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);

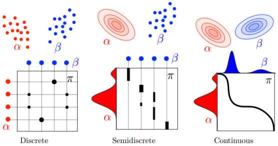

Fig. 1. Three main scenarios for Kantorovich OT

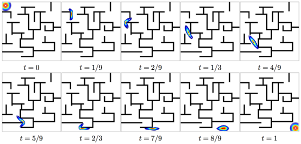

Fig. 2. Solving maze with OT

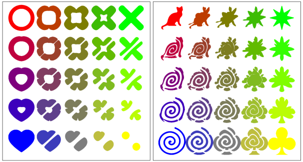

Fig. 3. 2D shape interpolation with OT

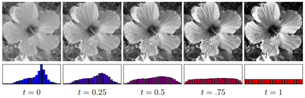

Fig. 4. Histogram equalization with OT

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.

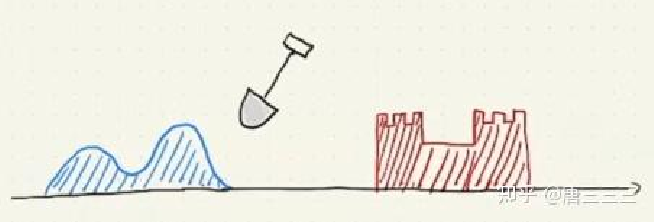

Fig. 5. The sand-moving problem.

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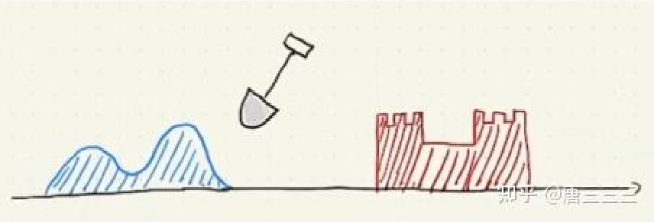

Fig. 5. The sand-moving problem.

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?

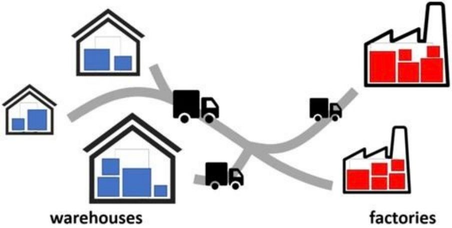

Fig. 6. The allocation problem.

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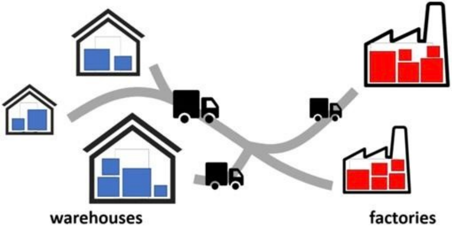


Fig. 6. The allocation problem.

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

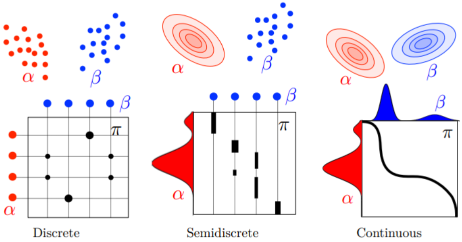
$$\sum_{i,j} d_{ij} v_{ij} \tag{3}$$

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 Kantorovich formulation

To give an general formulation of OT, we first recall the three main scenarios for OT.



[1] Leonid Kantorovich. "On the transfer of masses". In: *Doklady Akademii Nauk* 37.2 (1942).

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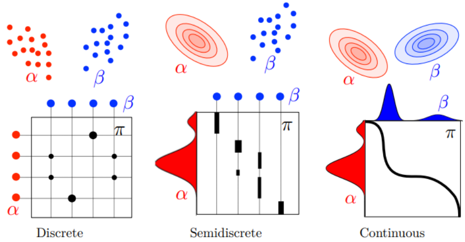

Given two probability measures μ on $\mathcal{X}$ and ν on $\mathcal{Y}$, and a cost function $c(x, y)$. The Kantorovich formulation[1] of OT is

$$\mathcal{L}_c(\mu, \nu) = \min_{\pi} \int_{\mathcal{X}\times\mathcal{Y}} c(x, y)\ d\pi(x, y), \tag{5}$$

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

$$\mu = \int_{\mathcal{Y}} \pi(\cdot, y)\ dy, \qquad \nu = \int_{\mathcal{X}} \pi(x, \cdot)\ dx. \tag{6}$$

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Metric properties of OT

Here we assume $\mathcal{X} = \mathcal{Y}$ and $c(x, y) = d(x, y)^p$ $(p > 1)$, where d is a distance on $\mathcal{X}$. Denote $\mathcal{M}_+^1(\mathcal{X})$ the set of probability measures on $\mathcal{X}$.

[2] Cédric Villani. *Optimal Transport: Old and New*. Vol. 338. Springer Verlag, 2009.

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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)

Assume $\mathcal{X}$ 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

$$\int_{\mathcal{X}} g \; d\mu_k \to \int_{\mathcal{X}} g \; d\mu, \quad \forall g \in \mathcal{C}(\mathcal{X}). \tag{7}$$

Theorem (Wasserstein distance and weak convergence[2])

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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Thank You