Optimal Transport: A Crash Course

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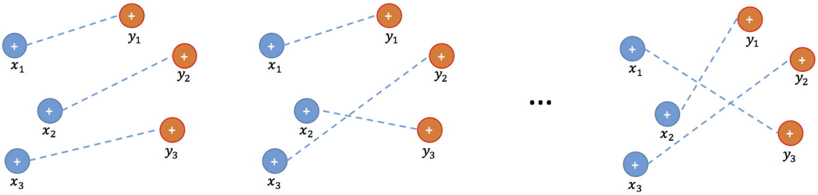
Introduction

What is Optimal Transport?

- The optimal transport problem seeks the most efficient way of transporting one distribution of mass into another.



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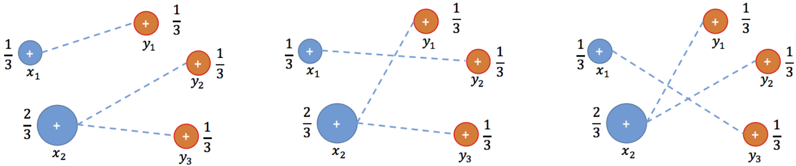

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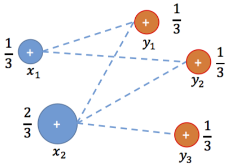

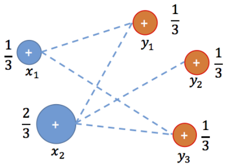

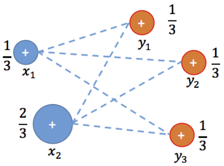

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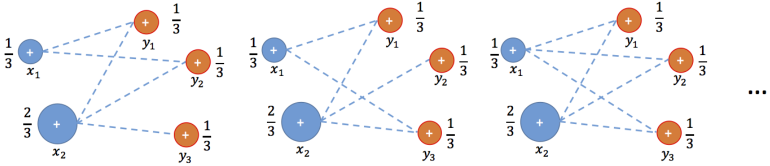

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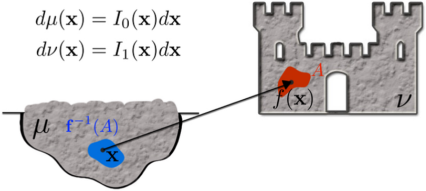
There are infinitely many transportation plans!

A little bit of history!

- The problem was originally studied by Gaspard Monge in the 18'th century.

Gaspard Monge
1746-1818

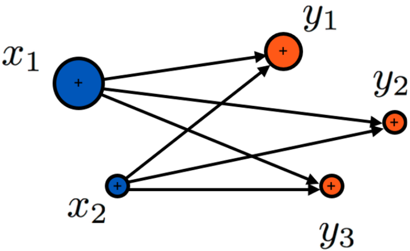


Le mémoire sur les déblais et les remblais
(The note on land excavation and infill)

A little bit of history!:

- Working on optimal allocation of scarce resources during World War II, Kantorovich revisited the optimal transport problem in 1942.

Leonid Kantorovich
1912-1986



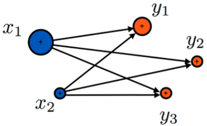
Resource allocation

A little bit of history!

- In 1975, he shared the Nobel Memorial Prize in Economic Sciences with Tjalling Koopmans "for their contributions to the theory of optimum allocation of resources."

Leonid Kantorovich
1912-1986

Tjalling Koopmans
1910-1985

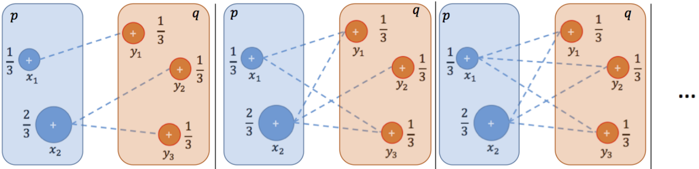


Resource allocation

Linear programming is born!

Kantorovich Formulation

- First lets focus on the common trait of these transportation plans.



$$\gamma = \begin{array}{c} \begin{array}{ccc} y_1 & y_2 & y_3 \end{array} \\ \begin{bmatrix} \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} \end{bmatrix} \end{array} \begin{array}{c} x_1 \\ x_2 \end{array} \qquad \gamma = \begin{array}{c} \begin{array}{ccc} y_1 & y_2 & y_3 \end{array} \\ \begin{bmatrix} \frac{1}{9} & 0 & \frac{2}{9} \\ \frac{2}{9} & \frac{1}{3} & \frac{1}{9} \end{bmatrix} \end{array} \begin{array}{c} x_1 \\ x_2 \end{array} \qquad \gamma = \begin{array}{c} \begin{array}{ccc} y_1 & y_2 & y_3 \end{array} \\ \begin{bmatrix} \frac{1}{9} & \frac{1}{9} & \frac{1}{9} \\ \frac{2}{9} & \frac{2}{9} & \frac{2}{9} \end{bmatrix} \end{array} \begin{array}{c} x_1 \\ x_2 \end{array} \qquad \cdots$$

$$\sum_i \gamma_{i\cdot} = [\frac{1}{3} \quad \frac{1}{3} \quad \frac{1}{3}] \qquad \sum_j \gamma_{\cdot j} = \begin{bmatrix} \frac{1}{3} \\ \frac{2}{3} \end{bmatrix}$$

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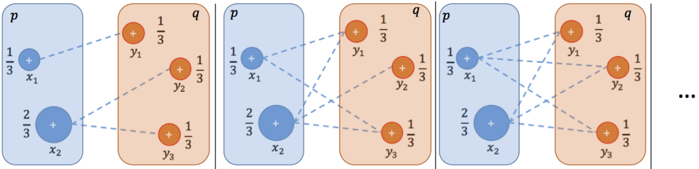

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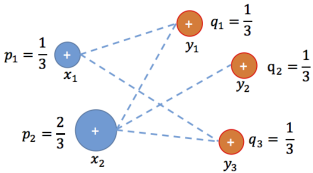
A transportation plan is a joint probability distribution with marginal distributions equal to the original distributions, p and q.



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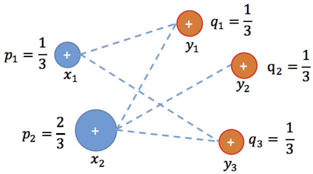
$$\sum_i \gamma_{ij} = q_j, \sum_j \gamma_{ij} = p_i$$

- Let $\mu = \sum_i p_i \delta_{x_i}$ and $\nu = \sum_j q_j \delta_{y_j}$ represent the mass distributions, where δ_{x_i} is a Dirac measure centered at x_i.



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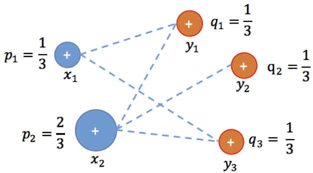

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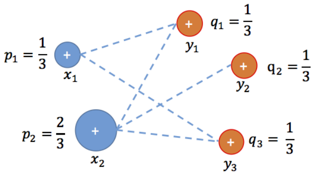
- Transportation from x_i to y_j would induce a cost $c_{ij} = c(x_i, y_j)$ (e.g. cost of gas for transportation distance)



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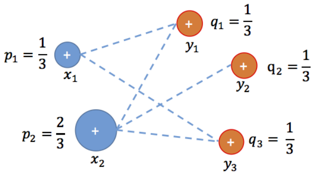
- Transportation from x_i to y_j would induce a cost $c_{ij} = c(x_i, y_j)$ (e.g. cost of gas for transportation distance)
- Optimal transport problem seeks the most efficient transportation plan with respect to the cost c:

$$\min_\gamma \sum_i \sum_j c_{ij}\gamma_{ij}$$

$$s.t. \ \sum_i \gamma_{ij} = q_j, \ \sum_j \gamma_{ij} = p_i, \gamma_{ij} \geq 0$$



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Optimal transport problem:

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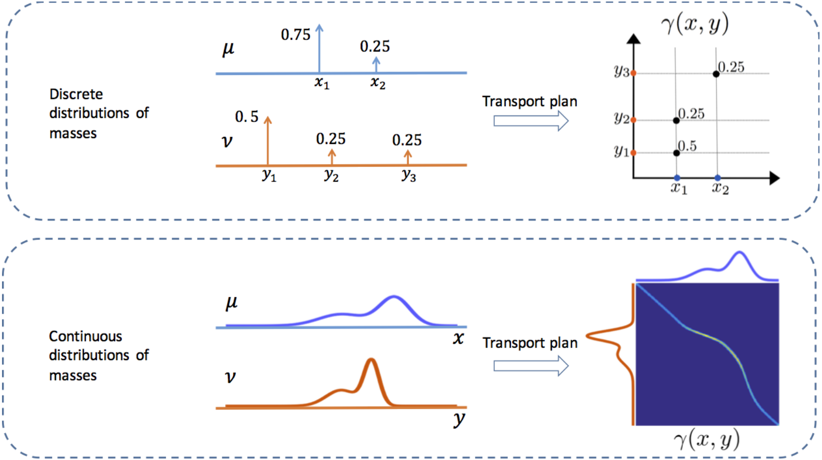
$$\gamma_{ij} \geq 0$$

- OT formulation for discrete mass distributions (point cloud distributions) is a linear programing problem
- The problem **is convex** but **not strictly convex**.
- Common solvers include: Simplex algorithm, Interior point methods (AKA Barrier methods), etc.

- What if we have two continuums of masses?



Kantorovich general formulation:

- A transport plan between measures μ and ν defined on X and Y is a probability measure $\gamma \in X \times Y$ with marginals,

$$\gamma(X, A) = \nu(A),\ \gamma(B, Y) = \mu(B) \tag{1}$$

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- Let $c(\cdot, \cdot) : X \times Y \to \mathbb{R}$ define the transportation cost from X to Y.
- The transport problem is then formulated as finding the transport plan that minimizes the expected cost, c, with respect to the joint probability measure γ,

$$\begin{aligned} KP(\mu, \nu) &= min_{\gamma \in \Gamma(\mu,\nu)} \int_{X \times Y} c(x, y) d\gamma(x, y) \\ \Gamma(\mu, \nu) &= \{\gamma \mid \gamma(A, Y) = \mu(A), \;\; \gamma(X, B) = \nu(B)\} \end{aligned} \tag{2}$$

Kantorovich: discrete formulation (Earth Mover's Distance)

- Let $\mu = \sum_{i=1}^{N} p_i \delta_{x_i}$ and $\nu = \sum_{j=1}^{M} q_j \delta_{y_j}$, where δ_{x_i} is a Dirac measure,

$$
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Kantorovich: general formulation

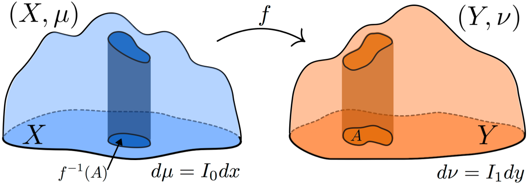
- Let $d\mu(x) = p(x)dx$ and $d\nu(x) = q(x)dx$,

$$\begin{aligned} KP(\mu,\nu) = &\quad \min_\gamma \quad \int_{X\times Y} c(x,y)d\gamma(x,y) \\ s.t. &\quad \int_Y d\gamma(x,y) = p(x),\ \int_X d\gamma(x,y) = q(y) \\ &\quad \gamma(x,y) \geq 0 \end{aligned}$$

Monge Formulation

Monge formulation and Transport Maps:

- A map, $f: X \to Y$, for measures μ and ν defined on spaces X and Y is called a transport map iff,



$$\int_{f^{-1}(A)} I_0(x)dx = \int_A I_1(y)dy \tag{3}$$

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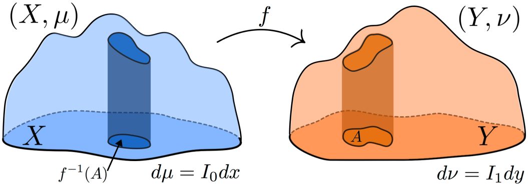

$$\int_{f^{-1}(A)} I_0(x)dx = \int_A I_1(y)dy \tag{3}$$

- Find the optimal transport map $f : X \to Y$ that minimizes the expected cost of transportation,

$$M(\mu, \nu) = \inf_{f \in MP} \int_X c(x, f(x)) I_0(x)dx \tag{4}$$

Monge formulation and Transport Maps:

- In the majority of engineering applications the cost is the Euclidean distance,

$$\begin{aligned} M(\mu,\nu) &= \inf_{f\in MP} \int_X |x-f(x)|^2 I_0(x)dx \\ MP &= \{f: X\to Y | \int_{f^{-1}(A)} I_0(x)dx = \int_A I_1(y)dy\} \end{aligned} \tag{5}$$

Note that the objective function and the constraint in Eq. (5) are both nonlinear with respect to f.

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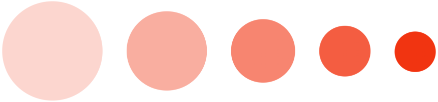
  Note that the objective function and the constraint in Eq. (5) are both nonlinear with respect to f.

- When f exists and it is differentiable, above constraint can be written in differential form as,

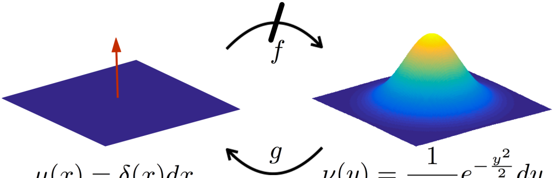
$$MP = \{f:X\to Y| det(Df(x))I_1(f(x)) = I_0(x), \forall x\in X\} \quad (6)$$



$$f(x) = \alpha x \Rightarrow det(Df(x))I(f(x)) = \alpha^d I(\alpha x)$$

A Transport Map May Not Exist:

- A transport map, f, exists only if μ is an absolutely continuous measure with compact support and $c(x, f(x))$ is convex.
- Here is an example where the transport map does not exists:



$$\mu(x) = \delta(x)dx \qquad \nu(y) = \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} dy$$

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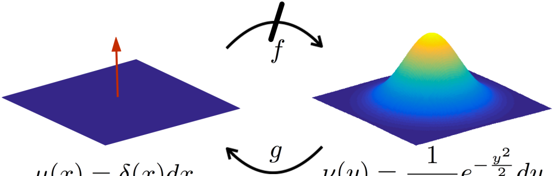

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- Monge formulation is not suitable for analyzing point cloud distributions or any particle like distributions. This is when Kantorovich's formulation comes to rescue!

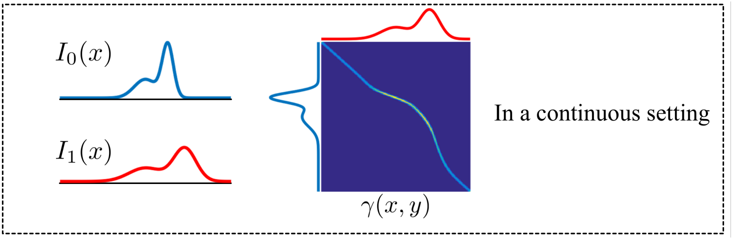
Kantorovich vs. Monge

- The following relationship holds between Monge's and Kantorovich's formulation,

$$KP(\mu,\nu) \leq M(\mu,\nu) \tag{7}$$

- When an optimal transport map exists, $f : X \to Y$, the optimal transport plan and the optimal transport map are related through,

$$\int_{X\times Y} c(x,y)d\gamma(x,y) = \int_X c(x,f(x))d\mu(x) \tag{8}$$



Existence and uniqueness

Brenier's theorem

- Let $c(x,y) = |x-y|^2$ and let μ be absolutely continuous with respect to the Lebesgue measure. Then, there exists a unique optimal transport map $f : X \to Y$ such that,

$$\int_{f^{-1}(A)} d\mu(x) = \int_A d\nu(y)$$

which is characterized as,

$$f(x) = x - \nabla\psi(x) = \nabla \underbrace{(\frac{1}{2}|x|^2 - \psi(x))}_{\phi(x)} \quad (9)$$

for some concave scalar function ψ. In other words, f is the gradient of a convex scalar function ϕ, and therefore it is curl free.

Dual Problem

Kantorovich problem and its dual

- Primal problem:

$$
\begin{aligned}
KP(\mu,\nu) = \quad & \min_{\gamma} \quad \int_{X\times Y} c(x,y)\,d\gamma(x,y) \\
& s.t. \quad \int_{Y} d\gamma(x,y) = p(x), \;\; \int_{X} d\gamma(x,y) = q(y) \\
& \qquad\quad \gamma(x,y) \geq 0
\end{aligned}
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- Dual problem:

$$\begin{aligned} DP(\mu,\nu) = \quad & \max_{\phi,\psi} \quad \int_X \phi(x)d\mu(x) + \int_Y \psi(y)d\nu(y) \\ & s.t. \quad \phi(x) + \psi(y) \leq c(x,y), \quad \forall (x,y) \in X\times Y \end{aligned}$$

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$$

- Note that $DP(\mu,\nu) \leq KP(\mu,\nu)$, where equality holds when the cost function, c, is nonnegative lower semi-continuous.

Dual problem and Kantorovich-Rubinstein theorem:

- Dual problem:

$$\begin{aligned} DP(\mu,\nu) = \quad & \max_\phi \quad \int_X \phi(x)d\mu(x) + \int_Y \phi^c(y)d\nu(y) \\ & s.t. \qquad \phi^c(y) = \inf_X c(x,y) - \phi(x) \end{aligned}$$

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Kantorovich-Rubinstein theorem

- Let μ and ν be two probability measures in the metric space (X, d).
- When the cost function is the ℓ_1 norm, $c(x,y) = |x-y|$, the Dual problem could be simplified into:

$$DP(\mu,\nu) = \quad \max_{\phi\in Lip_1(X)} \quad \int_X \phi(x)d\mu(x) - \int_X \phi(x)d\nu(x)$$

where $Lip_1(X) = \{\phi \;\;|\;\; |\phi(x)-\phi(y)| \leq d(x,y), \forall x,y \in X\}$.

Transport-Based Metrics

p-Wasserstein distance

- Let $P_p(\Omega)$ be the set of Borel probability measures with finite p'th moment defined on a given metric space (Ω, d). The p-Wasserstein metric, W_p, for $p \geq 1$ on $P_p(\Omega)$ is then defined as the optimal transport problem with the cost function $c(x, y) = d^p(x, y)$. Let μ and ν be in $P_p(\Omega)$, then,

$$W_p(\mu, \nu) = \left(\min_{\gamma \in \Gamma(\mu,\nu)} \int_{\Omega \times \Omega} d^p(x, y) d\gamma(x, y) \right)^{\frac{1}{p}} \tag{10}$$

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or equivalently when the optimal transport map, f^*, exists,

$$W_p(\mu, \nu) = \left(\min_{f \in MP} \int_{\Omega} d^p(x, f(x)) d\mu(x) \right)^{\frac{1}{p}} . \tag{11}$$

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- In most engineering applications $\Omega \subset \mathbb{R}^d$ and $d(x,y) = |x - y|$.

p-Wasserstein for 1D probability measures

- For absolutely continuous one-dimensional probability measures μ and ν on $\mathbb{R}$ with positive probability density functions I_0 and I_1, the optimal transport map has a closed form solution.

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$$\begin{cases} F_\mu(x) = \mu((-\infty, x)) \\ F_\nu(y) = \nu((-\infty, y)) \end{cases} \tag{12}$$

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In one dimension, there only exists one monotonically increasing transport map $f : \mathbb{R} \to \mathbb{R}$ such that $f \in MP$, and it is defined as,

$$f(x) := \min\{t \in \mathbb{R} \ : \ F_\nu(t) \geq F_\mu(x)\}. \tag{13}$$

or equivalently $f(x) = F_\nu^{-1} \circ F_\mu(x)$.

p-Wasserstein distance for 1D probability measures

$$W_p(\mu,\nu) = \left(\int_0^1 |F_\mu^{-1}(t) - F_\nu^{-1}(t)|^p dt\right)^{\frac{1}{p}} \tag{14}$$

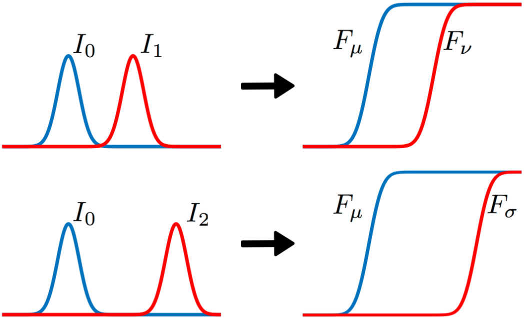

Figure: Note that, the Euclidean distance does not provide a sensible distance between I_0, I_1 and I_2 while the p-Wasserstein distance does.

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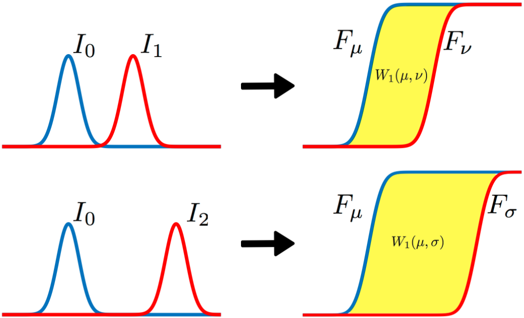

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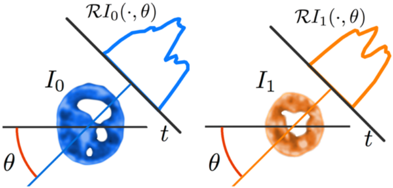
Sliced p-Wasserstein distance

- Slice an n-dimensional probability distribution $(n > 1)$ into one-dimensional representations through projections and measure p-Wasserstein distance between these representations.



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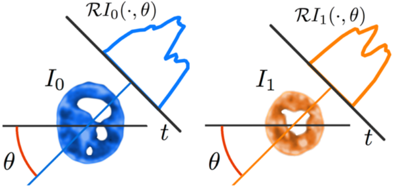

  - Where $\mathscr{R}$ denotes Radon transform and is defined as,

$$\mathscr{R}I(t,\theta) := \int_{\mathbb{S}^{d-1}} I(x)\delta(t-\theta\cdot x)dx$$
$$\forall t \in \mathbb{R},\ \forall\theta \in \mathbb{S}^{d-1}(\text{Unit sphere in } \mathbb{R}^d) \quad (16)$$

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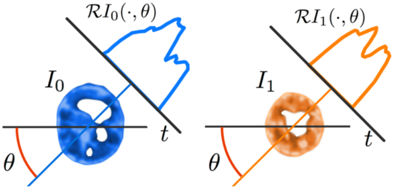

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  - and the p-Sliced-Wasserstein (p-SW) distance is defined as:

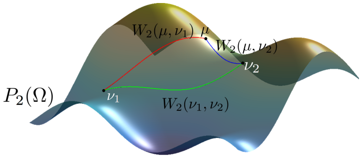
$$SW_p(I_0,I_1) = \left(\int_{\mathbb{S}^{d-1}} W_p^p(\mathscr{R}I_0(.,\theta),\mathscr{R}I_1(.,\theta))d\theta\right)^{\frac{1}{p}} \tag{17}$$

Geometric Properties

2-Wasserstein geodesics

- The set of continuous measures together with the 2-Wasserstein metric forms a Riemmanian manifold.

- Given the 2-Wasserstein space, $(P_2(\Omega), W_2)$, the geodesic between $\mu, \nu \in P_2(\Omega)$ is the shortest curve on $P_2(\Omega)$ that connects these measures.



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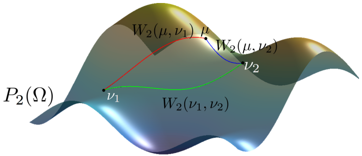

- Let ρ_t for $t \in [0, 1]$ parametrizes a curve on $P_2(\Omega)$ with $\rho_0 = \mu$ and $\rho_1 = \nu$, and let I_t denote the density of ρ_t, $I_t(x)dx = d\rho_t(x)$.

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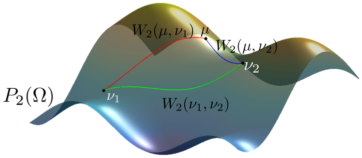

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- For the optimal transport map, $f(x)$, between μ and ν the geodesic is parametrized as,

$$I_t(x) \quad = \quad det(Df_t(x))I_1(f_t(x)), \quad f_t(x) = (1-t)x + tf(x) \qquad (18)$$

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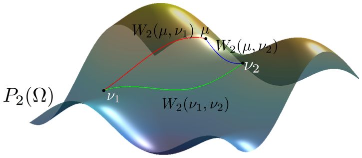

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- It is straightforward to show that,

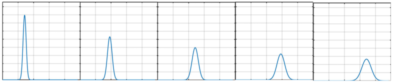
$$W_2(\mu, \rho_t) = tW_2(\mu, \nu) \tag{19}$$

2-Wasserstein geodesics

Geodesic in the 2-Wasserstein space

$$I_t(x) = det(Df_t(x))I_1(f_t(x))$$

$t = 0$ $t = 0.25$ $t = 0.5$ $t = 0.75$ $t = 1$



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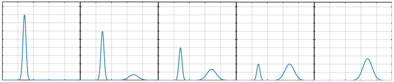

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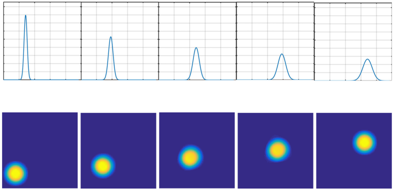

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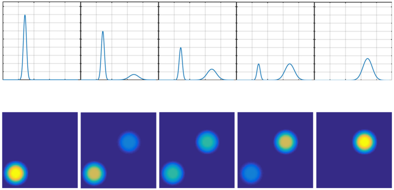

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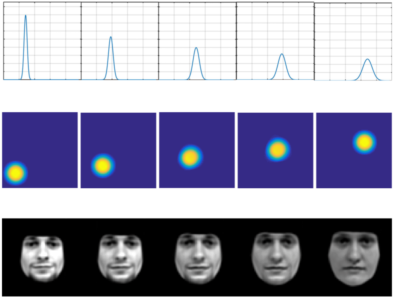

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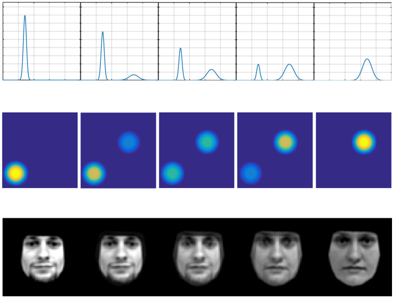

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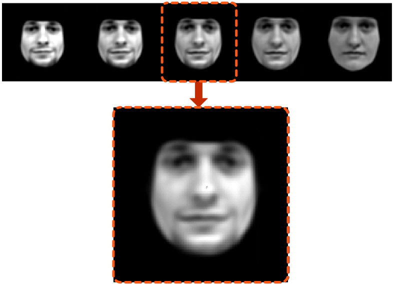

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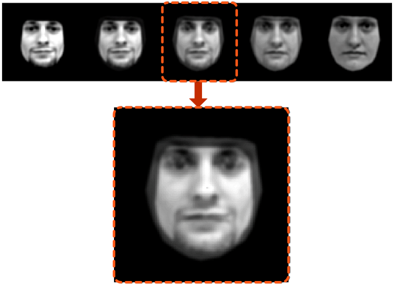

Numerical Solvers

Flow Minimization (Angenent, Haker, and Tannenbaum)

- The flow minimization method finds the optimal transport map following below steps:
    1. Obtain an initial mass preserving transport map using the Knothe-Rosenblatt coupling
    2. Update the initial map to obtain a curl free mass preserving transport map that minimizes the transport cost

$$f_{k+1} = f_k + \epsilon \frac{1}{I_0} Df_k(f_k - \nabla(\Delta^{-1} div(f_k))), \quad \Delta^{-1} : \text{Poisson solver} \quad (20)$$

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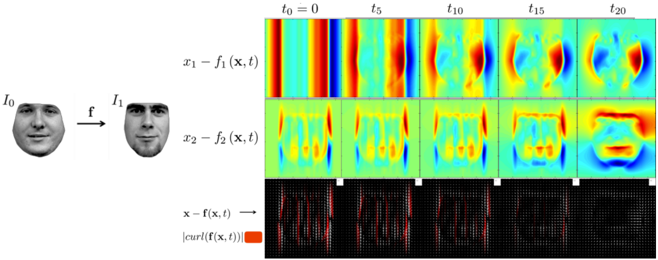

Angenent, S., et al. "Minimizing flows for the Monge–Kantorovich problem." SIAM 2003

Gradient descent on the dual problem (Chartrand et al.)

- For the strictly convex cost function, $c(x,y) = \frac{1}{2}|x-y|^2$, the dual of Kantorovich problem can be formalized as minimizing,

$$M(\eta) = \int_X \eta(x)d\mu(x) + \int_Y \eta^c(y)d\nu(y) \tag{21}$$

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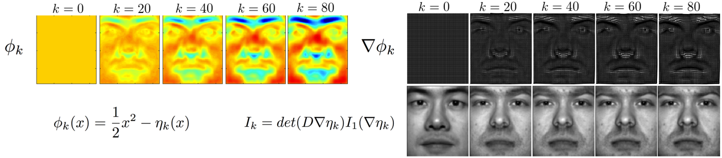
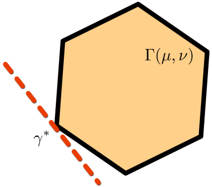


Chartrand, R., et al. "A gradient descent solution to the Monge-Kantorovich problem." AMS 2009

Linear programming

- Let $\mu = \sum_{i=1}^{N} p_i \delta_{x_i}$ and $\mu = \sum_{j=1}^{M} q_j \delta_{y_j}$, where δ_{x_i} is a Dirac measure,

$$\begin{aligned} KP(\mu,\nu) &= \min_\gamma \sum_i \sum_j c(x_i, y_j)\gamma_{ij} \\ s.t. &\quad \sum_j \gamma_{ij} = p_i,\ \sum_i \gamma_{ij} = q_j,\ \gamma_{ij} \geq 0 \end{aligned}$$



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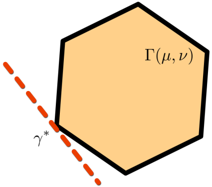

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Multi-Scale Approaches

  - To improve computational complexity of several multi-scale approaches have been proposed
  - The idea behind all these multi-scale techniques is to obtain a coarse transport plan and refine the transport plan iteratively.

Entropy Regularization

- Cuturi proposed a regularized version of the Kantorovich problem which can be solved in $\mathcal{O}(NlogN)$,

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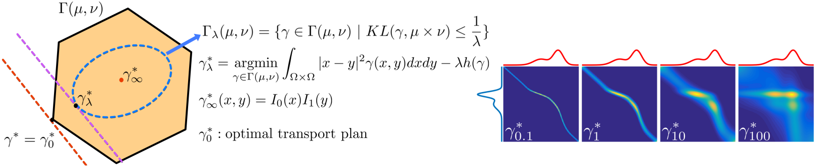

Cuturi, M. "Sinkhorn distances: Lightspeed computation of optimal transport." NIPS 2013.

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Coming Up Next

- Transport-based transformations

Thank you!