#### The Abel Symposium

## A variational regularity theory for optimal transportation and its application to matching

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#### **Optimal matching of random point clouds**

*Matching* of two locally finite point clouds  $\{X\}$  and  $\{Y\} \subset \mathbb{R}^d$ , amounts to a pairing  $\{(X, Y)\} \subset \mathbb{R}^d \times \mathbb{R}^d$ .

$$\begin{split} & \sum_{n=1}^{N} |Y_n - X_n|^2 \\ & \leq \sum_{n=1}^{N} |Y_{n-1} - X_n|^2 \\ & \iff \sum_{n=1}^{N} (Y_n - Y_{n-1}) \cdot X_n \ge 0. \end{split}$$

Simplest random setting:

 $\{X\}, \{Y\}$  indep. samples of **Poisson point processes**.

cyclical monotonicity  $\forall$  matched finite subset  $\{X_1, \dots, X_N\}$  $\{Y_1, \dots, Y_N = Y_0\}.$ 

**Optimality** means

#### The Poisson point process

Locally finite point cloud via Poisson point process of unit intensity (means that distance between points O(1))

canonical vs. grand-canonical definition





- Seek cyclically monotone matching of two independent Poisson point processes
- mean distance diverges in d = 1.



#### Matching depends on dimension d ...

Cyclically monotone matching of two independent Poisson point processes – distances diverge like square-root for d = 1.

Cause of divergence: mesoscopic fluctuations of number density n

$$= O(\frac{1}{\sqrt{L^d}});$$
 lower for higher  $d$ .

Number of excess points =  $O(\sqrt{L^d})$ ,

number of points in (width one) boundary layer =  $O(L^{d-1})$ .

... critical dimension d = 2







## **Impose statistical translation invariance** ("Stationarity") of matching

Cyclically monotone matching of two independent Poisson point processes  $\{X\}, \{Y\}$ .

Poisson point process is *stationary*:  $\forall \text{ shift vectors } z \in \mathbb{R}^d \qquad \{z + X\} =_{\mathsf{IAW}} \{X\}.$ 



Seek random point cloud  $\{(X, Y)\}$  in  $\mathbb{R}^d \times \mathbb{R}^d$  s. t. marginals are independent Poisson point processes, coupling is cyclically monotone almost surely, and  $\forall z \in \mathbb{R}^d$  {(z + X, z + Y)} =<sub>Law</sub> {(X, Y)}.

#### Critical dimension d = 2 rigorously captured

Interest in Combinatorics (eg. Ajtai et al. '84), Probability Theory (Talagrand '92+, Holroyd-Peres '11+), Physics (eg. Parisi et al. '14), Analysis (eg. Ambrosio et al. '16+).

Seek random point cloud  $\{(X, Y)\}$  in  $\mathbb{R}^d \times \mathbb{R}^d$  s. t. marginals are independent Poisson point processes, coupling is cyclically monotone almost surely, and  $\forall z \in \mathbb{R}^d \quad \{(z + X, z + Y)\} =_{\mathsf{law}} \{(X, Y)\}.$ 

**Theorem** (Huesmann&Sturm '13)

For d > 2 have existence.

Theorem (H.&Mattesini&0. '21)

For  $d \leq 2$  have non-existence.

### Proof via continuum/PDE perspective Optimal Transportation in Kantorowicz' formulation

Given two measures

seek transfer plan  $\pi$ , i. e.  $\pi(U \times \mathbb{R}^d) = \mu(U), \ \pi(\mathbb{R}^d \times V) = \lambda(V)$ that minimizes Euclidean transport cost  $\int_{\mathbb{R}^d \times \mathbb{R}^d} |y-x|^2 \pi(dxdy).$ 

Minimum =:  $W_2^2(\mu, \lambda)$  (squared) Wasserstein distance.

#### From optimal transportation to Monge-Ampère

Minimize  $\int_{\mathbb{R}^d \times \mathbb{R}^d} |y - x|^2 \pi(dxdy)$ among all  $\pi(dxdy)$  with marginals  $\mu(dx)$  and dy. Support of optimal transfer plan  $\pi$ is cyclically monotone; hence  $\exists$  convex  $\psi$ supp $\pi \subset \{(x, y) | y \in \text{sub-gradient } \partial \psi(x) \}$ .

 $\forall$  test functions  $\zeta \quad \int \zeta(\nabla \psi(x)) \mu(dx) = \int \zeta(y) dy.$ 

In smooth case, this amounts to  $detD^2\psi = \mu$ , an instance of the Monge-Ampère equation.

#### Nature of the Monge-Ampère equation

Recall Monge-Ampère:  $det D^2 \psi = 1$ . Fully non-linear with F(A) := det A - 1.

However elliptic: F(A) > F(A') for  $A > A' \ge 0$ ; satisfies comparison principle.

However degenerate:  $\leftrightarrow$  affine invariant (non-compact SL(d)). Cf. Laplacian F(A) = trA: rotation invariant (compact SO(d)).

Caffarelli's '90 breakthrough: comparison principle, affine invariance, compactness.



Pogorelov's example is worst case

Monge-Ampère equation at crossroads of fully nonlinear and variational.

# Parisi's heuristics for semi-discrete matching $\mu = \sum_{x \in X} \delta_x$ Poisson, $\lambda = dy$ Lebesgue

det $D^2\psi$ -1 =  $\mu$ -1  $\approx_{\text{law}} \xi$  on scales  $R \gg 1$ ,  $\xi$  = white noise, meaning  $\int \eta_R(\mu$ -1)  $\approx_{\text{law}} \int \eta_R \xi$ , with  $\eta_R(x) = \frac{1}{R^d} \eta(\frac{x}{R}), \ \eta \in C_0^{\infty}$  fixed.

Consider  $\Delta \phi = \xi$  (so that  $\nabla \phi$  behaves as Gaussian free field)  $\xi \sim R^{-\frac{d}{2}} \ll 1$  on scales  $R \gg 1 \implies D^2 \phi \ll 1$  on scales  $\gg 1 \implies \det(D^2(\phi + \frac{1}{2}|x|^2)) - 1 = \det(D^2\phi + \mathrm{id}) - 1 \approx \mathrm{tr} D^2\phi = \xi$ on scales  $\gg 1$ .

Hence expect  $\nabla \psi - x \approx_{\text{law}} \nabla \phi$  on scales  $\gg 1$ ; in terms of "displacement"  $(y-x)\pi(dxdy)$ :  $\frac{\int \eta_R(x)(y-x)\pi(dxdy)}{\int \eta_R(x)\pi(dxdy)} \approx_{\text{law}} \int \eta_R \nabla \phi.$ 

#### **Quantitative large-scale linearization**

Compare:  $\pi(dxdy)$  optimal for  $\mu(dx)$  and dywith  $-\triangle \phi = \mu - 1$ .

Rate function  $D(R) \uparrow$ ,  $\frac{D(R)}{R} \downarrow$ in strengthened sense of Dini  $\sum_{k=0}^{\infty} \frac{D(2^k R)}{2^k R} \leq 4 \frac{D(R)}{R}$ .

**Theorem 1** (Goldman&Huesmann&O.) Provided  $\frac{1}{|B_R|}W_{B_R}^2(\mu,\kappa_R) + R^2(\kappa_R-1)^2 \leq D(R) \quad \text{for all } R \geq 1,$ then  $\left|\frac{\int \eta_R(x)(y-x)\pi(dxdy)}{\int \eta_R(x)\pi(dxdy)} - \int \eta_R \nabla \phi\right| \lesssim \frac{D(R)}{R} \quad \text{for all } R \geq 1.$ 

Confirms (deterministic part of) Parisi's heuristics. Relies on large-scale regularity theory.

# Large-scale regularity via harmonic approximation Consider $\pi(dxdy)$ optimal for $\mu(dx)$ and $\lambda(dy)$ . Local energy $E := \int_{(B_6 \times \mathbb{R}^d) \cup (\mathbb{R}^d \times B_6)} |y - x|^2 \pi(dxdy)$ , Local data size<sup>2</sup> $D := W_{B_6}^2(\mu, \kappa = \text{const}) + (\kappa - 1)^2$ $+ \text{ same for } \lambda$

Theorem 2 (Goldman&Huesmann&O.)  $\forall \tau > 0 \quad \exists \epsilon(\tau, d) > 0, \ C(\tau, d) < \infty \quad \text{s. t.} \quad E + D \leq \epsilon \implies$   $\exists \nabla \phi \text{ harmonic,} \quad \int_{B_1} |\nabla \phi|^2 \leq C(E + D),$  $\int_{(B_1 \times \mathbb{R}^d) \cup (\mathbb{R}^d \times B_1)} |y - x - \nabla \phi(y)|^2 \pi(dxdy) \leq \tau E + CD.$ 

# Harmonic approximation: correct homogeneities ... $E := \int_{(B_6 \times \mathbb{R}^d) \cup (\mathbb{R}^d \times B_6)} |y - x|^2 \pi(dxdy), \text{ quadratic in solution,}$ $D := W_{B_6}^2(\mu, \kappa = \text{const}) + (\kappa - 1)^2 + \text{same for } \lambda, \text{ quadratic in data.}$

# Theorem 2 $\forall \tau > 0 \quad \exists \epsilon(\tau, d) > 0, \ C(\tau, d) < \infty \quad \text{s. t.} \quad E + D \leq \epsilon \implies$ $\exists \nabla \phi \text{ harmonic,} \quad \int_{B_1} |\nabla \phi|^2 \leq C(E + D),$ $\int_{(B_1 \times \mathbb{R}^d) \cup (\mathbb{R}^d \times B_1)} |y - x - \nabla \phi(y)|^2 \pi(dxdy) \leq \tau E + CD.$

Compare to  $\int_{B_1} L(\nabla u - \nabla \phi) \leq \tau \int_{B_6} L(\nabla u) + C \int_{B_6} |f|^2$ for  $-\nabla \cdot DL(\nabla u) = \nabla \cdot f$  with uniformly convex L.

#### ... and correct metric

#### **Definition of** $\nabla \phi$ **via Neumann-Poisson problem**

Consider trajectories  $[0,1] \ni t \mapsto X(t) := ty + (1-t)x$ .

Consider when & where trajectories  $\begin{pmatrix} \text{enter} \\ \text{exit} \end{pmatrix} B_R$ :  $\binom{\sigma}{\tau} := \binom{\min}{\max} \{ t \in [0, 1] | X(t) \in \overline{B}_R \},$ 

$$\int \zeta dg = \int \zeta(X(\sigma)) \pi(dxdy), \quad ^{X(1)} \int \zeta df = \int \zeta(X(\tau)) \pi(dxdy).$$



Define  $\nabla \phi$  by the Neumann-Poisson problem:  $-\Delta \phi = \frac{(\lambda - \mu)(B_R)}{|B_R|}$  in  $B_R$  and  $\nu \cdot \nabla \phi = f - g$  on  $\partial B_R$ . Optimize in  $R \in [2, 3]$ .

#### A numerical illustration in case of matching

Matching of  $\{X\}$  and  $\{Y\}$ ; consider a square Q



Define  $\nabla \phi$  by the Neumann-Poisson problem:

$$- \bigtriangleup \phi = \sum_{Y \in Q} \delta_Y - \sum_{X \in Q} \delta_X \quad \text{in } Q,$$
$$\nu \cdot \nabla \phi = \sum_{Y \in Q, X \notin Q} \delta_Z - \sum_{Y \notin Q, X \in Q} \delta_Z \quad \text{on } \partial Q.$$

#### A numerical illustration in case of matching

Recall 
$$- \bigtriangleup \phi = \sum_{Y \in Q} \delta_Y - \sum_{X \in Q} \delta_X$$
 in  $Q$ ,  
 $\nu \cdot \nabla \phi = \sum_{Y \in Q, X \notin Q} \delta_Z - \sum_{Y \notin Q, X \in Q} \delta_Z$  on  $\partial Q$ .

Check  $\nabla \phi \approx Y - X$  when averaged on scale R;



R larger – better agreement; side-length of Q = 75.

Finite Element discretization, simulations by R. Kriemann

#### Analogies to minimal surfaces (Schoen&Simon '82)

Approximate minimal surface by harmonic graph / approximate displacement by harmonic gradient.

Use: Object is minimizing under compact perturbations. Don't use: Euler-Lagrange equation (= first variation).

Mismatch of type of boundary condition for construction of harmonic competitor: graph vs. non-graph / flux vs. displacement; choice of good radius.

Use of strict convexity to convert energy gap into distance ("approximate orthogonality"); need to smooth out boundary data.

#### Summary and outlook

Variational regularity theory for optimal transportation, mimics  $\epsilon$ -regularity theory for minimal surfaces, is more robust than maximum principle-based approach, provides large-scale regularity theory for matching.

Extend non-existence result and regularity theory from p = 2 to  $p \in (1, \infty)$  (& L. Koch), and to entropic regularization (& R. Gvalani). Seek quantitative coupling of shot noise  $\mu - 1$  with white noise  $\xi$  in d > 2 (Komlós&Major&Tusnády '75).