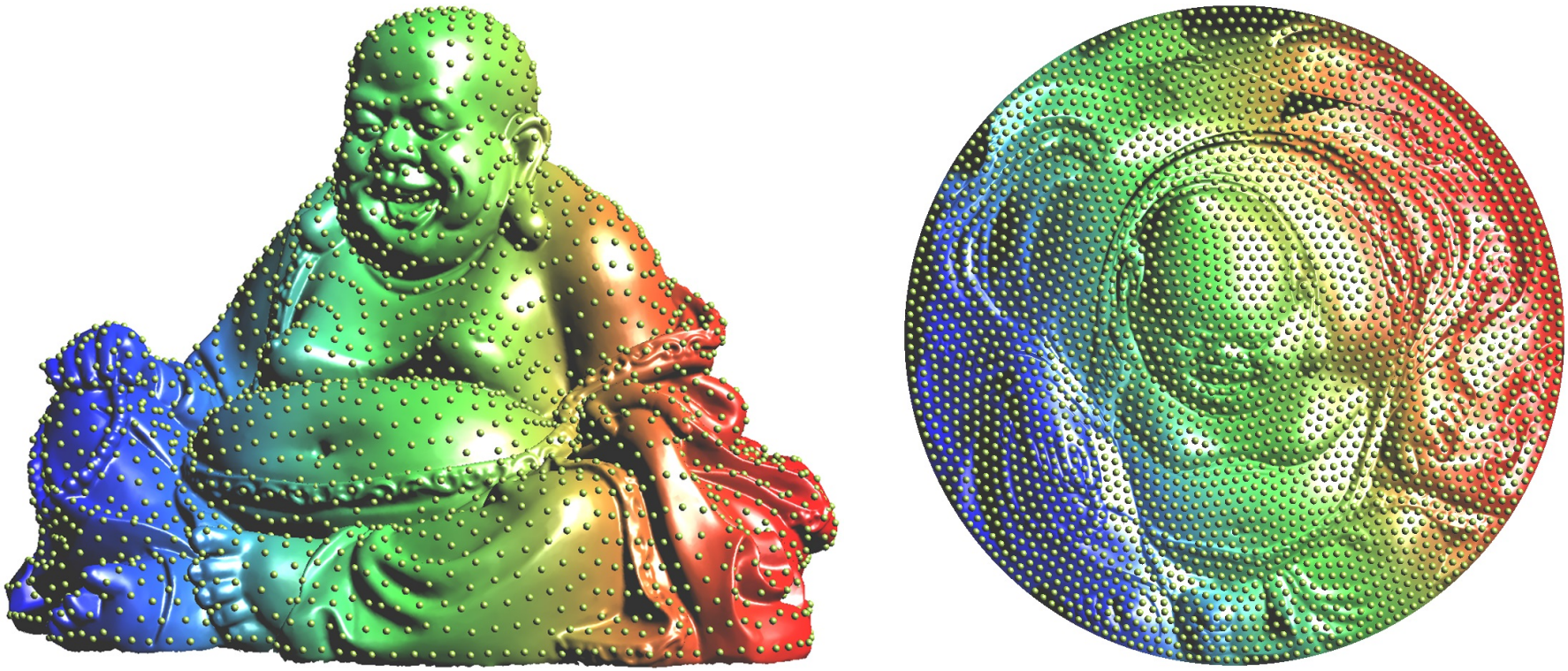


Figure: Brenier potential.

Optimal Transportation Map

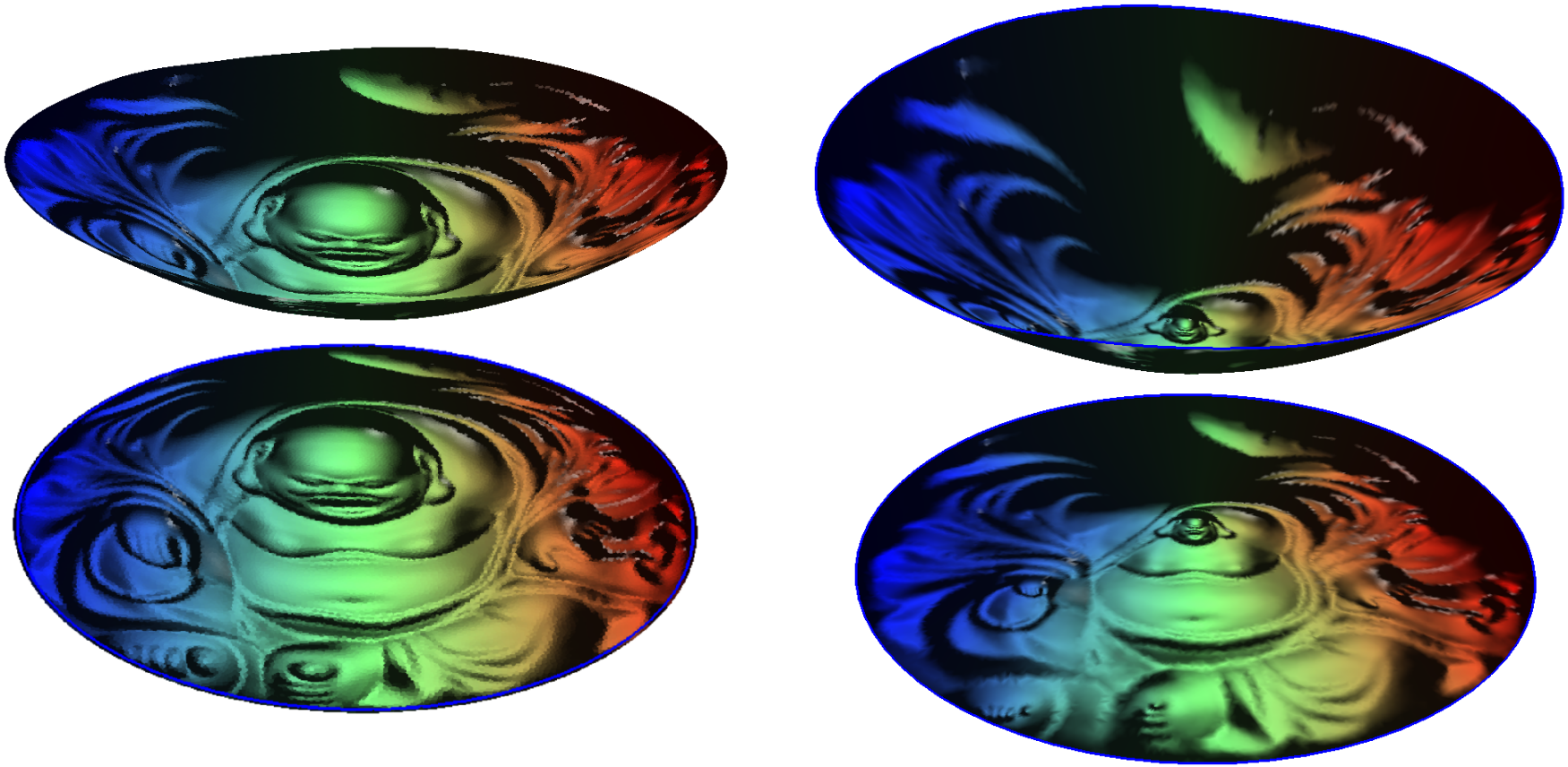


Figure: Brenier potential.

Duality Theories

Monge Problem

Assume Ω and Σ are two domains in the Euclidean space, $\mathbb{R}^d$, μ and ν are two probability measures on Ω and Σ respectively, $\mu \in \mathcal{P}(\Omega)$, $\nu \in \mathcal{P}(\Sigma)$, such that they have equal total measure:

$$\mu(\Omega) = \nu(\Sigma). \tag{1}$$

Definition (Measure-preserving Map)

A mapping $T : \Omega \to \Sigma$ is called *measure preserving*, if or any Borel set $B \subset \Sigma$,

$$\int_{T^{-1}(B)} d\mu = \int_B d\nu, \tag{2}$$

and is denoted as $T_{\#}\mu = \nu$ T pushes μ forward to ν.

Monge Problem

Suppose the density functions of μ and ν are given by $f : \Omega \to \mathbb{R}$ and $g : \Sigma \to \mathbb{R}$, namely

$$d\mu = f(x_1, x_2, \cdots, x_d) dx_1 \wedge dx_2 \wedge \cdots \wedge dx_d,$$
$$d\nu = g(y_1, y_2, \cdots, y_d) dy_1 \wedge dy_2 \wedge \cdots \wedge dy_d,$$

and $T : \Omega \to \Sigma$ is C^1 and measure-preserving,

$$f(x_1, \ldots, x_d) dx_1 \wedge \cdots \wedge dx_d = g(T(x)) dy_1 \wedge \cdots dy_d.$$

then T satisfies the Jacobi equation:

Definition (Jacobi Equation)

$$\det DT(x) = \frac{f(x)}{g \circ T(x)} \tag{3}$$

Monge Problem

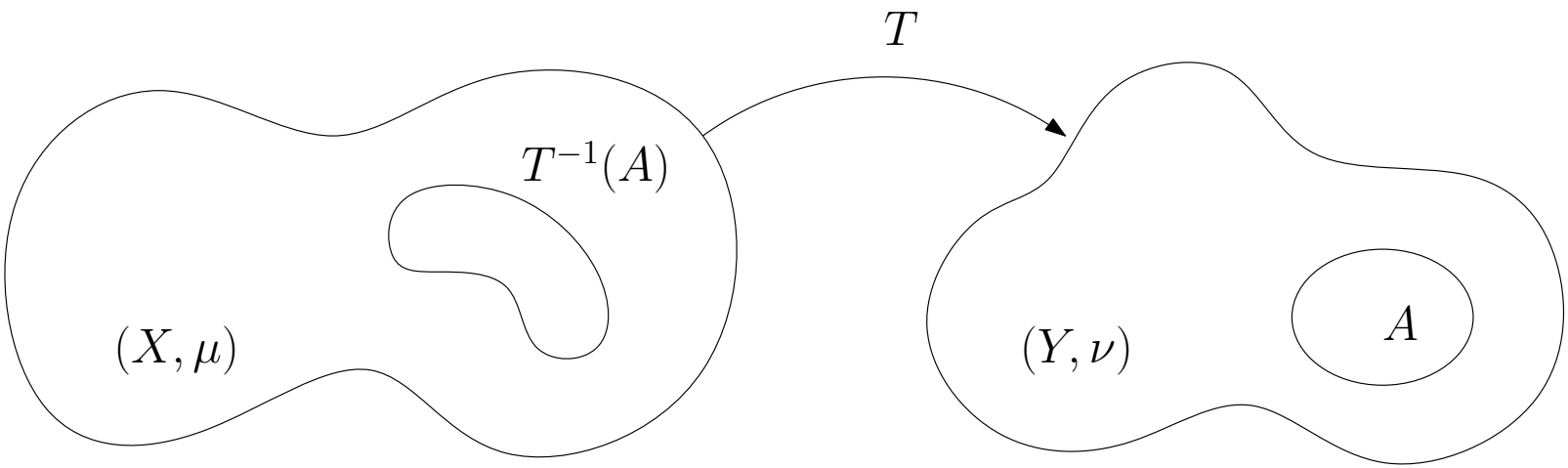


Figure: Measure-preserving map.

Monge Problem

Definition (Transportation Cost)

Given a cost function $c : \Omega \times \Sigma \to \mathbb{R}$, the total transportation cost for a map $T : \Omega \to \Sigma$ is defined as

$$\mathcal{C}(T) := \int_{\Omega} c(x, T(x)) d\mu(x).$$

Problem (Monge)

Amonge all the measure-preserving mappings, $T : \Omega \to \Sigma$ and $T_{\#}\mu = \nu$, find the one with the minimal total transportation cost,

$$MP : \qquad \min \left\{ \int_{\Omega} c(x, T(x)) d\mu(x) : \ T_{\#}\mu = \nu \right\}. \tag{4}$$

Monge Problem

Definition (Optimal Transportation Map)

The solution to the Monge problem is called an optimal transportation map between (Ω, μ) and (Σ, ν).

Suppose Ω coincides with Σ

Definition (Wasserstein Distance)

The total cost of the optimal transportation map $T : \Omega \to \Sigma$, $T_{\#}\mu = \nu$, is called the Wasserstein distance between μ and ν.

Suppose the cost is the square of the Euclidean distance $c(x, y) = |x - y|^2$, then the Wasserstein distance is defined as

$$\mathcal{W}_2^2(\mu, \nu) := \inf \left\{ \int_\Omega |x - T(x)|^2 d\mu(x) : \quad T_{\#}\mu = \nu \right\}.$$

Kantorovich Problem

Transportation Plan

Kantorovich relax the transportation map to transportation scheme, or transportation plan, which is represented by a joint probability distribution $\rho : \omega \times \Sigma \to \mathbb{R}$, $\rho(x, y)$ represents how much mass is transported from the source point x to the target point y.

Marginal Distribution

The marginal districution of ρ equals to μ and ν, namely we have the condition

$$(\pi_x)_{\#}\rho = \mu, \quad (\pi_y)_{\#}\rho = \nu, \tag{5}$$

where the projection maps

$$\pi_x(x, y) = x, \quad \pi_y(x, y) = y.$$

Kantorovich Problem

Transportation map vs. Transportation plan

Transportation map is a special case of transportation plan, namely a transportation map $T : \Omega \to \Sigma$ induces a transportation plan

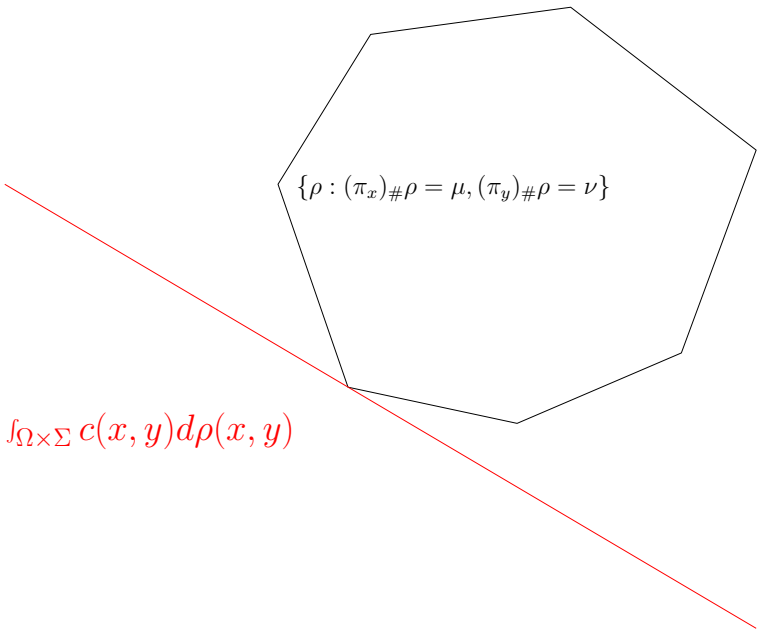
$$(Id, T)_{\#}\mu = \rho. \tag{6}$$

Kantorovich Problem

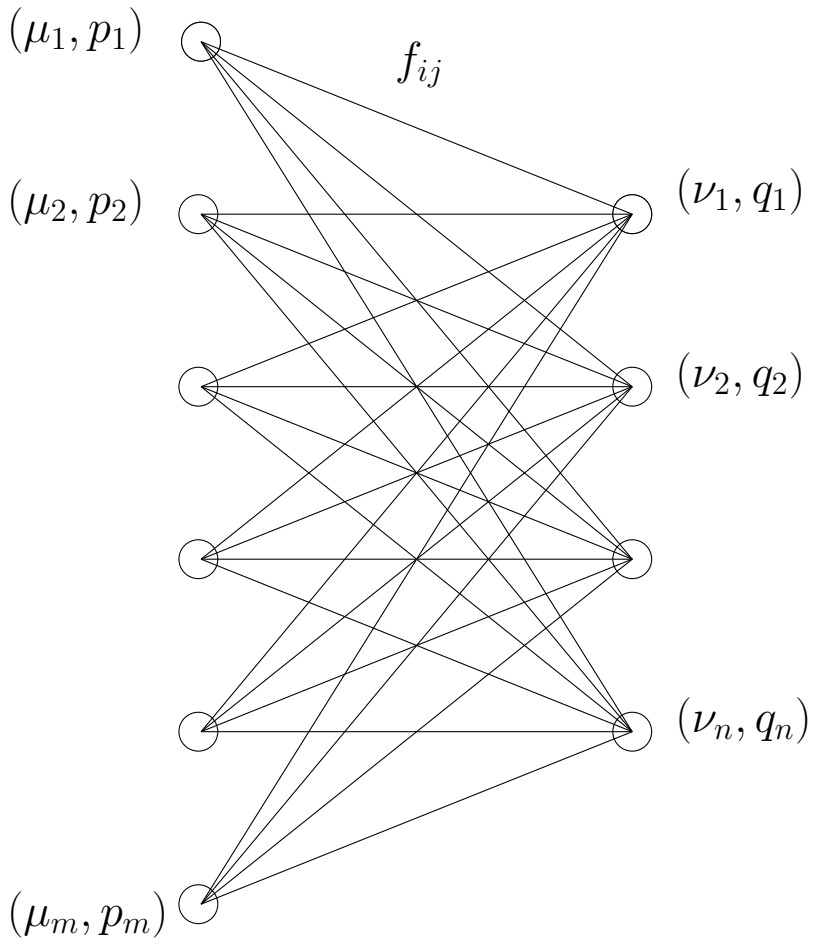
Problem (Kantorovich)

Find a transportation plan with the minimal toal transportation cost,

$$KP: \quad \min\left\{\int_{\Omega\times\Sigma} c(x,y)d\rho(x,y): \ (\pi_x)_{\#}\rho=\mu, \ (\pi_y)_{\#}\rho=\nu\right\}. \quad (7)$$



Kantorovich Problem



Problem (Linear Programming)

$$\min \sum_{ij} c(p_i, q_j) f_{ij},$$

such that

$$\forall i, \ \sum_j f_{ij} = \mu_i$$

$$\forall j, \ \sum_i f_{ij} = \nu_j.$$

Kantorovich Problem

Linear Programming

Kantorovich problem is to find a minimal value of a linear function defined on a convex polytope, so the solution exists. KP can be solved using linear programming method, such as simplx, interior point or ellipsoid algorithms.

Kantorovich Problem

In general situation, the support of a transportation plan ρ covers all the $\Omega \times \Sigma$. If the transportation map T exists, the support of $(Id, T)_{\#}\mu$ has 0 measure in $\Omega \times \Sigma$. KP doesn't discover the intrinsic structure, it is highly inefficient to compute optimal transportation map.

Kantorovich Problem

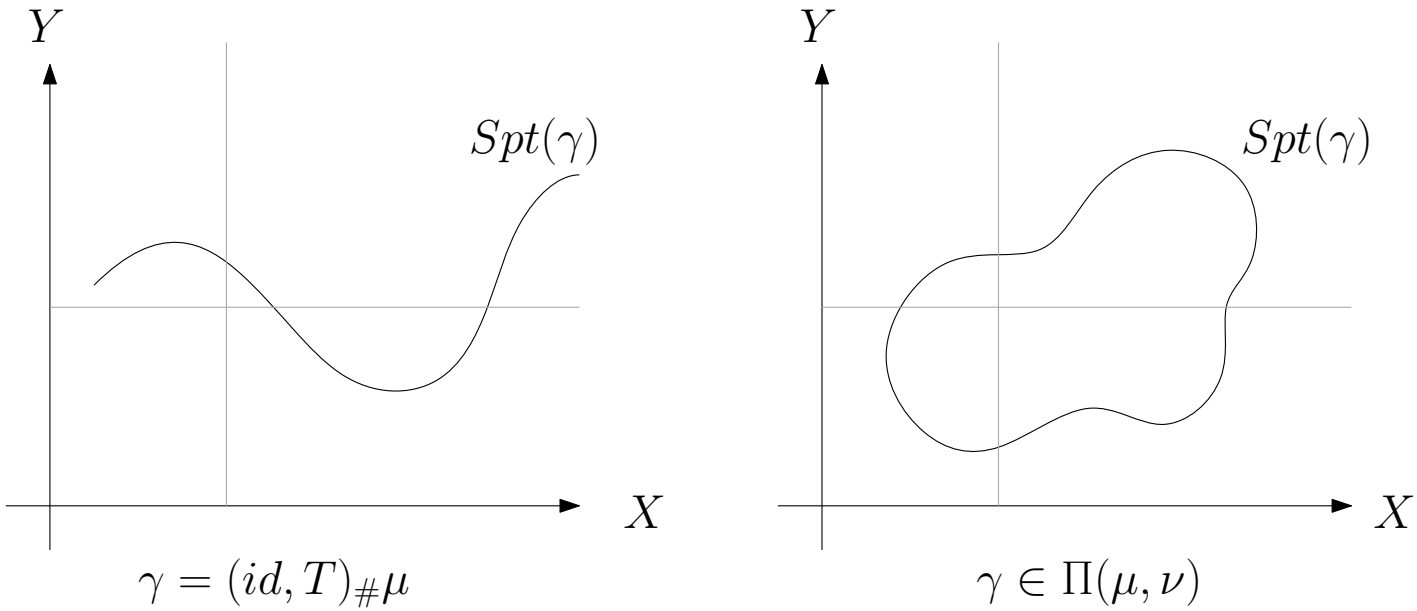


Figure: Caption

Kantorovich Dual Problem

Denote $\Pi(\mu,\nu) = \{\rho : (\pi_x)_{\#}\rho = \mu, (\pi_y)_{\#}\rho = \nu\}$. We consider the constraint $\rho \in \Pi(\mu,\nu)$. we have

$$\sup_{\varphi,\psi} \int_{\Omega} \varphi d\mu + \int_{\Sigma} \psi d\nu - \int_{\Omega\times\Sigma} (\varphi(x) + \psi(y)) d\rho = \begin{cases} 0 & \rho \in \Pi(\mu,\nu), \\ +\infty & \rho \notin \Pi(\mu,\nu), \end{cases} \tag{8}$$

where the superimum is taken among all bounded continuous functions, $\varphi \in C_b(\Omega)$ and $\psi \in C_b(\Sigma)$.

Kantorovich Dual Problem

We use this as a generalized Lagrange multiplier in (KP), and rewrite (KP) as

$$\min_{\rho} \int_{\Omega\times\Sigma} c d\rho + \sup_{\varphi,\psi} \int_{\Omega} \varphi d\mu + \int_{\Sigma} \psi d\nu - \int_{\Omega\times\Sigma} (\varphi(x)+\psi(y)) d\rho \qquad (9)$$

Under suitable conditions, such as Rockafella's conditions, we can exchange sup and inf

$$\sup_{\varphi,\psi} \int_{\Omega} \varphi d\mu + \int_{\Sigma} \psi d\nu + \inf_{\rho} \int_{\Omega\times\Sigma} (c(x,y) - (\varphi(x)+\psi(y))) d\rho. \qquad (10)$$

We can rewrite the infimum in ρ as a constraint on φ and ψ:

$$\inf_{\rho\geq 0} \int_{\Omega\times\Sigma} (c - \varphi\oplus\psi) d\rho = \begin{cases} 0 & \varphi\oplus\psi \leq c \text{ on } X\times Y \\ -\infty & \varphi\oplus\psi > c \end{cases}$$

where $\varphi\oplus\psi$ denotes the function $\varphi\oplus\psi(x,y) := \varphi(x)+\psi(y)$.

Kantovorich Dual Problem

This leads to the dual optimization problem.

Problem (Dual)

Given $\mu \in \mathcal{P}(\Omega)$ *and* $\nu \in \mathcal{P}(\Sigma)$ *and the cost function* $c : \Omega \times \Sigma \to [0, +\infty)$, *we consider the problem*

$$(DP) \quad \max \left\{ \int_{\Omega} \varphi d\mu + \int_{\Sigma} \psi d\nu : \varphi \in C_b(\Omega), \psi \in C_b(\Sigma) : \varphi \oplus \psi \leq c \right\}. \tag{11}$$

From the condition $\varphi \oplus \psi \leq c$, we obtain $\sup DP \leq \min KP$,

$$\int_{\Omega} \varphi d\mu + \int_{\Sigma} \psi d\nu = \int_{\Omega \times \Sigma} \varphi \oplus \psi d\rho \leq \int_{\Omega \times \Sigma} c d\rho$$

This is valid for all admissible pairs (φ, ψ) and every admissible ρ.

Kantovorich Dual Problem

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This is valid for all admissible pairs (φ, ψ) and every admissible ρ. This shows

$$\boxed{\max(DP) \leq \min(KP)}$$

c-transform

Definition (c-transform)

Given $\varphi \in L^1(\Omega)$, and the cost function $c : \Omega \times \Sigma \to \mathbb{R}$, the c-transform of φ is defined as $\varphi^c : \Sigma \to \mathbb{R}$,

$$\varphi^c(y) := \inf_{x \in \Omega} c(x, y) - \varphi(x), \tag{12}$$

The optimization of Kantorovich functional is equivalent to replace the Kantorovich potentials (φ_n, ψ_n) by the c-transforms of the other, namely

$$(\varphi, \psi) \to (\varphi, \varphi^c) \to (\varphi^{cc}, \varphi^c) \to (\varphi^{cc}, \varphi^{ccc}) \cdots$$

c-transform

Geometrically, if we fix a point $x \in \Omega$, then we get a supporting surface $\Gamma_x : \Sigma \to \mathbb{R}$,

$$\Gamma_x(y) := c(x, y) - \varphi(x),$$

the graph of the c-transform $\varphi^c(y)$ is the envelope of all these supporting surfaces.

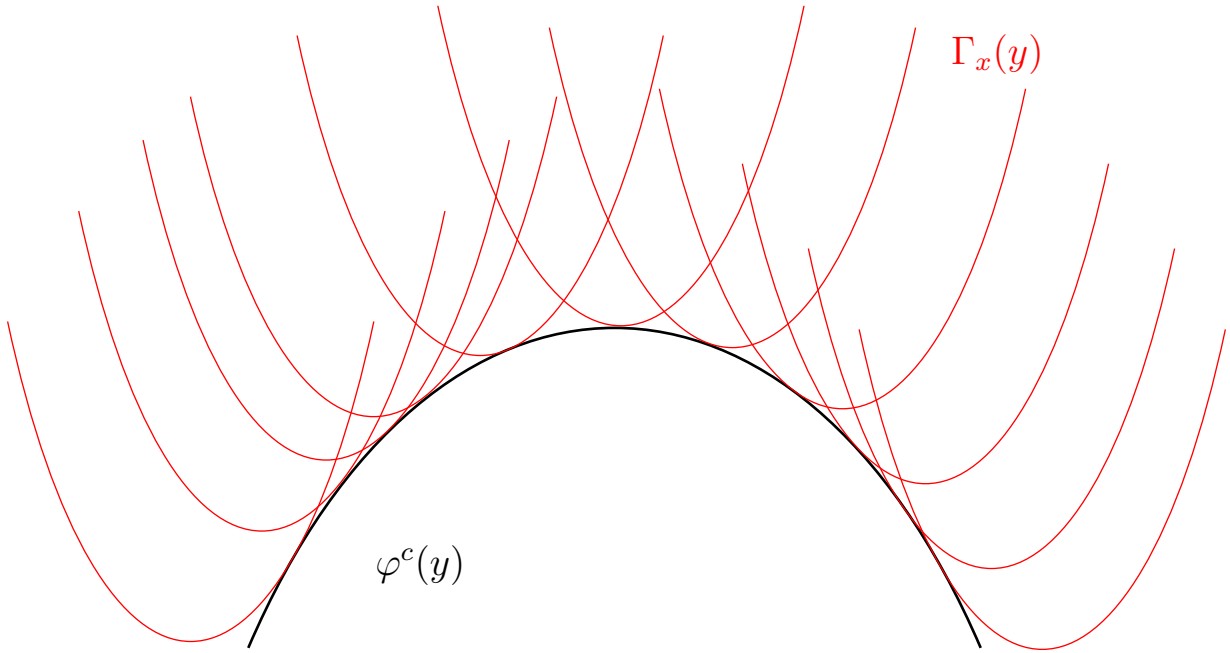


Figure: Geometric interpretation of c-transform.

Twisting Condition

By $\varphi^c(y) = \inf_x c(x,y) - \varphi(x)$, we obtain

$$\boxed{\nabla_x c(x, y(x)) = \nabla \varphi(x)}$$

Definition (Twisting condition)

Given a cost function $c : \Omega \times \Sigma \to \mathbb{R}$, if for any $x \in \Omega$, the mapping

$$\mathcal{L}_x(y) := \nabla_x c(x,y)$$

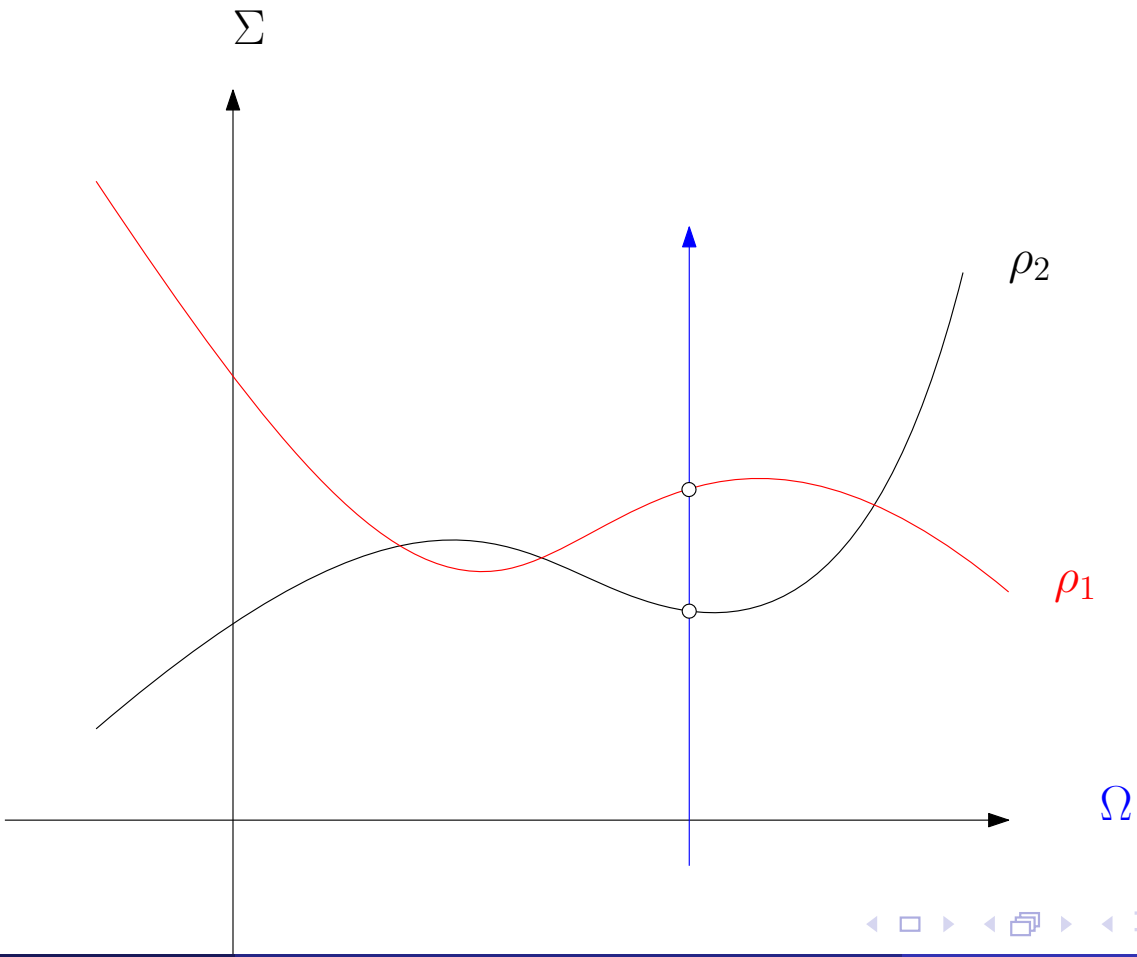
is injective, then we say c satisfies twisting condition.

If c satisfies the twisting condition, then an optimal plan is an optimal map.

Uniqueness of Optimal Transportation Map

Theorem (Uniqueness)

Suppose c satisfies the twisting condition, then the optimal transportation map is unique.



Uniqueness of Optimal Transportation Map

Proof.

Assume there are two optimal transportion maps $T_1, T_2 : (\Omega, \mu) \to (\Sigma, \nu)$, the corresponding optimal transportation plans are

$$\rho_k = (Id, T_k)_{\#}\mu, \quad k = 1, 2.$$

Then $\frac{1}{2}(\rho_1 + \rho_2)$ is also an optimal transportation. Since c satisfies the twisting condition, $\frac{1}{2}(\rho_1 + \rho_2)$ corresponds to an optimal transport map. But the blue line intersects the support of $\frac{1}{2}(\rho_1 + \rho_2)$ at two points, it is not a map. Contradiction. □

Dual Problem

By utilizing c-transform, we obtain

Problem (Dual Problem)

Given $\mu \in \mathcal{P}(\Omega)$, $\nu \in \mathcal{P}(\Sigma)$, the dual problem is

$$DP: \quad \max_{\varphi \in C_b(\Omega)} \left\{ \int_\Omega \varphi(x) d\mu(x) + \int_\Sigma \varphi^c(y) d\nu(y) \right\}. \tag{13}$$

Cyclic Monotonocity

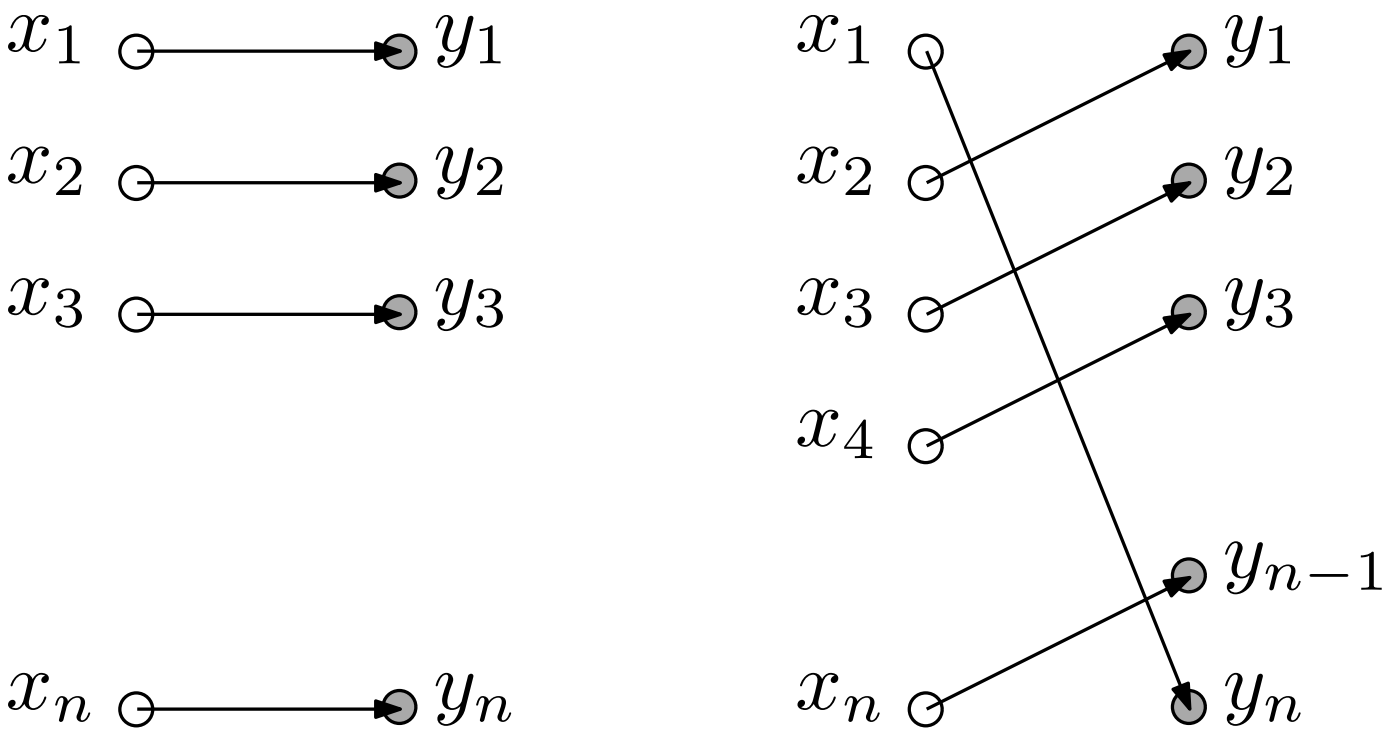


Figure: Cyclic monotonocity.

ρ is optimal, then for any $(x, y) \in \mathrm{Supp}(\rho)$, $\varphi(x) + \psi(y) = c(x, y)$.

Cyclic Monotonocity

Theorem

If $\Gamma \neq \emptyset$, Γ is cyclic monotonuous in $\Omega \times \Sigma$, then there exists a c-concave function φ, such that

$$\Gamma \subset \{(x, y) \in \Omega \times \Sigma : \varphi(x) + \varphi^c(y) = c(x, y)\}.$$

Theorem

If ρ is an optimal transport plan for the continuous cost c, then its support $supp(\rho)$ is cyclic monotonous.

Cyclic Monotonocity

Theorem (max (DP)=min (KP))

Suppose that Ω and Σ are Polish spaces and that $c : \Omega \times \Sigma \to \mathbb{R}$ is uniformly continuous and bounded. Then the problem (DP) admits a solution (φ, φ^c) and we have

$$\boxed{\max(DP) = \min(KP)}$$

Proof.

Suppose ρ is a solution to (KP), then $\mathrm{Supp}(\rho)$ satisfies cyclic monotonicity; hence there exists φ and φ^c, $\mathrm{Supp}(\rho) \subset \{\varphi + \varphi^c = c\}$, therefore

$$\min(KP) = \int_{\Omega\times\Sigma} c d\rho \leq \int_{\Omega} \varphi d\mu + \int_{\Sigma} \varphi^c d\nu \leq \max(DP).$$

Monge-Ampere Equation

Lemma

Suppose $c : \Omega \to \mathbb{R}$ is a C^2 strictly convex function, Ω is convex, then $\nabla c : \Omega \to \mathbb{R}^d$ is injective.

Proof.

Suppose there are two distinct points $x_0, x_1 \in \Omega$, such that $\nabla c(x_0) = \nabla c(x_1)$. Draw a line segment $\gamma : [0,1] \to \Omega$, $\gamma(0) = x_0$ and $\gamma(1) = x_1$. Then $f(t) = c \circ \gamma(t)$ is strictly convex

$$f'(t) = \langle \nabla c((1-t)x_0 + tx_1), x_1 - x_0 \rangle$$
$$f''(t) = (x_1 - x_0)^T D^2 c((1-t)x_0 + tx_1)(x_1 - x_0).$$

Therefore, $f'(1) = f'(0)$ and $f''(t) > 0$. Contradiction. □

Monge-Ampere Equation

Lemma

Suppose $c : \Omega \to \mathbb{R}$ is a strictly convex function, Ω is convex, then $\nabla c : \Omega \to \mathbb{R}^d$ is injective.

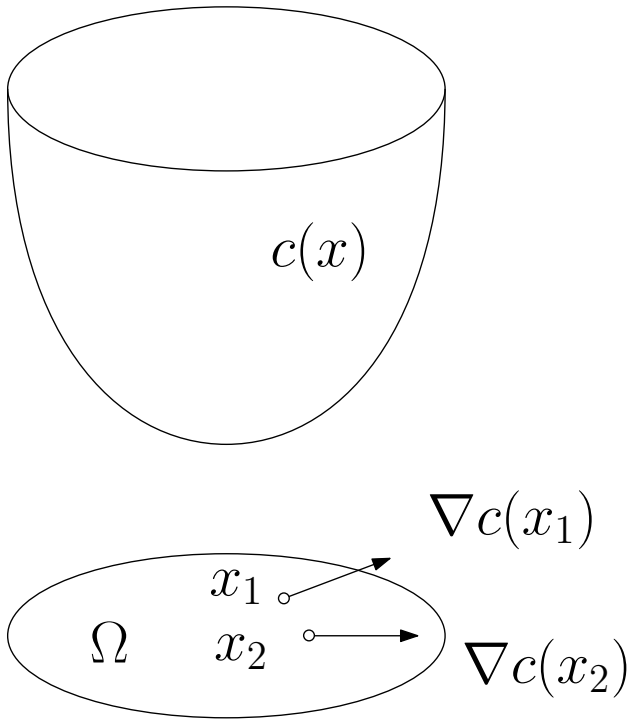


Figure: Injectivity of the gradient map of a strictly convex function.

Monge-Ampere Equation

Suppose the cost function is a strictly convex function, satisfying the condition $c(x, y) = c(x - y)$, then

$$D_x c(x, y) - D\varphi(x) = 0,$$

we obtain $D_x c(x - y) = D\varphi(x)$,

$$T(x) = y = x - (Dc)^{-1}(D\varphi(x)),$$

Brenier Problem

Theorem (Brenier)

Given $\mu \in \mathcal{P}(\Omega)$ and $\nu \in \mathcal{P}(\Sigma)$, and the cost function $c(x,y) = \frac{1}{2}|x-y|^2$, the optimal transportation map is the gradient of a function $u : \Omega \to \mathbb{R}$, $T(x) := \nabla u(x)$.

Proof.

We obtain

$$T(x) = x - D\varphi(x) = D\left(\frac{|x|^2}{2} - \varphi(x)\right) = Du(x).$$

Brenier Problem

Problem (Brenier)

Find a convex function $u : \Omega \to \mathbb{R}$, satisfying the Monge-Amperé equation,

$$det\left(\frac{\partial^2 u(x)}{\partial x_i \partial x_j}\right) = \frac{f(x)}{g \circ \nabla u(x)}. \tag{14}$$

Proof.

We plug $T(x) = Du(x)$ into the Jacobi equation, we obtain the Monge-Ampere equation,

$$\det DT = \frac{f(x)}{g \circ T(x)}$$

hence

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

Fluid Dynamics View

Fluid View

Consider a flow field of special gas. At each time $t \in [0, 1]$, at point $x \in \Omega$, the density of the gas is $\rho(x, t)$. For Lagrangian point of view, the trajectory of each particle (molecule) is a curve, denoted as $\gamma_x(t)$, with initial position and velocity

$$\gamma_x(0) = x, \quad \gamma_x'(t) = \mathbf{v}(\gamma_x(t)).$$

Diffeomorphism

Suppose the trajectories of different particles intersect at some time t, then globally there will be shock waves in the flow field. If there is no shocks, then at each time $t \in [0,1]$, the initial position x of each particle is mapped to the current position $\gamma_x(t)$, this gives a global diffeomorphism

$$g_t := g(\cdot, t) : x \mapsto \gamma_x(t),$$

at time t, the velocity of the particle is $\gamma_x'(t) = \mathbf{v}(\gamma_x(t))$, the global velocity field is denoted as $\mathbf{v}(x,t)$, then the diffeomorphism satisfies the ODE:

$$\frac{d}{dt} g(x,t) = \mathbf{v}(g(x,t),t). \tag{15}$$

Diffeomorphism

Given a smooth velocity field $\mathbf{v}(x,t)$, we can get the diffeomorphism group $g(x,t)$. Namely, if $\mathbf{v}(x,t)$ is smooth enough, no shock waves will appear,

$$\partial_t \log \det \left[\frac{\partial g(x,t)}{\partial x} \right] = \nabla \cdot \mathbf{v}(g(x,t),t). \tag{16}$$

McCann Interpolation

If the cost function is strictly convex, under Lagrangian point of view, all particles move with uniform speed in a straight line, their trajectories are

$$g_t(x) = (1-t)x + t(\nabla c)^{-1}(\nabla \varphi), \tag{17}$$

where φ is the optimal Kantorovich potential, this is called McCann interpolation.
McCann's interpolation gives geodesics in Wasserstein space. One can show that

$$\mathcal{W}_c((g_s)_{\#}\mu, (g_t)_{\#}\nu) = |s-t|\mathcal{W}_c(\mu,\nu), \quad \forall s,t \in [0,1].$$

Time Dependent Optimal Transport Problem

Given a differential cost function $c(\mathbf{v})$, defined on velocity vector, then the cost for a trajectory is

$$\mathcal{C}[g_t(x)] := \int_0^1 c(\dot{g}_t(x))dt.$$

Problem (Time Dependent Optimal Transport)

Find a flow field connecting μ and ν, that minimizes the total cost of all trajectories:

$$\inf \left\{ \int_\Omega \mathcal{C}[g_t(x)]d\mu(x) : \ g_0 = Id, \quad (g_1)_\# \mu = \nu \right\}. \tag{18}$$

Time Dependent Optimal Transport Problem

From mass-conservation law, we get the continuity equation:

$$\frac{d}{dt}\rho(x,t) + \nabla \cdot (\rho(x,t)\mathbf{v}(x,t)) = 0,$$

By McCann interpolation, the velocity field satisfies the Euler equation:

$$\frac{d}{dt}\mathbf{v}(x,t) + \mathbf{v}(x,t) \cdot \nabla \mathbf{v}(x,t) = 0.$$

The cost function information is implied by the initial conditon

$$\mathbf{v}(x,0) = (\nabla c)^{-1}(\nabla \varphi),$$

where φ is the optimal Kantorovich potential.

Benamou-Brenier Problem

Consider all flow fields connecting μ and ν, denote $(\rho(x,t), \mathbf{v}(x,t))$ as (ρ_t, v_t), then

$$\Gamma(\mu,\nu) := \left\{ (\rho_t, v_t) : \frac{\partial \rho_t}{\partial t} = -\nabla \cdot (\rho_t \mathbf{v}_t), \quad \rho_0 = \mu, \quad \rho_1 = \nu \right\}$$

Given any time $t \in [0,1]$, the Kinetic energy of the velocity field $\mathbf{v}(x,t)$ is defined as

$$E(\mathbf{v}_t) := \frac{1}{2} \int_\Omega \rho(x,t) \|\mathbf{v}(x,t)\|^2 dx.$$

Benamou-Brenier Problem

Problem (Benamou-Brenier)

Find the flow field in $\Gamma(\mu, \nu)$, that minimizes the total kinetic energy,

$$BB: \quad \min\left\{\frac{1}{2}\int_0^1 \int_\Omega \rho_t \|\mathbf{v}_t\|^2 dxdt : \ (\rho_t, \mathbf{v}_t)\right\} \tag{19}$$

Benamou-Brenier Problem

Use variational approach, assume $\rho_t \mathbf{w}_t$ is divergence free,

$$\frac{1}{2}\frac{d}{d\varepsilon}\int_0^1 \int \Omega \rho_t \langle \mathbf{v}_t + \varepsilon \mathbf{w}_t, \mathbf{v}_t + \varepsilon \mathbf{w}_t \rangle dxdt = \int_0^1 \int_\Omega \langle \mathbf{v}_t, \varepsilon \mathbf{w}_t \rangle dxdt = 0,$$

by Hodge decomposition theorem, $\mathbf{v})_t$ is orthogonal to all divergence free vector fields, so $\mathbf{v}_t = \nabla u_t$, where $u_t : \Omega \to \mathbb{R}$ is a family of funcitions. This can be obatined by McCann interpolation.

Benamou-Brenier Problem

Problem (Benamou-Brenier)

$$\mathcal{W}_2(\mu,\nu) := \min\left\{\int_0^1 \left\|\frac{\partial \rho}{\partial t}\right\|^2_{\rho(t)} dt, \rho_0 = \mu, \rho_1 = \nu, -\nabla\cdot(\rho\nabla u) = \frac{\partial \rho}{\partial t}\right\}$$

where

$$\left\|\frac{\partial \rho}{\partial t}\right\|^2_{\rho(t)} = \int_\Omega \rho|\nabla u|^2,$$

Otto's Interpretation

Given two geodesics $\rho_1(t), \rho_2(t) \subset \mathcal{P}(\Omega)$, $\rho_1(0) = \rho_2(0) = \rho$, the tangent vector at $\rho \in \mathcal{P}(\Omega)$,

$$\frac{\partial \rho_1}{\partial t} = -\nabla \cdot (\rho \nabla \varphi_1)$$
$$\frac{\partial \rho_2}{\partial t} = -\nabla \cdot (\rho \nabla \varphi_2)$$

the Riemannian inner product is

$$\left\langle \frac{\partial \rho_1}{\partial t}, \frac{\partial \rho_2}{\partial t} \right\rangle_\rho = \int_\Omega \rho \langle \nabla \varphi_1, \nabla \varphi_2 \rangle dx.$$

Entropy Flow

Definition (Entropy)

Given a probability measure $\rho \in \mathcal{P}(\Omega)$, its entropy is defined as

$$\mathrm{Ent}(\rho) := \int_{\Omega} \rho \log \rho dx.$$

Principle of maximum entropy

The principle of maximum entropy states that the probability distribution which best represents the current state of knowledge is the one with largest entropy, in the context of precisely stated prior data.

Entropy Flow

Consider a path $\rho(t) \subset \mathcal{P}(\Omega)$,

$$\frac{d}{dt}\mathrm{Ent}(\rho(t)) = \int_{\omega} \left(\dot{\rho} \log \rho + \rho \frac{\dot{\rho}}{\rho} \right) dx = \int_{\Omega} (1 + \log \rho) \dot{\rho} dx.$$

By continuity equation $\dot{\rho} = -\nabla \cdot (\rho \mathbf{v})$, assume $\Omega = \mathbb{R}^d$, hence

$$\int_{\Omega} \dot{\rho} dx = -\int_{\Omega} \nabla \cdot (\mathbf{v}\rho) dx = -\int_{\partial\Omega} \rho \mathbf{v} dx = 0.$$

We obtain

$$\frac{d}{dt}\mathrm{Ent}(\rho(t)) = \int_{\Omega} \log \rho \dot{\rho} dx = -\int_{\Omega} \log \rho \nabla \cdot (\rho \mathbf{v}),$$

Entropy Flow

At the same time

$$\nabla \cdot (\rho \log \rho \mathbf{v}) = \log \rho \nabla \cdot (\rho \mathbf{v}) + \langle \nabla \log \rho, \rho \mathbf{v} \rangle,$$

We obtain

$$\begin{aligned} \frac{d}{dt}\mathrm{Ent}(\rho(t)) &= -\int_{\Omega} \log \rho \nabla \cdot (\rho \mathbf{v}) \\ &= \int_{\Omega} \langle \nabla \log \rho, \rho \mathbf{v} \rangle - \int_{\partial \Omega} \rho \log \rho \mathbf{v} \\ &= \int_{\Omega} \langle \nabla \log \rho, \mathbf{v} \rangle \rho dx. \end{aligned}$$

This shows the Wasserstein gradient of Entropy is $\nabla \log \rho$.

Entropy Flow

In order to reduce the entropy, we let $\mathbf{v} = -\nabla \log \rho$, plug into the continuity equation:

$$\frac{\partial \rho_t}{\partial t} + \nabla \cdot (\rho_t \mathbf{v}_t) = 0,$$

hence

$$\frac{\partial \rho_t}{\partial t} - \nabla \cdot (\rho_t \nabla \log \rho_t) = 0$$

$$\frac{\partial \rho_t}{\partial t} - \nabla \cdot (\rho_t \frac{\nabla \rho_t}{\rho_t}) = 0$$

$$\frac{\partial \rho_t}{\partial t} - \Delta_t = 0$$

This shows Wasserstein gradient flow of entropy equals to the classical heat flow.

Entropy Flow

We let $\mathbf{v} = -\nabla \log \rho$, plug into the continuity equation:

$$\frac{d}{dt}\mathrm{Ent}(\rho(t)) = \int_\Omega \langle \nabla \log \rho, \mathbf{v} \rangle \rho dx = -\int_\Omega \frac{|\nabla \rho|^2}{\rho} dx = -4 \int_\Omega |\nabla \sqrt{\rho}|^2 dx.$$

This gives the dissipation speed of the entropy. Let t go to infinity, ρ_∞ becomes a uniform distribution.