An introduction to optimal transport

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July 9, 2025

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- Why should I care? What can I do with it? Applications?

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- Density functional theory (physics/chemistry): how does a system of electrons organize itself to minimize interaction energy.
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Both talks will focus on **ideas** and we will try to avoid getting bogged down in too many details.

Origins of optimal transport

- Gaspard Monge (1781): How do I fill a hole with dirt as efficiently as possible?

Monge's optimal transport problem

- Data: two positive functions, $f(x)$ and $g(y)$ on regions $X, Y \subset \mathbb{R}^n$, (the height of the dirt pile and depth of the hole) and a cost function, $c(x, y)$ (the cost per unit to transport dirt from x to y).

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- Assume $\int_X f(x)dx = \int_Y g(y)dy = 1$ (ie, the total volume of the pile and the hole are the same).
- We look for a transport map $T : X \to Y$ so that, for each $A \subseteq Y$, $\int_{T^{-1}(A)} f(x)dx = \int_A g(y)dy$ (the total amount of dirt moved into the set A is the same as the volume of that part of the hole). In this case, we write $T_\# f = g$.

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- If T is a diffeomorphism, (ie. $1 - 1$, onto, smooth with a smooth inverse), this means T satisfies the change of variables equation: $f(x) = |\det DT(x)| g(T(x))$.
- Among all T's with this property, we seek to minimize

$$\int_X c(x, T(x)) f(x) dx.$$

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- Therefore, choose $T(x)$ so that

$$\int_{-\infty}^{x} f(t)dt = \int_{-\infty}^{T(x)} g(s)ds$$

For probabilistically minded people, this is $T = (F_g)^{-1} \circ F_f$, where F_g and F_f are the cummulative distribution functions.

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- In this case, the gradient $\nabla u(x) := (\frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, ..., \frac{\partial u}{\partial x_n})(x)$ gives us a vector at each $x = (x_1, x_2, ..., x_n)$. We can think of this as a function $\nabla u : \mathbb{R}^n \to \mathbb{R}^n$.

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- A symmetric $n \times n$ matrix A is said to be positive definite if $V^T AV \geq 0$ for all $V \in \mathbb{R}^n$.
- We say $u : \mathbb{R}^n \to \mathbb{R}$ is convex if $D^2u(x)$ is positive definite for each $x \in \mathbb{R}^n$.

Optimal transport in higher dimensions: Brenier's theorem

- Suppose $X, Y \subseteq \mathbb{R}^n$ and $c(x,y) = |x-y|^2 = \sum_{i=1}^n (x_i - y_i)^2$ (this is the cost function that turns out to give the cleanest theory, and is also the most useful in applications).

Theorem (Brenier 1987)

There exists a unique solution T to Monge's problem.
Furthermore, $T(x) = \nabla u(x)$ is the gradient of a convex function.

- Note: in one dimension, this just means $T(x) = \frac{du}{dx}(x)$, implying $T'(x) = \frac{d^2u}{dx^2}(x) \geq 0$. So T is increasing, as we saw before.
- It is not even obvious beforehand that there exists a map of this form satisfying the constraint $T_{\#} f = g$. This fact alone (a consequence of Brenier's theorem) is important in some applications (in these situations the optimization problem doesn't even show up; it is just the existence of the map T that matters).

Application: isoperimetric inequality

Isoperimetric inequality: The surface area of any set $M \subseteq \mathbb{R}^n$ is greater than or equal to the surface area of a ball with the same volume.

$$Vol(M) = Vol(B_R(0)) \implies S(M) \geq S(B_R(0))$$

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Proof:

- Take $f(x) = \chi_M$, $g(y) = \chi_{B_R(0)}$.
- $\nabla u(x)$ the Brenier map $\implies det(D^2u(x)) = f(x)/g(\nabla u(x)) = 1$ (change of variables).
- Arithmetic mean dominates geometric mean (as u is convex, D^2u has positive eigenvalues) $\implies det^{1/n}(D^2u(x)) \leq \frac{1}{n}\Delta u(x)$

Proof

$$
\begin{aligned}
\frac{1}{n}S(B_R(0))R = Vol(B_R(0)) &= Vol(M) \\
&= \int_M 1 d^n x \\
&= \int_M det^{1/n}(D^2 u(x))dx \\
&\leq \int_M \frac{1}{n}\Delta u(x)dx \\
&= \frac{1}{n}\int_{\partial M} \nabla u(x) \cdot \vec{N} d^{n-1}S(x) \\
&\leq \frac{1}{n}\int_{\partial M} R d^{n-1}S(x) \\
&= \frac{1}{n}S(M)R
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- We prove an inequality about surfaces/curves/bodies in $\mathbb{R}^n$ by working with simple inequalities under the integral sign (geometric-arithmetic mean, Cauchy-Schwartz on $\mathbb{R}^n$).
- This is a **common theme** in applications of optimal transport in geometry.

Some background on the theory

- How do we prove Brenier's theorem?
- More generally, what tools do we use to understand solutions to optimal transport problems?

Kantorovich's relaxed version

- Kantorovich (1942) was interested in the optimal allocation of resources. Given a distribution of mines $f(x)$ producing iron and a distribution $g(y)$ of factories consuming iron, and a cost $c(x, y)$ to move iron from point x to y, which mine should supply which factory to minimize the total transport cost?

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- Monge-Kantorovich problem: Minimize

$$\int_{X\times Y} c(x,y)\gamma(x,y)dxdy$$

among functions (actually, a generalization of functions) $\gamma(x,y)\geq 0$ such that $\int_X \gamma(x,y)dx = g(y)$ and $\int_Y \gamma(x,y)dy = f(x)$.

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among functions (actually, a generalization of functions) $\gamma(x,y) \geq 0$ such that $\int_X \gamma(x,y)dx = g(y)$ and $\int_Y \gamma(x,y)dy = f(x)$.
- Interpretation: $\gamma(x,y)$ represents the amount of iron that goes from mine x to factory y. In Monge's version, each mine x can supply only one factory $y = T(x)$, but that is not true here: mine x can split its iron among several, or even infinitely many, factories. This is a *relaxation* of Monge's problem.

Kantorovich's relaxed version (cont'd)

- This is now a linear minimization problem (an infinite dimensional linear program), and is much easier to deal with technically than Monge's functional, $\int_X c(x, T(x))f(x)dx$ and constraint $T_\# f = g$ (ie, $f(x) = |\det DT(x)| g(T(x))$).

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- Kantorovich duality: the Kantorovich problem is equivalent (*dual*) to maximizing

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among functions $u(x)$ and $v(y)$ that satisfy $u(x) + v(y) \leq c(x, y)$.

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- Kantorovich shared the Nobel prize in 1975 with Tjalling Koopmans for developing this theory.

Idea of proof of Brenier's Theorem

- For $c(x,y) = |x-y|^2$, the solutions to the dual problem turn out to be (more or less) convex functions. The constraint is saturated along the solutions (ie, $u(x)+v(y) = c(x,y)$ when x and y are coupled together).

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- Differentiating, after some manipulation, yields,

$$\nabla u(x) = y$$

which basically means there is only one $y = \nabla u(x) := T(x)$ which gets coupled to x.

Some applications

- Optimal transport has many diverse applications, in PDE, fluid mechanics, statistics, image recognition, operations research, functional/geometric inequalites, meteorology, finance...
- I'll briefly describe three selected applications here. At the end of the lecture, we'll vote on which one is the most interesting, and discuss the winner in more depth on Wednesday.

Choice one: matching theory in economics

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- *What on earth does this have to do with optimal transport?*

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- Their work on matching theory garnered Alvin Roth and Lloyd Shapley the 2012 Nobel Prize in economics.

Choice two: density functional theory in physics

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- The development of density functional theory earned Walter Kohn the Nobel prize in chemistry in 1998. 12 of the 100 most cited papers in the history of science are on this topic (and two of the top 10).

Choice three: Ricci curvature and entropy in geometry

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- One of the pioneers of this field, Cedric Villani, won the Fields medal in 2010.

Vote!

- Matching theory (economics).

Vote!

- Density functional theory (physics/chemistry).

Vote!

- Ricci curvature and entropy (geometry).

Some references

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