Optimal Transport

Theory, Computation and Applications

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Optimal Transport

Principal concern: the distance between two probability measures.
First introduced in 1781 by Monge.
Relative subjects: probability theory, geometry, graph theory, machine learning...
Applications:

- Image registration and warping;
- Reflector design;
- Retrieving information from shadowgraphy and proton radiography;
- Seismic tomography and reflection seismology.

Some well-known researchers:

- Gasoard Monge (France);
- Leonid Kantorovich (Russia);
- Yann Brenier (France);
- Xianfeng Gu (顾险峰, China);

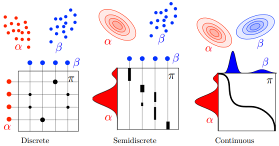

Fig. 1. Three main scenarios for Kantorovich OT

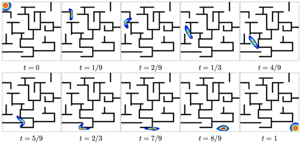

Fig. 2. Solving maze with OT

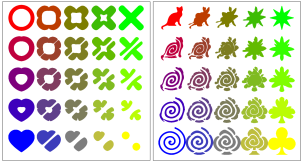

Fig. 3. 2D shape interpolation with OT

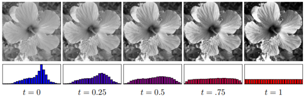

Fig. 4. Histogram equalization with OT

The sand-moving problem

A child wants to make a pile of sand in the shape of a castle.
Cost: 1 kcal per shovel and per meter horizontally.
Target: Minimize the total cost.

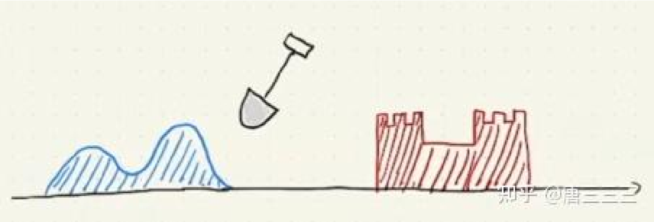

Fig. 5. The sand-moving problem.

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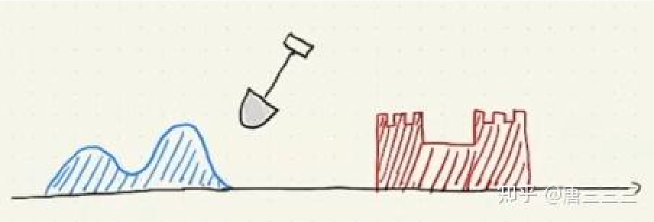

Fig. 5. The sand-moving problem.

Let's denote the source shape by $f(x)$ and the target by $g(x)$. The sand-moving problem cound be formulated as: find a **transport mapping** $T : \mathbb{R} \to \mathbb{R}$ to minimize

$$\int_{\mathbb{R}} |T(x) - x| f(x)\ dx, \tag{1}$$

which satisfies

$$\int_{T(U)} g(x)\ dx = \int_U f(x)\ dx \text{ for all open interval } U \subset \mathbb{R}. \tag{2}$$

The allocation problem

There are some steel coils to be transported from warehouses to factories. The transport cost is $1 per coil and per kilometer. How to minimize the total cost?

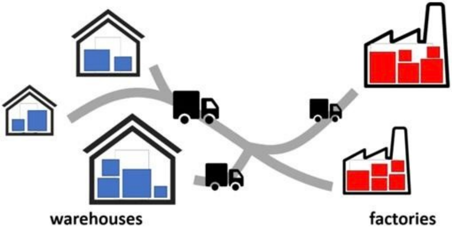

Fig. 6. The allocation problem.

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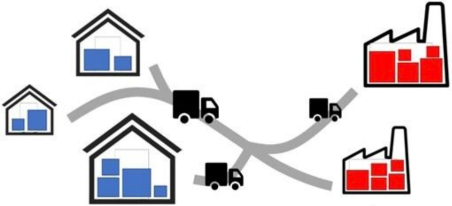

Fig. 6. The allocation problem.

Assume the i-th warehouse has a_i coils and the j-th factory needs b_i coils. And assume the distance between the i-th warehouse and the j-th factory is d_{ij}. The allocation problem could be formulated as: find a **transport matrix** v_{ij} to minimize

$$\sum_{i,j} d_{ij} v_{ij} \tag{3}$$

which satisfies

$$a_i = \sum_j v_{ij}, \quad \forall i, \qquad \text{and} \qquad b_j = \sum_i v_{ij}, \quad \forall j. \tag{4}$$

The Monge formulation

Denote $\mathcal{M}_+^1(\mathcal{X})$ the set of probability measures on $\mathcal{X}$.

Definition (push-forward)

Suppose $\mu \in \mathcal{M}_+^1(\mathcal{X})$ *and a map* $T : \mathcal{X} \to \mathcal{Y}$. *Say* $\nu \in \mathcal{M}_+^1(\mathcal{Y})$ *is the push-forward of* μ *by* T *if*

$$\int_{\mathcal{Y}} h(y)\ d\nu(y) = \int_{\mathcal{X}} h(T(x))\ d\mu(x), \quad \forall h \in \mathcal{C}(\mathcal{Y}). \tag{5}$$

Write $T_{\#}\mu := \nu$.

Example (push-forward of a discrete measure)

Suppose α *is a discrete measure*

$$\alpha = \sum_{i=1}^{n} a_i \delta_{x_i}.$$

Then the push-forward of α *by* T *is*

$$T_{\#}\alpha = \sum_{i=1}^{n} a_i \delta_{T(x_i)}.$$

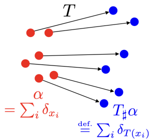

Fig. 7. push-forward of a discrete measure

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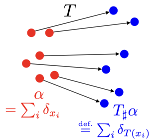

Fig. 7. push-forward of a discrete measure

Given two probability measures μ on $\mathcal{X}$ and ν on $\mathcal{Y}$, and a cost function $c(x, y)$. Optimal transport could be generally formulated as the Monge problem:

$$\min_{T} \left\{ \int_{\mathcal{X}} c(x, T(x))\ d\mu(x) : T_{\#}\mu = \nu \right\} \tag{6}$$

The Monge problem between discrete measures is introduced by Monge[1].

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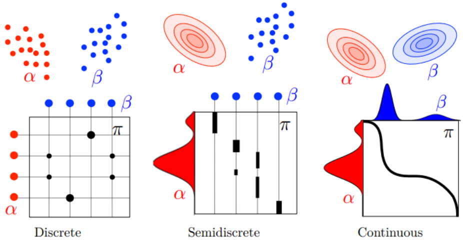
The Kantorovich formulation

Here's another general formulation of OT, we first recall the three main scenarios for OT.



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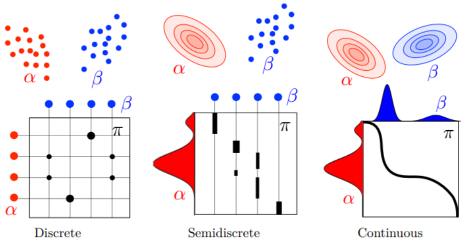

Given two probability measures μ on $\mathcal{X}$ and ν on $\mathcal{Y}$, and a cost function $c(x, y)$. Optimal transport could be generally formulated as the Kantorovich problem[2]:

$$\mathcal{L}_c(\mu, \nu) = \min_{\pi} \int_{\mathcal{X}\times\mathcal{Y}} c(x, y)\ d\pi(x, y), \tag{7}$$

where π is a measure on $\mathcal{X} \times \mathcal{Y}$, whose marginals are μ and ν, that is,

$$\mu = \int_{\mathcal{Y}} \pi(\cdot, y)\ dy, \qquad \nu = \int_{\mathcal{X}} \pi(x, \cdot)\ dx. \tag{8}$$

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Wasserstein disrtance

Here we suppose $\mathcal{X} = \mathcal{Y}$ and $c(x, y) = d(x, y)^p$ $(p > 1)$, where d is a distance on $\mathcal{X}$.

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Theorem (Wasserstein distance)

Under the above assumptions, $\mathcal{L}_c(\mu, \nu)^{1/p}$ is a distance on $\mathcal{M}_+^1(\mathcal{X})$.

The distance $\mathcal{W}_p(\mu, \nu) := \mathcal{L}_c(\mu, \nu)^{1/p}$ is called p-Wasserstein distance.

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Definition (weak convergence)

Suppose $\mathcal{X}$ *is compact. Say* $(\mu_k)_{k \geq 1} \subset \mathcal{M}_+^1(\mathcal{X})$ *converges weakly to* $\mu \in \mathcal{M}_+^1(\mathcal{X})$ *if*

$$\int_{\mathcal{X}} g \; d\mu_k \to \int_{\mathcal{X}} g \; d\mu, \quad \forall g \in \mathcal{C}(\mathcal{X}). \tag{9}$$

Theorem (Wasserstein distance and weak convergence[3])

On a compact domain $\mathcal{X}$, $(\mu_k)_{k \geq 1} \subset \mathcal{M}_+^1(\mathcal{X})$ *converges weakly to* $\mu \in \mathcal{M}_+^1(\mathcal{X})$ *if and only if* $\mathcal{W}_p(\mu_k, \nu) \to 0$.

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Equivalence between the Kantorovich and Monge problems

Theorem (Kantorovich dual problem)

The Kantorovich problem can be solved in the dual space by

$$\mathcal{L}_c(\mu,\nu) = \sup_{(f,g)\in\mathcal{R}(c)} \int_{\mathcal{X}} f(x)\ d\mu(x) + \int_{\mathcal{Y}} g(y)\ d\nu(y), \tag{10}$$

where the set of admissible dual potential is

$$\mathcal{R}(c) := \{(f,g) \in \mathcal{C}(\mathcal{X}) \times \mathcal{C}(\mathcal{Y}) : \forall (x,y), f(x) + g(y) \leq c(x,y)\}. \tag{11}$$

The pair (f,g) is called Kantorovich potentials.

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Theorem (Brenier)

In the case $\mathcal{X} = \mathcal{Y} = \mathbb{R}^d$ and $c(x, y) = \|x - y\|_2^2$, if at least one of the two input measures (denoted μ) has a density ρ_μ with respect to the Lebesgue measure, then the optimal π in the Kantorovich formulation is unique and is supported on the graph $(x, T(x))$ of a Monge map $T : \mathbb{R}^d \to \mathbb{R}^d$. This means that $\pi = (\mathrm{Id}, T)_{\#}\mu$, i.e.

$$\int_{\mathcal{X}\times\mathcal{Y}} h(x, y)\ d\pi(x, y) = \int_{\mathcal{X}} h(x, T(x))\ d\mu(x), \quad \forall h \in \mathcal{C}(\mathcal{X} \times \mathcal{Y}). \tag{12}$$

Furthermore, this map T is uniquely defined as the gradient of a convex function φ, $T(x) = \nabla\varphi(x)$, where φ is the unique (up to an additive constant) convex function such that $(\nabla\varphi)_{\#}\mu = \nu$. This convex function is related to the dual potential f solving (10) as

$$\varphi(x) = \frac{\|x\|_2^2}{2} - f(x). \tag{13}$$

1-D case

Thank You