Theory of Optimal Mass Transportation

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Thanks for the invitation.



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

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Motivation



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Mesh Parameterization



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Conformal parameterization: angle-preserving



Infinitesimal circles are mapped to infinitesimal circle.

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Area-preserving Parameterization

Area-preserving parameterization



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

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Surface Parameterization

Area-preserving parameterization



(a) Cortical surface

(b) Conformal (c) Area-preserving

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Surface Parameterization



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Surface Parameterization



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

Volume Parameterization



Volume Parameterization



volume-preserving map

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Registration



Conformal Parameterization for Surface Matching

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



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



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Optimal Mass Transport Map

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



Registration based on Optimal Mass Transport Map



Geometric Clustering



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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.



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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".

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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?



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Optimal Mass Transport Mapping



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Optimal Transport Problem



Earth movement cost.

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Optimal Mass Transportation

Problem Setting

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

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

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



Optimal Mass Transportation

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

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

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.



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

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

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

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Problem

Is there an optimal mapping $T: U \rightarrow V$ 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

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

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Three categories:

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

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Kantorovich's Approach

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

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

(v, V) is

$$\{(v_1,\mathbf{q}_1),(v_2,\mathbf{q}_2),\cdots,(v_n,\mathbf{q}_n)\}.$$

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

$$\sum_{i} f_{ij} = \mu_i, \sum_{i} f_{ij} = \nu_j.$$

mn unknowns in total. The complexity is quite high.



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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

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

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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 $\nabla f: U \rightarrow V$ 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, \dots, p_k in \mathbb{R}^n and $A_1, \dots, A_k > 0$, find a transport map $T : U \to \{p_1, \dots, p_k\}$ with $vol(T^{-1}(p_i)) = A_i$, so that T minimizes the transport cost

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

Theorem (Aurenhammer-Hoffmann-Aronov 1998)

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

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

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Power Diagram vs Optimal Transport Map



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Power Diagram vs Optimal Transport Map

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- 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.

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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 v_i such that $\sum v_i = \mu(\Omega)$, there exists a weights vector W such that $\mu(Pow_W(p_i)) = v_i$.

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Power Diagram vs Optimal Transport Map

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

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

using envelope theorem,

$$\frac{\partial f_{\mathcal{T}_W}(W)}{\partial w_i} = -\mu(\mathsf{Pow}_W(p_i)),$$

the convex energy is defined as

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

the gradient is

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

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

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

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Comparison

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

- Alexandrov 1950, proved the existence using the non-constructive topological method, and the uniqueness using Brunn-Minkowski inequality.
- 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.
- 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.

- 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.

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Convex Geometry



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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

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



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Minkowski problem - General Case

Minkowski Problem

Given *k* unit vectors $\mathbf{n}_1, \dots, \mathbf{n}_k$ not contained in a half-space in \mathbb{R}^n and $A_1, \dots, A_k > 0$, 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, \dots, F_k , such that • *area*(F_i) = A_i , • $n_i \perp F_i$.



Minkowski problem - General Case

Theorem (Minkowski)

P exists and is unique up to translations.



Given $\mathbf{h} = (h_1, \dots, h_k), h_i > 0$, 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

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



Minkowski's Proof

Define the admissible height space

$$\mathscr{H} := \{\mathbf{h} | h_i > 0, area(F_i) \ge 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.



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



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Minkowski Sum



Definition (Minkowski Sum)

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

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

Let

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

then

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

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Theorem (Brunn-Minkowski)

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

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

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.

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 :

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

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



Theorem (Alexandrov 1950)

Given Ω compact convex domain in \mathbb{R}^n , p_1, \dots, p_k distinct in \mathbb{R}^n , $A_1, \dots, A_k > 0$, 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.



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Voronoi Decomposition



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Voronoi Diagram

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

$$W_i = \{\mathbf{x} | |\mathbf{x} - \mathbf{p}_i|^2 \le |\mathbf{x} - \mathbf{p}_j|^2, \forall j\}.$$



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

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



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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.

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

$$|\mathbf{x} - \mathbf{p}_i|^2 - 2h_i - |\mathbf{p}_i|^2 \le |\mathbf{x} - \mathbf{p}_j|^2 - 2h_j - |\mathbf{p}_j|^2.$$



Theorem (Gu-Luo-Sun-Yau 2013)

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

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

satisfies $\int_{W_i \cap \Omega} \mathbf{s}(\mathbf{x}) d\mathbf{x} = A_i$, where $W_i = \{\mathbf{x} | \nabla f(\mathbf{x}) = \mathbf{p}_i\}$. Furthermore, **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.

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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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For $\mathbf{h} = (h_1, \dots, h_k)$ 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.

Variational Proof

Proof.

Second, we can show the symmetry

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

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

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

hence

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

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Third, because

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

due to

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

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

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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.

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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 \mathcal{H}_0 . The gradient ∇G on the boundary of \mathcal{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.

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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 $\int^{h} \sum w_i(\eta) d\eta_i$ equals to the volume of the truncated cylinder.

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The concave energy is

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

Geometrically, the energy is the volume beneath the parabola.



The gradient of the energy is the areas of the cells

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

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

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

- Initialize h = 0
- Compute the Power Voronoi diagram, and the dual Power Delaunay Triangulation
- Sompute the cell areas, which gives the gradient ∇E
- Compute the edge lengths and the dual edge lengths, which gives the Hessian matrix of *E*, *Hess*(*E*)
- Solve linear system

$$\nabla E = Hess(E)dh$$

Update the height vector

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

where λ is a constant to ensure that no cell disappears

Repeat step 2 through 6, until $||d\mathbf{h}|| < \varepsilon$.

- Minkowski problem and the optimal mass transportation problem are closely related by the Monge-Ampere equation
- Obscrete variational framework for sovling Monge-Ampere equation with explicit geometric meaning
- 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/



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Thanks

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



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