Discrete Optimal Mass Transportation Theory

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Thanks

Thanks for the invitation.

Collaborators

The work is collaborated with Shing-Tung Yau, Feng Luo, Jian Sun, Na Lei, Li Cui and Kehua Su etc.

Motivation

Mesh Parameterization

Conformal Parameterization

Conformal parameterization: angle-preserving

Infinitesimal circles are mapped to infinitesimal circle.

Area-preserving Parameterization

Area-preserving parameterization

Infinitesimal circles are mapped to infinitesimal ellipses, preserving the areas.

Surface Parameterization

Area-preserving parameterization

(a) Cortical surface

(b) Conformal

(c) Area-preserving

Surface Parameterization

Surface Parameterization

(a) Gargoyle model; (b) Angle-preserving; (c) Area-preserving.

Volume Parameterization

harmonic map volume-preserving map

Volume Parameterization

harmonic map

volume-preserving map

Registration

Conformal Parameterization for Surface Matching

Existing method, 3D surface matching is converted to image matching by using conformal mappings.

Conformal Parameterization for Surface Matching

Disadvantages: conformal parameterization may induce exponential area shrinkage, which produces numerical instability and matching mistakes.

Optimal Mass Transport Map

Advantage: the parameterization is area-preserving, improves the robustness.

Registration based on Optimal Mass Transport Map

(a) Armadillo #1 (b) Armadillo #2

(c) OMT Map #1

(d) Conformal Map #1

(e) Curvature difference hist.

(f) OMT Map #2

(g) Conformal Map #2

(h) Area distortion hist.

Geometric Clustering

Wasserstein Distance

Given a metric surface $(S, \mathbf{g})$, a Riemann mapping $\varphi : (S, \mathbf{g}) \to \mathbb{D}^2$, the conformal factor $e^{2\lambda}$ gives a probability measure on the disk. The shape distance is given by the Wasserstein distance.

Fig. 9: **The computation of Wasserstein distance**

Expression Classification

Fig. 10: **Face surfaces for expression clustering. The first row is "sad", the second row is "happy" and the third row is "surprise".**

Expression Classification

Compute the Wasserstein distances, embed isometrically using MDS method, perform clustering.

From Shape to IQ

Can we tell the IQ from the shape of the cortical surface?

Optimal Mass Transport Mapping

Optimal Transport Problem

Earth movement cost.

Optimal Mass Transportation

Problem Setting

Find the best scheme of transporting one mass distribution (μ, U) to another one (ν, V) such that the total cost is minimized, where U, V are two bounded domains in $\mathbb{R}^n$, such that

$$\int_U \mu(x)dx = \int_V \nu(y)dy,$$

$0 \leq \mu \in L^1(U)$ and $0 \leq \nu \in L^1(V)$ are density functions.

Optimal Mass Transportation

For a transport scheme s (a mapping from U to V)

$$s : \mathbf{x} \in U \to \mathbf{y} \in V,$$

the total cost is

$$C(s) = \int_U \mu(\mathbf{x}) c(\mathbf{x}, s(\mathbf{x})) d\mathbf{x}$$

where $c(\mathbf{x}, \mathbf{y})$ is the cost function.

Cost Function $c(x,y)$

The cost of moving a unit mass from point x to point y.

$$Monge(1781): c(x,y) = |x-y|.$$

This is the natural cost function. Other cost functions include

$$\begin{aligned} c(x,y) &= |x-y|^p, p \neq 0 \\ c(x,y) &= -\log|x-y| \\ c(x,y) &= \sqrt{\varepsilon + |x-y|^2}, \varepsilon > 0 \end{aligned}$$

Any function can be cost function. It can be negative.

Optimal Transportation Map

Problem

Is there an optimal mapping $T : U \to V$ such that the total cost $\mathscr{C}$ is minimized,

$$\mathscr{C}(T) = \inf\{\mathscr{C}(s) : s \in \mathscr{S}\}$$

where $\mathscr{S}$ is the set of all measure preserving mappings, namely $s : U \to V$ satisfies

$$\int_{s^{-1}(E)} \mu(x)dx = \int_E \nu(y)dy, \forall \textit{ Borel set } E \subset V$$

Solutions

Three categories:

1. Discrete category: both (μ, U) and (ν, V) are discrete,
2. Semi-continuous category: (μ, U) is continuous, (ν, V) is discrete,
3. Continuous category: both (μ, U) and (ν, V) are continuous.

Kantorovich's Approach

Both (μ, U) and (ν, V) are discrete. μ and ν are Dirac measures. (μ, U) is represented as

$$\{(\mu_1, \mathbf{p}_1), (\mu_2, \mathbf{p}_2), \cdots, (\mu_m, \mathbf{p}_m)\},$$

(ν, V) is

$$\{(\nu_1, \mathbf{q}_1), (\nu_2, \mathbf{q}_2), \cdots, (\nu_n, \mathbf{q}_n)\}.$$

A transportation plan $f : \{\mathbf{p}_i\} \to \{\mathbf{q}_j\}$, $f = \{f_{ij}\}$, f_{ij} means how much mass is moved from $(\mu_i, \mathbf{p}_i)$ to $(\nu_j, \mathbf{q}_j)$, $i \leq m, j \leq n$. The optimal mass transportation plan is:

$$\min_f f_{ij} c(\mathbf{p}_i, \mathbf{q}_j)$$

with constraints:

$$\sum_{j=1}^{n} f_{ij} = \mu_i, \sum_{i=1}^{m} f_{ij} = \nu_j.$$

Optimizing a linear energy on a convex set, solvable by linear programming method.

Kantorovich's Approach

Kantorovich won Nobel's prize in economics.

$$\min_f \sum_{ij} f_{ij} c(\mathbf{p}_i, \mathbf{p}_j),$$

such that

$$\sum_j f_{ij} = \mu_i, \sum_i f_{ij} = \nu_j.$$

mn unknowns in total. The complexity is quite high.

Brenier's Approach

Theorem (Brenier)

If $\mu, \nu > 0$ and U is convex, and the cost function is quadratic distance,

$$c(\mathbf{x}, \mathbf{y}) = |\mathbf{x} - \mathbf{y}|^2$$

then there exists a convex function $f : U \to \mathbb{R}$ unique upto a constant, such that the unique optimal transportation map is given by the gradient map

$$T : \mathbf{x} \to \nabla f(\mathbf{x}).$$

Brenier's Approach

Continuous Category: In smooth case, the Brenier potential $f : U \to \mathbb{R}$ statisfies the Monge-Ampere equation

$$det\left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right) = \frac{\mu(\mathbf{x})}{\nu(\nabla f(\mathbf{x}))},$$

and $\nabla f : U \to V$ minimizes the quadratic cost

$$\min_f \int_U |\mathbf{x} - \nabla f(\mathbf{x})|^2 d\mathbf{x}.$$

Semi-Continuous Category

Discrete Optimal Mass Transportation Problem

Given a compact convex domain U in $\mathbb{R}^n$ and $p_1, \cdots, p_k$ in $\mathbb{R}^n$ and $A_1, \cdots, A_k > 0$, find a transport map $T : U \to \{p_1, \cdots, p_k\}$ with $vol(T^{-1}(p_i)) = A_i$, so that T minimizes the transport cost

$$\int_U |\mathbf{x} - T(\mathbf{x})|^2 d\mathbf{x}.$$

Power Diagram vs Optimal Transport Map

Theorem (Aurenhammer-Hoffmann-Aronov 1998)

Given a compact convex domain U in $\mathbb{R}^n$ and $p_1, \cdots, p_k$ in $\mathbb{R}^n$ and $A_1, \cdots, A_k > 0$, $\sum_i A_i = vol(U)$, there exists a unique power diagram

$$U = \bigcup_{i=1}^{k} W_i,$$

$vol(W_i) = A_i$, the map $T : W_i \mapsto p_i$ minimizes the transport cost

$$\int_U |\mathbf{x} - T(\mathbf{x})|^2 d\mathbf{x}.$$

Power Diagram vs Optimal Transport Map

Power Diagram vs Optimal Transport Map

1. F. Aurenhammer, F. Hoffmann and B. Aronov, Minkowski-type theorems and least squares partitioning, in Symposium on Computational Geometry, 1992, pp. 350-357.
2. F. Aurenhammer, F. Hoffmann and B. Aronov, Minkowski-type Theorems and Least-Squares Clustering, vol 20, 61-76, Algorithmica, 1998.
3. Bruno Lévy, "A numerical algorithm for L_2 semi-discrete optimal transport in 3D", arXiv:1409.1279, Year 2014.
4. X. Gu, F. Luo, J. Sun and S.-T. Yau, "Variational Principles for Minkowski Type Problems, Discrete Optimal Transport, and Discrete Monge-Ampere Equations", arXiv:1302.5472, Year 2013.

Power Diagram vs Optimal Transport Map

In Aurenhammer et al.'s and Levy's works, the main theorems are:

Theorem

Given a set of points P and a set of weights $W = (w_i)$, the assignment $T_{P,W}$ defined by the power diagram is an optimal transport map.

Theorem

Given a measure μ with density, a set of points (p_i) and prescribed mass ν_i such that $\sum \nu_i = \mu(\Omega)$, there exists a weights vector W such that $\mu(Pow_W(p_i)) = \nu_i$.

Power Diagram vs Optimal Transport Map

In Levy's proof, the following energy is examined: Let $T : \Omega \to P$ be an arbitrary assignment,

$$f_T(W) := \int_\Omega \|x - T(x)\|^2 - w_{T(x)} d\mu,$$

using envelope theorem,

$$\frac{\partial f_{T_W}(W)}{\partial w_i} = -\mu(\mathrm{Pow}_W(p_i)),$$

the convex energy is defined as

$$g(W) = f_{T_W}(W) + \sum_i v_i w_i,$$

the gradient is

$$\frac{\partial g(W)}{\partial w_i} = -\mu(\mathrm{Pow}_W(p_i)) + v_i,$$

Comparison

The key differences between Aurenhammer 1998, Lévy 2014 works and Gu-Luo-Sun-Yau 2013 are:

1. What is the geometric meaning of the convex energy ?
2. What is the explicit formula for Hessian matrix ? What is the geometric meaning of the Hessian matrix ?
3. The convexity of the admissible weight space (height space). The argument that the critical point is an interior point in the admissible weight space.
4. Gradient descend, Quasi-Newton vs Newton's method.

Comparison

The same theorem has been proved several times in different fields, from different perspectives.

1. Alexandrov 1950, proved the existence using the non-constructive topological method, and the uniqueness using Brunn-Minkowski inequality.
2. Aurenhammer 1998, Lévy 2014 used the variational method to prove the existence and the uniqueness by a convex energy, formulated from L^2 transportation cost. The gradient formula is given.
3. Gu-Luo-Sun-Yau 2013 used the variational approach, proved the existence and the uniqueness by a convex energy, started from the volume of a convex polytope, furthermore the convexity of the space of admissible power weights (heights), and the interior critical point arguments are emphasized, which are based on Brunn-Minkowski inequality. Both the gradient and the Hessian are given.

Remarks

- Only the convexity of the energy is insufficient to guarantee the existence of the solution, it is further required that the domain is convex and the critical point is interior;
- The Brunn-Minkowski inequality is fundamentally essential;
- The L_2 cost and the volume are Legendre dual to each other.

Convex Geometry

Minkowski problem - 2D Case

Example

A convex polygon P in $\mathbb{R}^2$ is determined by its edge lengths A_i and the unit normal vectors $\mathbf{n}_i$.

Take any $\mathbf{u} \in \mathbb{R}^2$ and project P to $\mathbf{u}$, then $\langle \sum_i A_i \mathbf{n}_i, \mathbf{u} \rangle = \mathbf{0}$, therefore

$$\sum_i A_i \mathbf{n}_i = \mathbf{0}.$$

Minkowski problem - General Case

Minkowski Problem

Given k unit vectors $\mathbf{n}_1, \cdots, \mathbf{n}_k$ not contained in a half-space in $\mathbb{R}^n$ and $A_1, \cdots, A_k > 0$, such that

$$\sum_i A_i \mathbf{n}_i = \mathbf{0},$$

find a compact convex polytope P with exactly k codimension-1 faces $F_1, \cdots, F_k$, such that

1. $area(F_i) = A_i$,
2. $\mathbf{n}_i \perp F_i$.

Minkowski problem - General Case

Theorem (Minkowski)

P exists and is unique up to translations.

Minkowski's Proof

Given $\mathbf{h} = (h_1, \cdots, h_k)$, $h_i > 0$, define a compact convex polytope

$$P(\mathbf{h}) = \{\mathbf{x} | \langle \mathbf{x}, \mathbf{n}_i \rangle \leq h_i, \forall i\}$$

Let $Vol : \mathbb{R}_+^k \to \mathbb{R}_+$ be the volume $Vol(\mathbf{h}) = vol(P(\mathbf{h}))$, then

$$\frac{\partial Vol(\mathbf{h})}{\partial h_i} = area(F_i)$$

Minkowski's Proof

Define the admissible height space

$$\mathscr{H} := \{\mathbf{h} | h_i > 0, area(F_i) \geq 0, i = 1, 2, \cdots, k\} \cap \{\sum h_i A_i = 1\},$$

By using Brunn-Minkowski inequality, one can show that $\mathscr{H}$ is convex and compact. The smooth function $Vol(\mathbf{h})$ reaches its maximum. Furthermore, on $\partial\mathscr{H}$, the gradient of $Vol(\mathbf{h})$ points inside, therefore, the maximum is an interior point. Using Lagrangian multiplier, the solution (up to scaling) to MP is the critical point of Vol.

Minkowski's Proof

Uniqueness part is proved using Brunn-Minkowski inequality, which implies $(Vol(\mathbf{h}))^{\frac{1}{n}}$ is concave in $\mathbf{h}$.

Minkowski Sum

Definition (Minkowski Sum)

Given two point sets $P, Q \subset \mathbb{R}^n$, their Minkowski sum is given by

$$P \oplus Q = \{p + q | p \in P, q \in Q\}$$

Let

$$P(\mathbf{h}) = \{\mathbf{x} | \langle \mathbf{x}, \mathbf{n}_i \rangle \leq h_i, \forall i\}$$

then

$$P(\mathbf{h}_1) \oplus P(\mathbf{h}_2) = P(\mathbf{h}_1 + \mathbf{h}_2).$$

Brunn-Minkowski inequality

Theorem (Brunn-Minkowski)

For every pair of nonempty compact subsets A and B of $\mathbb{R}^n$ and every $0 \leq t \leq 1$,

$$[Vol(tA \oplus (1-t)B)]^{\frac{1}{n}} \geq t[vol(A)]^{\frac{1}{n}} + (1-t)[vol(B)]^{\frac{1}{n}}.$$

For convex sets A and B, the inequality is strick for $0 < t < 1$ unless A and B are homothetic i.e. are equal up to translation and dilation.

Piecewise Linear Convex Function

A Piecewise Linear convex function

$$f(\mathbf{x}) := \max\{\langle \mathbf{x}, \mathbf{p}_i \rangle + h_i | i = 1, \cdots, k\}$$

produces a convex cell decomposition W_i of $\mathbb{R}^n$:

$$W_i = \{\mathbf{x} | \langle \mathbf{x}, \mathbf{p}_i \rangle + h_i \geq \langle \mathbf{x}, \mathbf{p}_j \rangle + h_j, \forall j\}$$

Namely, $W_i = \{\mathbf{x} | \nabla f(\mathbf{x}) = \mathbf{p}_i\}$.

Alexandrov Theorem

Theorem (Alexandrov 1950)

Given Ω compact convex domain in $\mathbb{R}^n$, $p_1, \cdots, p_k$ distinct in $\mathbb{R}^n$, $A_1, \cdots, A_k > 0$, such that $\sum A_i = Vol(\Omega)$, there exists PL convex function

$$f(\mathbf{x}) := \max\{\langle \mathbf{x}, \mathbf{p}_i \rangle + h_i | i = 1, \cdots, k\}$$

unique up to translation such that

$$Vol(W_i) = Vol(\{\mathbf{x} | \nabla f(\mathbf{x}) = \mathbf{p}_i\}) = A_i.$$

Alexandrov's proof is topological, not variational. It has been open for years to find a constructive proof.

Voronoi Decomposition

Voronoi Diagram

Voronoi Diagram

Given $p_1, \cdots, p_k$ in $\mathbb{R}^n$, the Voronoi cell W_i at p_i is

$$W_i = \{\mathbf{x} | |\mathbf{x} - p_i|^2 \leq |\mathbf{x} - p_j|^2, \forall j\}.$$

Power Distance

Power Distance

Given $\mathbf{p}_i$ associated with a sphere $(\mathbf{p}_i, r_i)$ the power distance from $\mathbf{q} \in \mathbb{R}^n$ to $\mathbf{p}_i$ is

$$pow(\mathbf{p}_i, \mathbf{q}) = |\mathbf{p}_i - \mathbf{q}|^2 - r_i^2.$$

Power Diagram

Given $p_1, \cdots, p_k$ in $\mathbb{R}^n$ and power weights $h_1, \cdots, h_k$, the power Voronoi cell W_i at p_i is

$$W_i = \{\mathbf{x} | |\mathbf{x} - p_i|^2 + h_i \leq |\mathbf{x} - p_j|^2 + h_j, \forall j\}.$$

PL convex function vs. Power diagram

Lemma

Suppose $f(x) = \max\{\langle \mathbf{x}, \mathbf{p}_i \rangle + h_i\}$ *is a piecewise linear convex function, then its gradient map induces a power diagram,*

$$W_i = \{\mathbf{x} | \nabla f = \mathbf{p}_i\}.$$

Proof.

$\langle \mathbf{x}, \mathbf{p}_i \rangle + h_i \geq \langle \mathbf{x}, \mathbf{p}_j \rangle + h_j$ is equivalent to

$$|\mathbf{x} - p_i|^2 - 2h_i - |p_i|^2 \leq |x - p_j|^2 - 2h_j - |p_j|^2.$$

□

Variational Proof

Theorem (Gu-Luo-Sun-Yau 2013)

Ω is a compact convex domain in $\mathbb{R}^n$, $p_1, \cdots, p_k$ distinct in $\mathbb{R}^n$, $s : \Omega \to \mathbb{R}$ is a positive continuous function. For any $A_1, \cdots, A_k > 0$ with $\sum A_i = \int_\Omega s(\mathbf{x}) d\mathbf{x}$, there exists a vector $(h_1, \cdots, h_k)$ so that

$$f(\mathbf{x}) = \max\{\langle \mathbf{x}, \mathbf{p}_i \rangle + h_i\}$$

satisfies $\int_{W_i \cap \Omega} s(\mathbf{x}) d\mathbf{x} = A_i$, where $W_i = \{\mathbf{x} | \nabla f(\mathbf{x}) = \mathbf{p}_i\}$. Furthermore, $\mathbf{h}$ is the maximum point of the convex function

$$E(\mathbf{h}) = \sum_{i=1}^{k} A_i h_i - \int_{\mathbf{0}}^{\mathbf{h}} \sum_{i=1}^{k} w_i(\eta) d\eta_i,$$

where $w_i(\eta) = \int_{W_i(\eta) \cap \Omega} s(\mathbf{x}) d\mathbf{x}$ is the volume of the cell.

Variational Proof

X. Gu, F. Luo, J. Sun and S.-T. Yau, “Variational Principles for Minkowski Type Problems, Discrete Optimal Transport, and Discrete Monge-Ampere Equations”, arXiv:1302.5472

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Variational Proof

Proof.

For $\mathbf{h} = (h_1, \cdots, h_k)$ in $\mathbb{R}^k$, define the PL convex function f as above and let $W_i(\mathbf{h}) = \{\mathbf{x} | \nabla f(\mathbf{x}) = \mathbf{p}_i\}$ and $w_i(\mathbf{h}) = vol(W_i(\mathbf{h}))$. First, we show the admissible height space

$$\mathscr{H} = \{\mathbf{h} \in \mathbb{R}^k | w_i(\mathbf{h}) > 0, \forall i\}$$

is non-empty open convex set in $\mathbb{R}^k$ by using the Brunn-Minkowski inequality. $\square$

Variational Proof

Proof.

Second, we can show the symmetry

$$\frac{\partial w_i}{\partial h_j} = \frac{\partial w_j}{\partial h_i} \leq 0$$

for $i \neq j$. Thus the differential 1-form $\sum w_i(\mathbf{h}) dh_i$ is closed in $\mathscr{H}$. Therefore $\exists$ a smooth $F : \mathscr{H} \to \mathbb{R}$ so that

$$\frac{\partial F}{\partial h_i} = w_i(h),$$

hence

$$F(\mathbf{h}) := \int^{\mathbf{h}} \sum_{i=1}^{k} w_i(\eta) d\eta_i.$$

$\square$

Variational Proof

Proof.

Third, because

$$\frac{\partial w_i(\mathbf{h})}{\partial h_i} = 0$$

due to

$$\sum w_i(\mathbf{h}) = \mathrm{vol}(\Omega).$$

Therefore the Hessian of F is diagonally dominated, $F(\mathbf{h})$ is convex in $\mathscr{H}$. $\square$

Variational Proof

Proof.

Fourth, F is strictly convex in

$$\mathscr{H}_0 = \{\mathbf{h} \in \mathscr{H} | \sum_{i=1}^{k} h_i = 0\}$$

and that

$$\nabla F(\mathbf{h}) = (w_1(\mathbf{h}), w_2(\mathbf{h}), \cdots, w_k(\mathbf{h})).$$

If F is strictly convex on an open convex set Ω in $\mathbb{R}^k$, then $\nabla F : \Omega \to \mathbb{R}^k$ is one-one. This shows the uniqueness part of the Alexandrov's theorem. □

Variational Proof

Proof.

Fifth, it can be shown that the convex function

$$G(\mathbf{h}) = \sum A_i h_i - F(\mathbf{h})$$

has a maximum point in $\mathscr{H}_0$. The gradient ∇G on the boundary of $\mathscr{H}_0$ points to the interior. Therefore, the maximum point is an interior point, which is the solution to Alexandrov's theorem. This gives the existence proof. $\square$

Geometric Interpretation

One can define a cylinder through $\partial\Omega$, the cylinder is truncated by the xy-plane and the convex polyhedron. The energy term $\int^{\mathbf{h}} \sum w_i(\eta) d\eta_i$ equals to the volume of the truncated cylinder.

Computational Algorithm

The concave energy is

$$E(h_1, h_2, \cdots, h_k) = \sum_{i=1}^{k} A_i h_i - \int_{\mathbf{0}}^{\mathbf{h}} \sum_{j=1}^{k} w_j(\eta) d\eta_j,$$

Geometrically, the energy is the volume beneath the parabola.

Computational Algorithm

The gradient of the energy is the areas of the cells

$$\nabla E(h_1, h_2, \cdots, h_k) = (A_1 - w_1, A_2 - w_2, \cdots, A_k - w_k)$$

Computational Algorithm

The Hessian of the energy is the length ratios of edge and dual edges,

$$\frac{\partial w_i}{\partial h_j} = \frac{|e_{ij}|}{|\bar{e}_{ij}|}$$

Computational Algorithm

1. Initialize $\mathbf{h} = \mathbf{0}$
2. Compute the Power Voronoi diagram, and the dual Power Delaunay Triangulation
3. Compute the cell areas, which gives the gradient ∇E
4. Compute the edge lengths and the dual edge lengths, which gives the Hessian matrix of E, $Hess(E)$
5. Solve linear system

$$\nabla E = Hess(E) d\mathbf{h}$$

6. Update the height vector

$$(h) \leftarrow \mathbf{h} - \lambda d\mathbf{h},$$

   where λ is a constant to ensure that no cell disappears
7. Repeat step 2 through 6, until $\|d\mathbf{h}\| < \varepsilon$.

Summary

1. Minkowski problem and the optimal mass transportation problem are closely related by the Monge-Ampere equation
2. Discrete variational framework for sovling Monge-Ampere equation with explicit geometric meaning
3. General framework for shape comparison/classification based on Wasserstein distance

Thanks

Code and Data

The code and the data sets can be downloaded from the following link:

http://www3.cs.stonybrook.edu/~ gu/software/omt/

Thanks

For more information, please email to gu@cs.stonybrook.edu.

Thank you!