Semi-discrete unbalanced optimal transport and quantization

David Bourne, Bernhard Schmitzer, Benedikt Wirth

WWU MÜNSTER

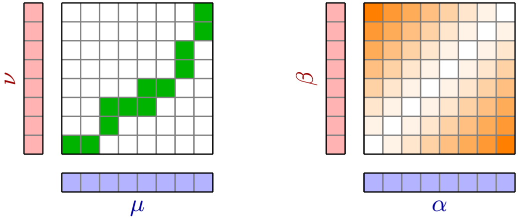
December 11, 2018

Overview

1. Introduction
2. Semi-discrete unbalanced transport
3. Quantization
4. Crystallization

Overview

Overview and notation



Optimal transport à la Kantorovich [Kantorovich, 1942]

- **couplings:** $\Pi(\mu,\nu) := \{\pi \in \mathcal{M}_+(X \times X) \mid \mathrm{P}_{1\sharp}\pi = \mu,\ \mathrm{P}_{2\sharp}\pi = \nu\}$
- **primal:** $\mathcal{C}_{\mathrm{OT}}(\mu,\nu) := \inf \left\{ \int_{X\times X} c(x,y)\, \mathrm{d}\pi(x,y) \middle| \pi \in \Pi(\mu,\nu) \right\}$
- **dual:**

$$\mathcal{C}_{\mathrm{OT}}(\mu,\nu) = \sup \left\{ \int_X \alpha\, \mathrm{d}\mu + \int_X \beta\, \mathrm{d}\nu \middle| \alpha,\beta \in C(X),\ \alpha(x) + \beta(y) \le c(x,y) \right\}$$

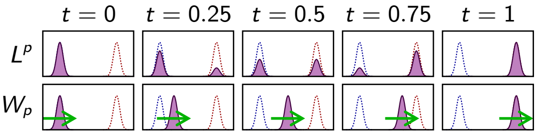
Wasserstein distance on probability measures $\mathcal{P}(X)$

$$W_p(\mu,\nu) := (\mathcal{C}_{\mathrm{OT}}(\mu,\nu))^{1/p} \text{ for } c(x,y) := d(x,y)^p, \quad p \in [1,\infty)$$

Today: $X \subset \mathbb{R}^n$ convex; **'radial' costs:** $c(x,y) = \ell(d(x,y))$,
$\ell : [0,\infty) \to [0,\infty]$ strictly increasing, continuous on its domain, $\ell(0) = 0$

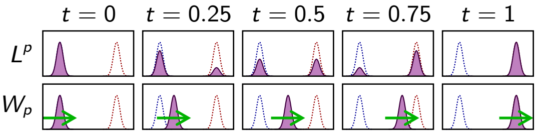
Wasserstein distances: displacement interpolation

- (X, d) length space $\Rightarrow (\mathcal{P}(X), W_p)$ is length space
- $d(x, y)$ is **length of shortest continuous path** between x and y



Wasserstein distances: displacement interpolation

- (X, d) length space $\Rightarrow$ $(\mathcal{P}(X), W_p)$ is length space
- $d(x, y)$ is **length of shortest continuous path** between x and y



Dynamic formulation: Benamou–Brenier formula (on $X = \mathbb{R}^d$)

- (weak) **continuity equation**: mass ρ, momentum $\omega = \rho \cdot v$

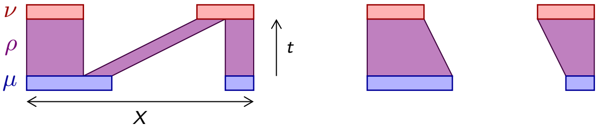
$$\mathcal{CE}(\mu, \nu) := \left\{(\rho, \omega) \in \mathcal{M}([0,1] \times X)^{1+d} : \partial_t \rho + \nabla \omega = 0,\ \rho_0 = \mu,\ \rho_1 = \nu\right\}$$

- **least action principle**: minimize Lagrangian / kinetic energy

$$W_p(\mu, \nu)^p = \inf_{(\rho,\omega) \in \mathcal{CE}(\mu,\nu)} \int_{[0,1]\times X} \frac{|\omega|^p}{\rho^{p-1}}\, \mathrm{d}x\mathrm{d}t$$

- $(\mathcal{P}(X = \mathbb{R}^d), W_2)$ 'looks like' **Riemannian manifold** [Otto, 2001]

Unbalanced transport: dynamic formulation



Unbalanced Benamou–Brenier formula

- **unbalanced continuity equation**: mass ρ, momentum ω, **source** ζ

$$\mathcal{CE}(\mu,\nu) = \left\{(\rho,\omega,\zeta) \in \mathcal{M}([0,1]\times X)^{1+d+1} : \partial_t\rho + \nabla\omega = \zeta,\ \rho_0 = \mu,\ \rho_1 = \nu\right\}$$

- **unbalanced action principle**

$$\mathcal{C}_{\text{UB}}(\mu,\nu) = \inf_{(\rho,\omega,\zeta)\in\mathcal{CE}(\mu,\nu)} \int_{[0,1]\times X} \cancel{\frac{\omega^2}{\rho}}\,\Phi(\rho,\omega,\zeta)\,\mathrm{d}x\mathrm{d}t$$

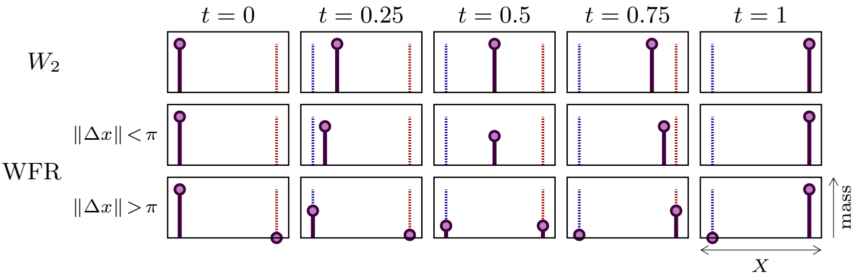
  - [Dolbeault et al., 2009]
  - [Piccoli and Rossi, 2016]: TV/L_1-type penalty
  - [Maas et al., 2015, 2017]: L_2 and L_2-L_1-type penalty
  - [Kondratyev et al., 2016; Chizat, Peyré, Schmitzer, and Vialard, 2018b; Liero et al., 2018]: Wasserstein–Fisher–Rao distance $\Phi(\rho,\omega,\zeta) := \frac{\omega^2+\zeta^2}{\rho}$
  - [Schmitzer and Wirth, 2017]: unbalanced W_1-type transport

Wasserstein–Fisher–Rao distance: basic properties

[Chizat, Peyré, Schmitzer, and Vialard, 2018b,a]

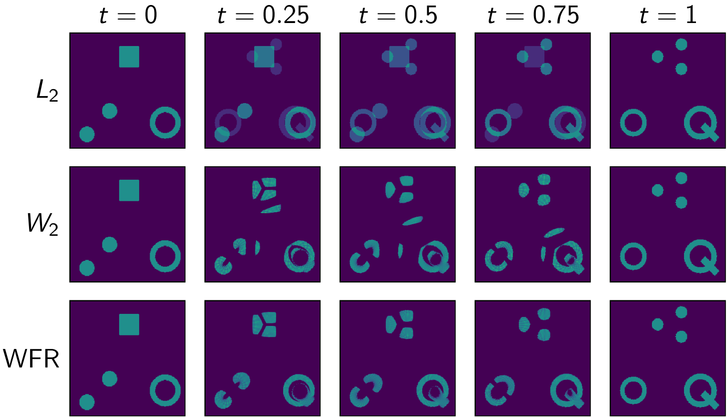
$$\mathrm{WFR}(\mu,\nu)^2 := \inf_{(\rho,\omega,\zeta)\in\mathcal{CE}(\mu,\nu)} \int_{[0,1]\times X} \frac{\omega^2+\zeta^2}{\rho}\,\mathrm{d}x\mathrm{d}t$$

- **Thm:** WFR is geodesic distance on **non-negative measures**.
- **Thm:** Geodesic between two Dirac measures is Dirac measure for intermediate times. Minimizing trajectories for $\mathrm{WFR}(\delta_{x_0} m_0, \delta_{x_1} m_1)$:
  - $\|x_0 - x_1\| < \pi$: **'travelling Dirac'**: $\rho_t = \delta_{x(t)} \cdot m(t)$
  - $\|x_0 - x_1\| > \pi$: **'teleportation'**: $\rho_t = \delta_{x_0} \cdot m_0(t) + \delta_{x_1} \cdot m_1(t)$
  - $\|x_0 - x_1\| = \pi$: **cut locus**



- **Thm:** general geodesics = superpositions of Dirac geodesics

Wasserstein–Fisher–Rao distance: numerical example



- ✗ ‘fading’ with **Euclidean** distance L_2
- ‘artifacts’ with **Wasserstein-2** distance W_2
- ✓ no artifacts with **unbalanced transport** distance WFR

Unbalanced transport: Kantorovich-type formulations

[Liero, Mielke, and Savaré, 2018]

Optimal entropy transport problems

$$\mathcal{C}_{\mathsf{UB}}(\mu,\nu) := \inf \left\{ \int_{X \times X} c \, \mathrm{d}\pi + \mathcal{F}(\mathsf{P}_{1\sharp}\pi|\mu) + \mathcal{F}(\mathsf{P}_{2\sharp}\pi|\nu) \,\middle|\, \pi \in \mathcal{M}_+(X \times X) \right\}$$

- **marginal discrepancy** $\mathcal{F}(\rho|\mu) := \begin{cases} \int_X F\left(\frac{\mathrm{d}\rho}{\mathrm{d}\mu}\right) \mathrm{d}\mu & \text{if } \rho \ll \mu, \\ +\infty & \text{else.} \end{cases}$
- $F : [0,\infty) \to [0,\infty]$ convex, lower semi-continuous, super-linear

Dual problem

$$\mathcal{C}_{\mathsf{UB}}(\mu,\nu) = \sup \left\{ -\int_X F^*(-\alpha)\, \mathrm{d}\mu - \int_X F^*(-\beta)\, \mathrm{d}\nu \,\middle|\, \alpha, \beta \in C(X),\ \alpha \oplus \beta \leq c \right\}$$

- $z \mapsto -F^*(-z)$: increasing, concave
- recover balanced case for $F = \iota_{\{1\}}$, $-F^*(-s) = s$.

Example: Wasserstein–Fisher–Rao / Hellinger–Kantorovich distance

- $\mathcal{F} = \mathrm{KL}$, $c_{\mathsf{WFR}}(x,y) = \begin{cases} -2\log\left[\cos\left(d(x,y)\right)\right] & \text{if } d(x,y) < \frac{\pi}{2}, \\ \infty & \text{else} \end{cases}$

Semi-discrete transport

- $\mu \ll \mathcal{L}$, $\nu = \sum_{i=1}^{M} m_i \, \delta_{x_i}$
- form of optimal coupling: $\pi = \sum_{i=1}^{M} \mu \llcorner C_i(w) \otimes \delta_{x_i}$
- $(C_i(w))_{i=1}^{M}$ **generalized Laguerre cells** for weight vector $w \in \mathbb{R}^m$:

$$\begin{aligned} C_i(w) = \big\{ & x \in X \mid c(x, x_i) < \infty, \\ & c(x, x_i) - w_i \leq c(x, x_j) - w_j \text{ for all } j \in \{1, \dots, M\} \big\} \end{aligned}$$

and **residual** $R = \big\{ x \in X \mid c(x, x_i) = \infty \text{ for all } i \in \{1, \dots, M\} \big\}$

Example: $(C_i(w))_{i=1}^{M}$ are **Voronoi cells** for $c(x, y) = d(x, y)$, $w = (0, \dots, 0)$

Tessellation formulation of semi-discrete transport

$$\mathcal{C}_{\mathrm{OT}}(\mu, \nu) = \sup \left\{ \sum_{i=1}^{M} \left[\int_{C_i(w)} [c(x, x_i) - w_i] \, \mathrm{d}\mu(x) + w_i \cdot m_i \right] \middle| \, w \in \mathbb{R}^M \right\}$$

- **efficient numerical methods** [Aurenhammer, Hoffmann, and Aronov, 1998; Kitagawa, Mérigot, and Thibert, 2016; Lévy, 2015]

Overview

1. Introduction
2. Semi-discrete unbalanced transport
3. Quantization
4. Crystallization

Semi-discrete unbalanced transport

Dual tessellation formulation:

- form of optimal coupling: $\pi = \sum_{i=1}^{M} \rho \llcorner C_i(w) \otimes \delta_{x_i}$, in general $\rho \neq \mu$

$$\mathcal{C}_{\mathrm{UB}}(\mu,\nu) = \sup \left\{ -\sum_{i=1}^{M} \left[\int_{C_i(w)} F^*(-c(x,x_i)+w_i)\,\mathrm{d}\mu(x) + F^*(-w_i)\cdot m_i \right] \right. \\ \left. + F(0)\cdot\mu(R) \middle| w \in \mathbb{R}^M \right\}$$

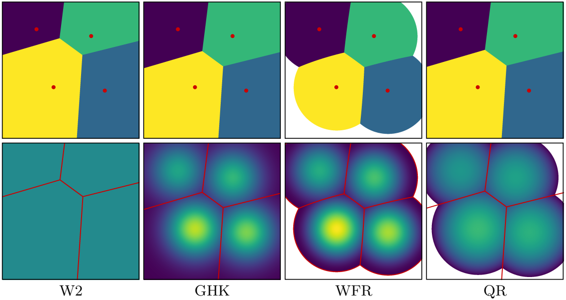
- recover balanced case for $F = \iota_{\{1\}}$, $-F^*(-s) = s$.

Primal tessellation formulation:

$$\mathcal{C}_{\mathrm{UB}}(\mu,\nu) = \inf \left\{ \sum_{i=1}^{M} \int_{C_i(w)} c(x,x_i)\,\mathrm{d}\rho(x) + \mathcal{F}(\rho|\mu) + \sum_{i=1}^{M} F\big(\tfrac{\rho(C_i(w))}{m_i}\big)\cdot m_i \right| \\ \left. w \in \mathbb{R}^M,\ \rho \in \mathcal{M}_+(\Omega),\ \rho(R) = 0 \right\}$$

Comparison of different models

- **Wasserstein-2 (W2):** $c = d^2$, $F = \iota_{\{1\}}$, $\mathcal{F}(\cdot|\mu) = \iota_{\{\mu\}}$
  - $C_i(w)$: weighted Laguerre cells, $R = \emptyset$; $\rho = \mu$,
- **Gaussian Hellinger–Kantorovich (GHK):** $c = d^2$, $\mathcal{F} = \mathrm{KL}$
  - still $R = \emptyset$; $\rho \neq \mu$ but $\operatorname{spt} \rho = \operatorname{spt} \mu$ since $F'(0) = -\infty$
- **Wasserstein–Fisher–Rao (WFR):** $c = c_{\mathrm{WFR}}$, $\mathcal{F} = \mathrm{KL}$
  - $c_{\mathrm{WFR}}(x, y) = \infty$ for $d(x, y) \geq \frac{\pi}{2}$, usually $R \neq \emptyset$; but $\operatorname{spt} \rho = \operatorname{spt} \mu \setminus R$
- **Quadratic regularization (QR):** $c = d^2$, $F(s) = (1 - s)^2$
  - $R = \emptyset$ but still usually $\operatorname{spt} \rho \subsetneq \operatorname{spt} \mu$ since $F'(0) > -\infty$



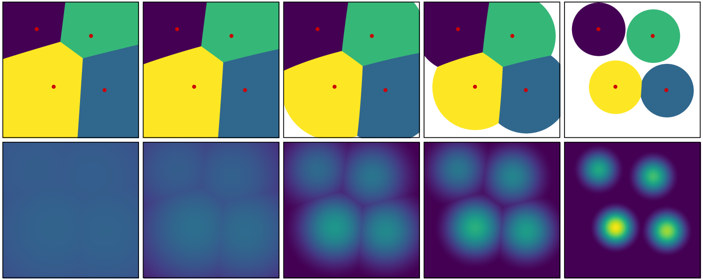
Length-scale in semi-discrete unbalanced transport

Trade-off: transport vs mass change

- **scaled cost:** $c_\varepsilon(x,y) = \ell(\frac{d(x,y)}{\varepsilon})$ with $\varepsilon > 0$
- assume $F(1) = 0 \leq F(s)$,
  $\Rightarrow$ **prefer to balance mass:** argmin $\mathcal{F}(\cdot|\mu) \ni \mu$

$$\mathcal{C}^{\varepsilon}_{\mathsf{UB}}(\mu,\nu) := \inf\left\{\int_{X\times X} c_\varepsilon \, \mathrm{d}\pi + \mathcal{F}(\mathrm{P}_{1\sharp}\pi|\mu) + \mathcal{F}(\mathrm{P}_{2\sharp}\pi|\nu) \middle| \pi \in \mathcal{M}_+(X\times X)\right\}$$

- $\varepsilon \to \infty$: transport very cheap, almost balanced
- $\varepsilon \to 0$: transport prohibitive, almost pure mass change



$\varepsilon = 1$ $\varepsilon = 1/2$ $\varepsilon = 1/4$ $\varepsilon = 1/5$ $\varepsilon = 1/8$

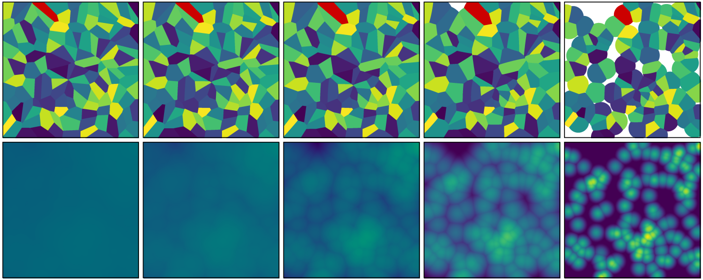
Length-scale in semi-discrete unbalanced transport

Trade-off: transport vs mass change

- **scaled cost:** $c_\varepsilon(x,y) = \ell(\frac{d(x,y)}{\varepsilon})$ with $\varepsilon > 0$
- assume $F(1) = 0 \leq F(s)$,
  $\Rightarrow$ **prefer to balance mass:** $\operatorname{argmin} \mathcal{F}(\cdot|\mu) \ni \mu$

$$\mathcal{C}_{\text{UB}}^{\varepsilon}(\mu,\nu) := \inf \left\{ \int_{X \times X} c_\varepsilon \, \mathrm{d}\pi + \mathcal{F}(\mathrm{P}_{1\sharp}\pi|\mu) + \mathcal{F}(\mathrm{P}_{2\sharp}\pi|\nu) \middle| \pi \in \mathcal{M}_+(X \times X) \right\}$$

- $\varepsilon \to \infty$: transport very cheap, almost balanced
- $\varepsilon \to 0$: transport prohibitive, almost pure mass change



$\varepsilon = 4/5$ | $\varepsilon = 2/5$ | $\varepsilon = 1/5$ | $\varepsilon = 1/10$ | $\varepsilon = 1/20$

Overview

1. Introduction
2. Semi-discrete unbalanced transport
3. Quantization
4. Crystallization

Quantization

- approximate $\mu \ll \mathcal{L}$ by M Dirac masses in OT-sense

$$\min \left\{ \mathcal{C}_{\mathrm{OT}}(\mu, \nu) \middle| \nu = \sum_{i=1}^{M} m_i \, \delta_{x_i}, \, x_1, \ldots, x_M \in X, \, m_1, \ldots, m_M \geq 0 \right\}$$

- applications: optimal location planning, discretization for particle methods, clustering, pattern formation...
- optimize over $(m_i)_{i=1}^M$:

$$= \min \left\{ J_M(x_1, \ldots, x_M) | x_1, \ldots, x_M \in X \right\}$$

- J_M? mass of μ always goes to nearest x_i ($c = \ell \circ d$), set m_i accordingly

$$\pi = \sum_{i=1}^{M} \mu \llcorner V_i(x_1, \ldots, x_M) \otimes \delta_{x_i}, \quad m_i = \mu(V_i), \quad V_i(\ldots) : \text{Voronoi cells}$$

$$J_M(x_1, \ldots, x_M) = \sum_{i=1}^{M} \int_{V_i} c(\cdot, x_i) \, \mathrm{d}\mu$$

Unbalanced quantization

- approximate $\mu \ll \mathcal{L}$ by M Dirac masses in unbalanced OT-sense

$$\min \left\{ \mathcal{C}_{\text{UB}}(\mu, \nu) \middle| \nu = \sum_{i=1}^{M} m_i \, \delta_{x_i}, \, x_1, \ldots, x_M \in X, \, m_1, \ldots, m_M \geq 0 \right\}$$

- assume $F(1) = 0 \leq F(s)$: prefer to balance mass
- optimize over $(m_i)_{i=1}^{M}$:

$$= \min \left\{ J_M(x_1, \ldots, x_M) \middle| x_1, \ldots, x_M \in X \right\}$$

$$\pi = \sum_{i=1}^{M} \rho \llcorner V_i(x_1, \ldots, x_M) \otimes \delta_{x_i}, \quad m_i = \rho(V_i), \quad V_i(\ldots) : \text{Voronoi cells}$$

$$J_M(x_1, \ldots, x_M) = \inf_{\rho} \sum_{i=1}^{M} \int_{V_i} c(\cdot, x_i) \, \mathrm{d}\rho + \mathcal{F}(\rho|\mu) + \sum_{i=1}^{M} F\left(\tfrac{\rho(V_i)}{m_i}\right) \cdot m_i$$

$$= \inf_{\rho \ll \mu} \sum_{i=1}^{M} \int_{V_i} \left[c(\cdot, x_i) \, \tfrac{\mathrm{d}\rho}{\mathrm{d}\mu} + F\left(\tfrac{\mathrm{d}\rho}{\mathrm{d}\mu}\right) \right] \mathrm{d}\mu = \sum_{i=1}^{M} \int_{V_i} -F^*(-c(\cdot, x_i)) \, \mathrm{d}\mu$$

- optimal free marginal: $\frac{\mathrm{d}\rho}{\mathrm{d}\mu} \in \partial F^*(-c(\cdot, x_i))$ on V_i

(Unbalanced) quantization: Lloyd's algorithm

Balanced:

$$\pi^{(\ell)} = \sum_{i=1}^{M} \mu \llcorner V_i(x_1^{(\ell)}, \dots, x_M^{(\ell)}) \otimes \delta_{x_i^{(\ell)}} \qquad \text{(optimize coupling)}$$

$$x_i^{(\ell+1)} = \operatorname*{argmin}_{z \in X} \int_{V_i^{(\ell)}} c(\cdot, z) \, \mathrm{d}\mu \qquad \text{(optimize locations)}$$

- $x_i^{(\ell+1)}$: generalized center of mass of $V_i^{(\ell)}$
- [Sabin and Gray, 1986; Du et al., 1999; Emelianenko et al., 2008; Bourne and Roper, 2015]

(Unbalanced) quantization: Lloyd's algorithm

Balanced:

$$\pi^{(\ell)} = \sum_{i=1}^{M} \rho^{(\ell)} \llcorner V_i(x_1^{(\ell)}, \ldots, x_M^{(\ell)}) \otimes \delta_{x_i^{(\ell)}} \qquad \text{(optimize coupling)}$$

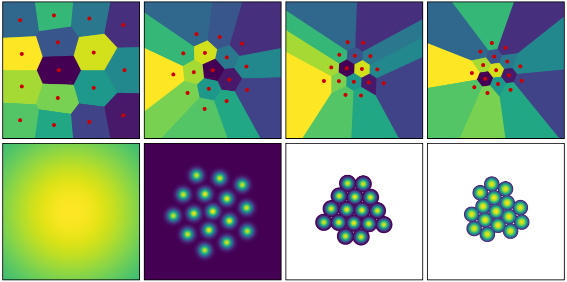
$$x_i^{(\ell+1)} = \operatorname*{argmin}_{z \in X} \int_{V_i^{(\ell)}} -F^*(-c(\cdot, z))\, \mathrm{d}\mu \qquad \text{(optimize locations)}$$

- $x_i^{(\ell+1)}$: generalized center of mass of $V_i^{(\ell)}$
- [Sabin and Gray, 1986; Du et al., 1999; Emelianenko et al., 2008; Bourne and Roper, 2015]

Unbalanced:

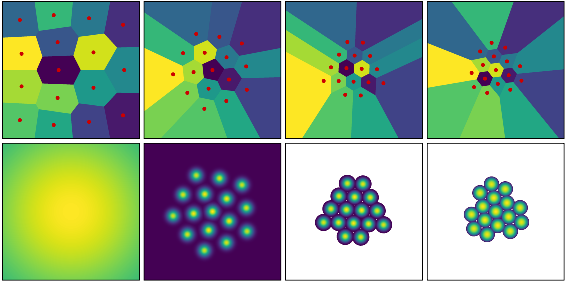
- replace $\mu \to \rho^{(\ell)}$ with $\frac{\mathrm{d}\rho^{(\ell)}}{\mathrm{d}\mu} \in \partial F^*(-c(\cdot, x_i^{(\ell)}))$ on $V_i^{(\ell)}$

Unbalanced quantization: numerical examples



W2 GHK WFR QR

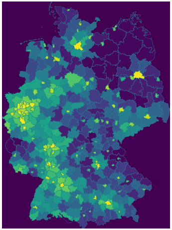
Unbalanced quantization: numerical examples

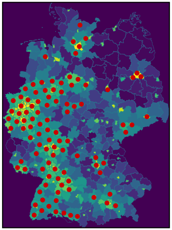


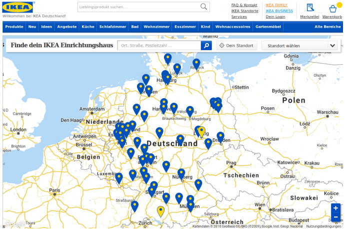
W2 GHK WFR QR

Example: unbalanced optimal location problem

population density μ discrete locations ν IKEA in Germany







Overview

Crystallization in 2D: Lebesgue measure

Balanced: $X \subset \mathbb{R}^2$, convex polygon, at most six sides; μ Lebesgue measure on X

$$J_{M,\varepsilon}(x_1, \dots, x_M) = \sum_{i=1}^{M} \int_{V_i} \ell\left(\tfrac{d(\cdot, x_i)}{\varepsilon}\right) \mathrm{d}\mu$$

- L. Fejes Tóth's Theorem on Sums of Moments:

$$\lim_{M \to \infty} \min_{(x_1, \dots, x_M)} J_{M,\varepsilon_M}(x_1, \dots, x_M) = |X| \cdot B\left(\frac{\lim_{M \to \infty} M\, \varepsilon_M^2}{|X|}\right)$$

with energy density of regular hexagonal tiling with point density z:

$$B(z) = z \int_{\mathrm{Hex}(1/z)} \ell(d(x, 0))\, \mathrm{d}x$$

Crystallization in 2D: Lebesgue measure

Balanced: $X \subset \mathbb{R}^2$, convex polygon, at most six sides; μ Lebesgue measure on X

$$J_{M,\varepsilon}(x_1,\ldots,x_M) = \sum_{i=1}^{M} \int_{V_i} -F^*(-\ell(\tfrac{d(\cdot,x_i)}{\varepsilon}))\,\mathrm{d}\mu$$

- L. Fejes Tóth's Theorem on Sums of Moments:

$$\lim_{M\to\infty} \min_{(x_1,\ldots,x_M)} J_{M,\varepsilon_M}(x_1,\ldots,x_M) = |X| \cdot B\left(\frac{\lim_{M\to\infty} M\,\varepsilon_M^2}{|X|}\right)$$

  with energy density of regular hexagonal tiling with point density z:

$$B(z) = z \int_{\mathrm{Hex}(1/z)} -F^*(-\ell(d(x,0)))\,\mathrm{d}x$$

Unbalanced: $F(1) = 0 \leq F(s)$; $F(0) \in (0,\infty)$

- B is non-negative, decreasing, convex, continuous
  - $B(0) = F(0)$: pure mass change
  - $B(\infty) = 0$: pure transport, cost vanishes

Crystallization in 2D: varying density

Thm: $X \subset \mathbb{R}^2$ polygon with at most six sides; $\mu \ll \mathcal{L}$, $m := \frac{\mathrm{d}\mu}{\mathrm{d}\mathcal{L}}$ Lipschitz continuous

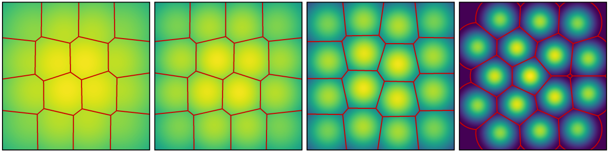
- $M\,\varepsilon_M^2 \to \infty$: pure transport, $\lim_{M\to\infty} \min_{(x_1,\dots,x_M)} J_{M,\varepsilon_M} = 0$
- $M\,\varepsilon_M^2 \to 0$: pure mass change
  $\lim_{M\to\infty} \min_{(x_1,\dots,x_M)} J_{M,\varepsilon_M} = \mu(X)\cdot F(0)$
- $M\,\varepsilon_M^2 \to P \in (0,\infty)$:

$$\lim_{M\to\infty} \min_{(x_1,\dots,x_M)} J_{M,\varepsilon_M} = \inf\left\{ \int_X B(D(x))\,\mathrm{d}\mu(x) \,\middle|\, D \in L_{1,+}(X),\ \int_X D(x)\,\mathrm{d}x = P \right\}$$

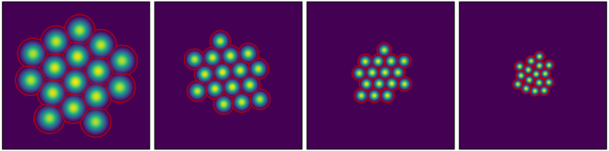
  - Lebesgue: $D(x) = \frac{P}{|X|} = \text{const}$
  - $D(x) \in \partial B^*(\lambda/m(x))$ for a.e. $x \in X$, λ: Lagrange multiplier
  - W2: $D(x) \propto \sqrt{m(x)}$
  - unbalanced: D may be zero on areas with $m > 0$

Crystallization in 2D: numerical examples I

Fixed M, decrease ε:

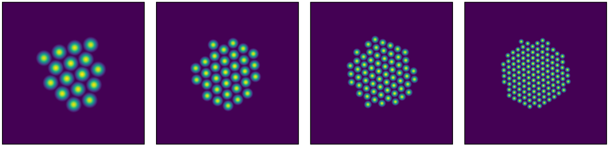


$\varepsilon = 15.391$ | $\varepsilon = 8.886$ | $\varepsilon = 4.867$ | $\varepsilon = 2.591$



$\varepsilon = 1.650$ | $\varepsilon = 1.106$ | $\varepsilon = 0.770$ | $\varepsilon = 0.541$

$M \to \infty$, fixed $M\,\varepsilon_M^2$:

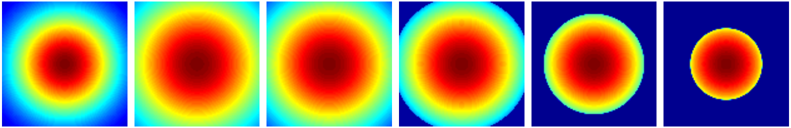


$M = 16, \varepsilon_M = 1.000$ | $M = 32, \varepsilon_M = 0.707$ | $M = 64, \varepsilon_M = 0.500$ | $M = 128, \varepsilon_M = 0.354$

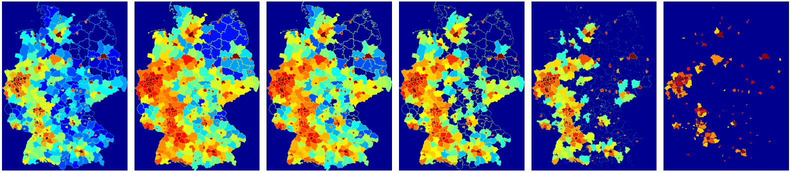
Crystallization in 2D: numerical examples II

- $P = \lim_{M\to\infty} M\,\varepsilon_M^2$: asymptotic average density
- $D(x)$: asymptotic local density

Examples for D:



input | $P = 2.4$ | $P = 0.69$ | $P = 0.28$ | $P = 0.12$ | $P = 0.049$

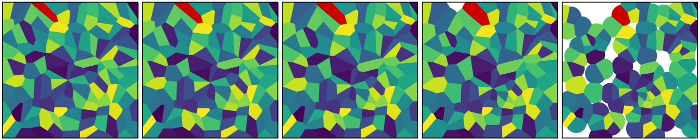


input | $P = .90$ | $P = 0.25$ | $P = 0.093$ | $P = 0.035$ | $P = 0.008$

Overview

1. Introduction
2. Semi-discrete unbalanced transport
3. Quantization
4. Crystallization

Conclusion



Semi-discrete unbalanced transport

- tessellation formulation
- length scales: transport vs mass change

Quantization

- applications: optimal location planning, discretization, pattern formation. . .
- Lloyd's algorithm
- 'neglected' regions

Crystallization

- locally triangular grids
- non-trivial local point density

PhD position available: numerical optimal transport at TU München

References I

F. Aurenhammer, F. Hoffmann, and B. Aronov. Minkowski-type theorems and least-squares clustering. *Algorithmica*, 20(1):61–76, 1998. doi: 10.1007/PL00009187.

D. P. Bourne and S. M. Roper. Centroidal power diagrams, Lloyd's algorithm, and applications to optimal location problems. *SIAM J. Numer. Anal.*, 53(6): 2545–2569, 2015. doi: 10.1137/141000993.

L. Chizat, G. Peyré, B. Schmitzer, and F.-X. Vialard. Unbalanced optimal transport: Dynamic and Kantorovich formulations. *J. Funct. Anal.*, 27(11):3090–3123, 2018a. doi: 10.1016/j.jfa.2018.03.008.

L. Chizat, G. Peyré, B. Schmitzer, and F.-X. Vialard. An interpolating distance between optimal transport and Fisher–Rao metrics. *Found. Comp. Math.*, 18(1): 1–44, 2018b.

J. Dolbeault, B. Nazaret, and G. Savaré. A new class of transport distances between measures. *Calc. Var. Partial Differential Equations*, 34(2):193–231, 2009. doi: 10.1007/s00526-008-0182-5.

Q. Du, V. Faber, and M. Gunzburger. Centroidal Voronoi tessellations: Applications and algorithms. *SIAM Rev.*, 41(4):637–676, 1999.

M. Emelianenko, L. Ju, and A. Rand. Nondegeneracy and weak global convergence of the Lloyd algorithm in $\mathbb{R}^d$. *SIAM J. Numer. Anal.*, 46(3):1423–1441, 2008.

References II

L. V. Kantorovich. O peremeshchenii mass. *Doklady Akademii Nauk SSSR*, 37(7–8): 227–230, 1942.

J. Kitagawa, Q. Mérigot, and B. Thibert. Convergence of a Newton algorithm for semi-discrete optimal transport. arXiv:1603.05579, 2016.

S. Kondratyev, L. Monsaingeon, and D. Vorotnikov. A new optimal transport distance on the space of finite Radon measures. *Adv. Differential Equations*, 21(11-12): 1117–1164, 2016.

B. Lévy. A numerical algorithm for L2 semi-discrete optimal transport in 3D. *ESAIM Math. Model. Numer. Anal.*, 49(6):1693–1715, 2015.

M. Liero, A. Mielke, and G. Savaré. Optimal entropy-transport problems and a new Hellinger–Kantorovich distance between positive measures. *Inventiones mathematicae*, 211(3):969–1117, 2018.

J. Maas, M. Rumpf, C. Schönlieb, and S. Simon. A generalized model for optimal transport of images including dissipation and density modulation. *ESAIM Math. Model. Numer. Anal.*, 49(6):1745–1769, 2015.

J. Maas, M. Rumpf, and S. Simon. Transport based image morphing with intensity modulation. In F. Lauze, Y. Dong, and A. B. Dahl, editors, *Scale Space and Variational Methods (SSVM 2017)*, pages 563–577. Springer, 2017. doi: 10.1007/978-3-319-58771-4_45.

References III

F. Otto. The geometry of dissipative evolution equations: the porous medium equation. *Comm. Partial Differential Equations*, 26(1-2):101–174, 2001.

B. Piccoli and F. Rossi. On properties of the generalized Wasserstein distance. *Archive for Rational Mechanics and Analysis*, 222(3):1339–1365, 2016. doi: 10.1007/s00205-016-1026-7.

M. Sabin and R. Gray. Global convergence and empirical consistency of the generalized Lloyd algorithm. *IEEE Trans. on Inform. Theory*, 32(2):148–155, 1986.

B. Schmitzer and B. Wirth. Dynamic models of Wasserstein-1-type unbalanced transport. to appear in ESAIM: Control, Optimisation and Calculus of Variations, arXiv:1705.04535, 2017.