Convergence rates for discretized optimal transport

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Based on joint work with F. Chazal and A. Delalande

1. Motivations

• Given $\mu \in \operatorname{Prob}(\mathbb{R})$, there exists a unique nondecreasing $T_{\mu} \in \mathrm{L}^1([0,1])$ satisfying $T_{\mu\#}\rho = \mu$, with $\rho =$ Lebesgue measure on [0,1].

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$$T_{\mu\#}\lambda = \mu \iff \forall B \subseteq \mathbb{R}, \ \lambda(T_{\mu}^{-1}(B)) = \mu(B)$$

 $\iff \forall x \in \mathbb{R}, \ \lambda([0, T_{\mu}^{-1}(x)]) = \mu((-\infty, x])$

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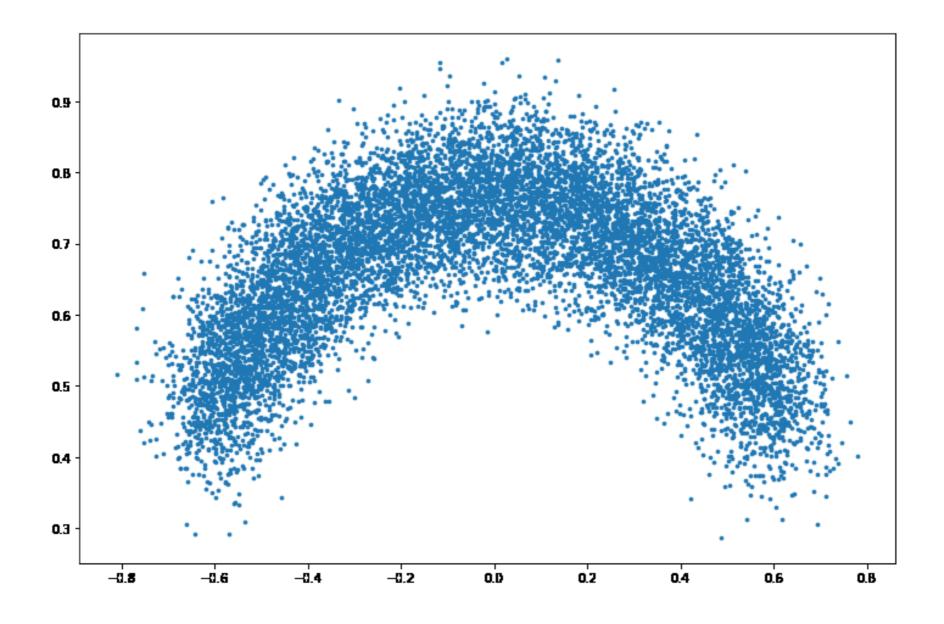
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- $ightharpoonup T_{\mu}$ is unique ho-a.e. but the convex function ϕ_{μ} is not necessarily unique.
- ▶ $T_{\mu} : \operatorname{spt}(\rho) \to \mathbb{R}^d$ is monotone: $\langle T_{\mu}(x) T_{\mu}(y) | x y \rangle \ge 0$.

Numerical Example: Monge-Kantorovich Depth

Source: $\rho = \text{uniform probability density on } B(0,1) \subseteq \mathbb{R}^2$

Target: $\mu = \frac{1}{N} \sum_{1 \le i \le N} \delta_{y_i}$ with $N = 10^4$ points



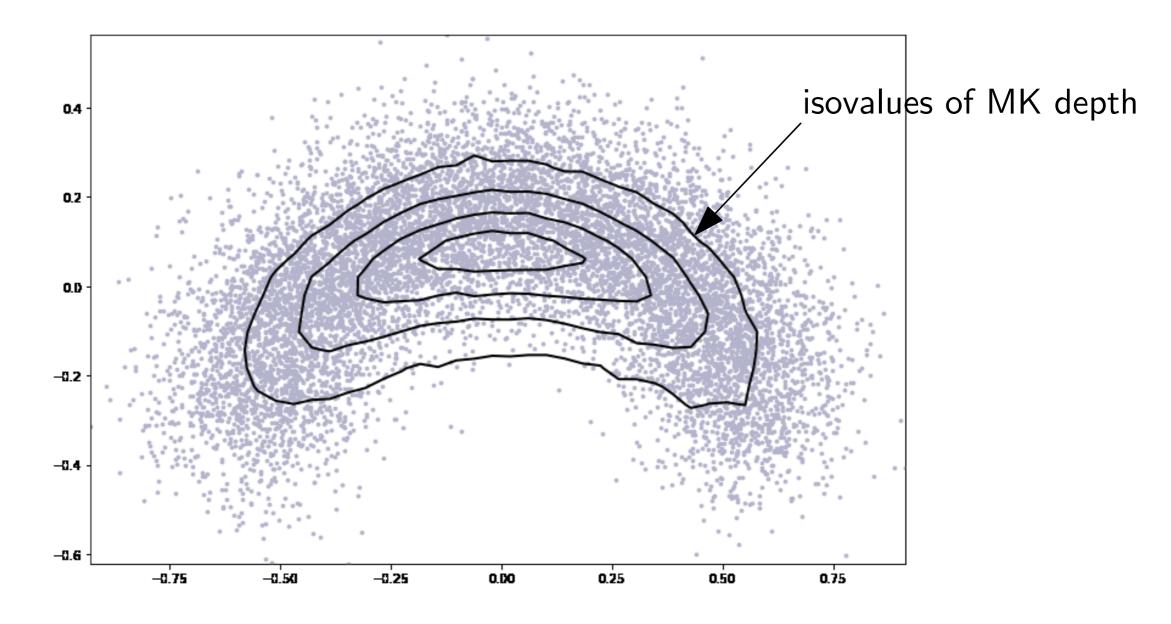
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▶ Let $\operatorname{Prob}_p(\mathbb{R}^d) = \{ \mu \in \operatorname{Prob}(\mathbb{R}^d) \mid \int ||x||^p d\mu < +\infty \}.$

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► On $\operatorname{Prob}(X)$, with $X \subseteq \mathbb{R}^d$ compact, W_p metrizes narrow convergence i.e. $\lim_{n \to +\infty} W_p(\mu_n, \mu) = 0 \iff \forall \phi \in \mathcal{C}^0(X), \lim_{n \to +\infty} \int \phi \, \mathrm{d} \, \mu_n = \int \phi \, \mathrm{d} \, \mu$.

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The previous embedding is false in higher dimension: $(Prob_p, W_p)$ is *curved*.

▶ We fix a reference measure, $\rho = \text{Leb}_X$ with $X \subseteq \mathbb{R}^d$ convex compact with |X| = 1.

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point	$x \in M$	$\mu \in \operatorname{Prob}_2(\mathbb{R}^d)$
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- \longrightarrow Representing family of probability measures by family of functions in $\mathrm{L}^2(
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$$\mu := \arg\min_{1 \le i \le k} \sum_{1 \le i \le k} \alpha_i W_2^2(\mu, \mu_i).$$

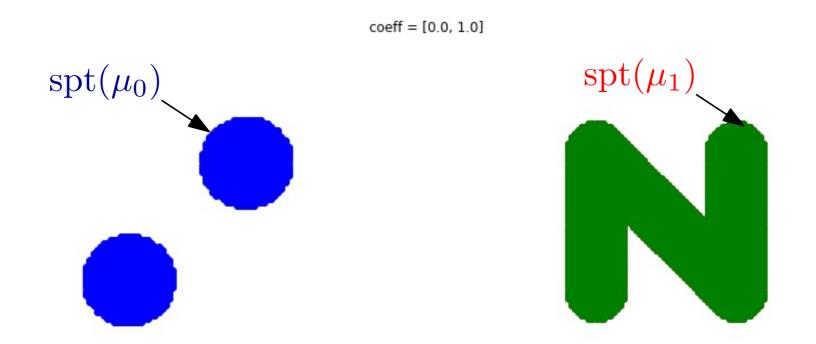
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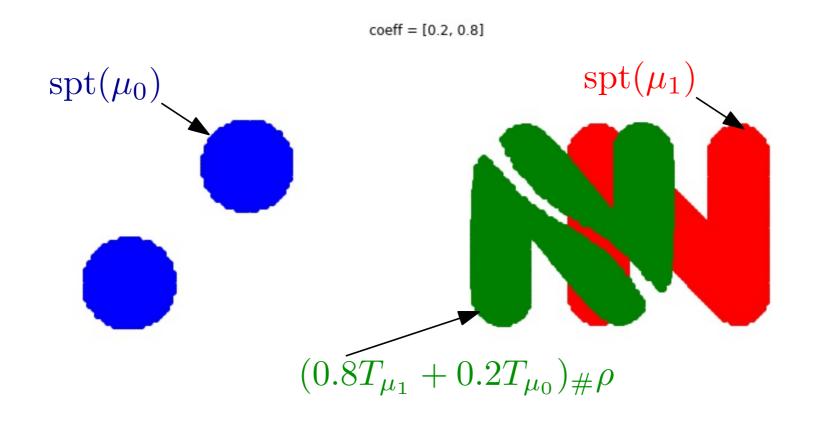
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- ▶ "Linearized" Wasserstein barycenters: $\mu := \left(\frac{1}{\sum_i \alpha_i} \sum_i \alpha_i T_{\mu_i}\right)_{\#} \rho$.
 - \longrightarrow Simple expression once the transport maps $T_{\mu_i}: \rho \to \mu_i$ have been computed.



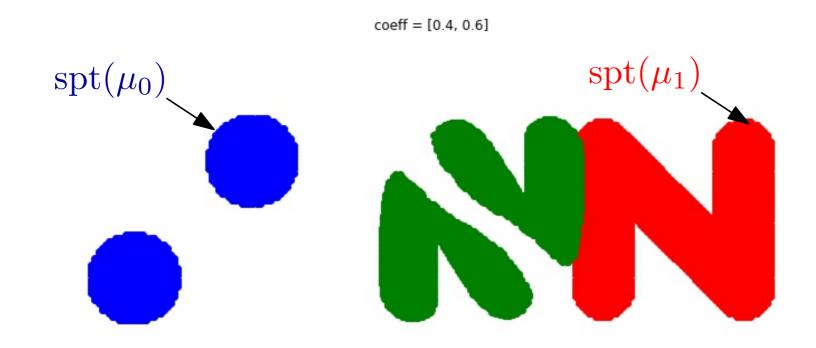
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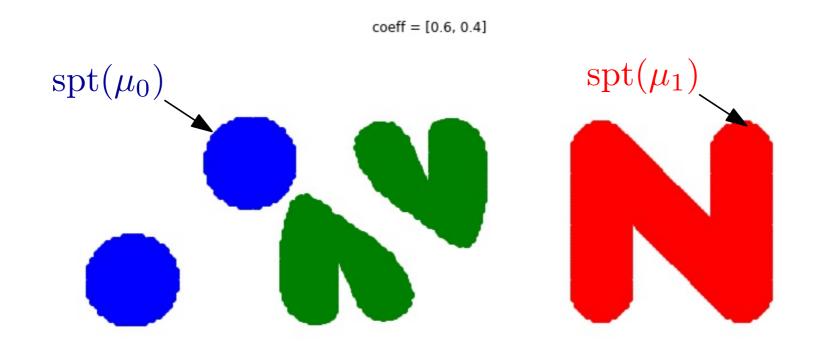
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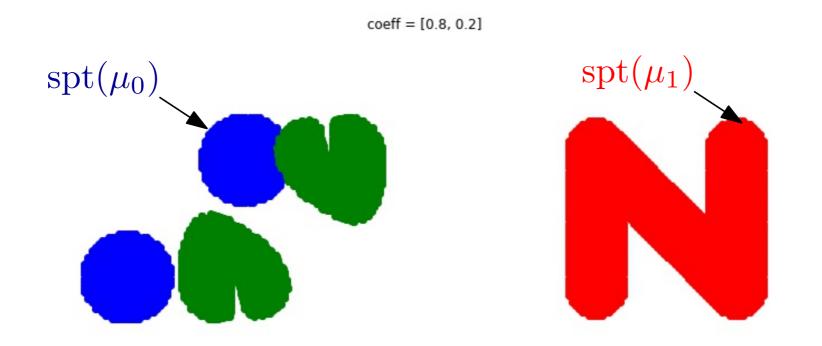
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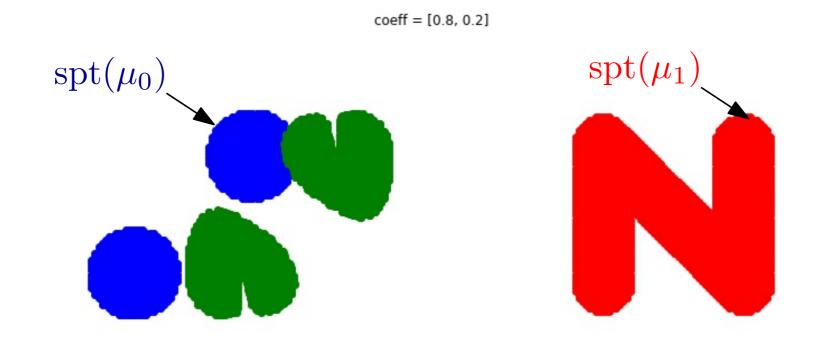
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What amount of the Wasserstein geometry is preserved by the embedding $\mu \mapsto T_{\mu}$?

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To solve numerically an OT problem between $\rho \in \operatorname{Prob}^{\mathrm{ac}}(\mathbb{R}^d)$ and $\mu \in \operatorname{Prob}([0,1]^d)$:

ightharpoonup Approximate μ by a discrete measure, for instance

$$\mu_k = \sum_{i_1 \leq ... \leq i_k} \mu(B_{i_1,...,i_k}) \delta_{(i_1/k,...,i_k/k)}$$

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Motivation 3: numerical analysis of optimal transport

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2. Continuity of $\mu \mapsto T_{\mu}$.

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Then
$$T_{\mu_{\theta}}(x) = \begin{cases} x_{\theta} & \langle x_{\theta} | x \rangle \geq 0 \\ x_{\theta+\pi} & \text{if not} \end{cases}$$
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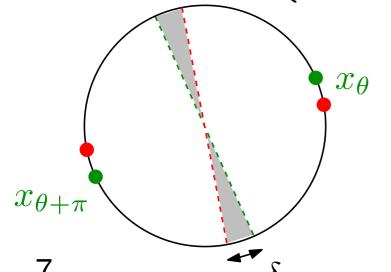
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, so that $\|T_{\mu_{\theta}} - T_{\mu_{\theta+\delta}}\|_{\mathrm{L}^{2}(\rho)}^{2} \geq C\delta$



Since on the other hand, $W_2(\mu_{\theta}, \mu_{\theta+\delta}) \leq C\delta$,

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Thm: Assume $\rho \in \operatorname{Prob}^{\operatorname{ac}}(X)$ and $\mu, \nu \in \operatorname{Prob}(Y)$ with $X, Y \subseteq \mathbb{R}^d$ compact If T_{μ} is L-Lipschitz, then $\|T_{\mu} - T_{\nu}\|_2^2 \leq C \operatorname{W}_1(\mu, \nu)$ with $C = 4L \operatorname{diam}(X)$.

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► **Prop** → **Thm:** Kantorovich-Rubinstein theorem

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$$(T_{\mu} = \nabla \phi_{\mu} \text{ L-Lipschitz} \iff \psi_{\mu} = \phi_{\mu}^{*} \text{ is L-strongly convex})$$

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- ▶ Proof of Berman's theorem relies on techniques from complex geometry.

2. Global, dimension-independent, Hölder-continuity of $\mu\mapsto T_{\mu}$.

Thm (M., Delalande, Chazal '19): Let X convex compact with |X|=1 and $\rho=\mathrm{Leb}_X$, and let Y be compact. Then, there exists C s.t. for all $\mu,\nu\in\mathrm{Prob}(Y)$, $\|T_\mu-T_\nu\|_{\mathrm{L}^2(X)}\leq C\,\mathrm{W}_2(\mu,\nu)^{1/5}.$

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- ▶ The constant C depend polynomially on diam(X), diam(Y).
- ▶ Proof relies on the semidiscrete setting, i.e. the bound is established in the case

$$\mu = \sum_{i} \mu_{i} \delta_{y_{i}}, \ \nu = \sum_{i} \nu_{i} \delta_{y_{i}}.$$

and one concludes using a density argument.

Let $\rho, \nu \in \operatorname{Prob}_1^{\operatorname{ac}}(\mathbb{R}^d)$ and $\Gamma(\rho, \mu) = \operatorname{couplings}$ between ρ, μ , $\mathcal{T}(\rho, \mu) = \max_{\gamma \in \Gamma(\rho, \mu)} \int \langle x | y \rangle \, \mathrm{d} \, \gamma(x, y)$

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Kantorovich duality

Legendre-Fenchel transform:

$$\psi^*(x) = \max_y \langle x|y\rangle - \psi(y)$$

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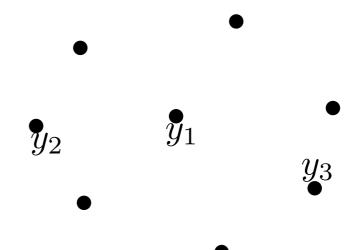
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Legendre-Fenchel transform:

$$\psi^*(x) = \max_y \langle x|y\rangle - \psi(y)$$

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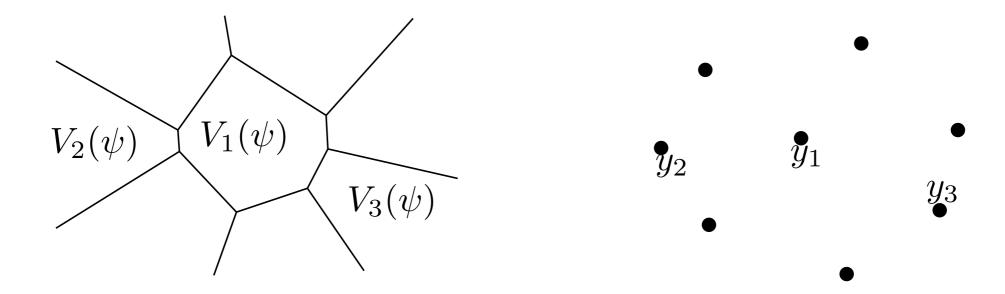
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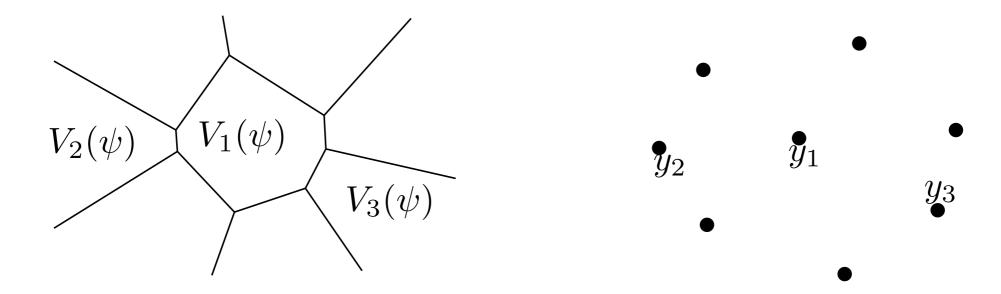
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Thus,
$$\mathcal{T}(\rho,\mu) = \min_{\psi \in \mathbb{R}^N} \sum_i \int_{V_i(\psi)} \langle x | y_i \rangle - \psi_i \, \mathrm{d} \, \rho(x) + \sum_i \mu_i \psi_i$$

Optimality condition and economic interpretation

$$\mathcal{T}(\rho,\mu) = \min_{\psi \in \mathbb{R}^N} \Phi(\psi) - \sum_i \mu_i \psi_i$$
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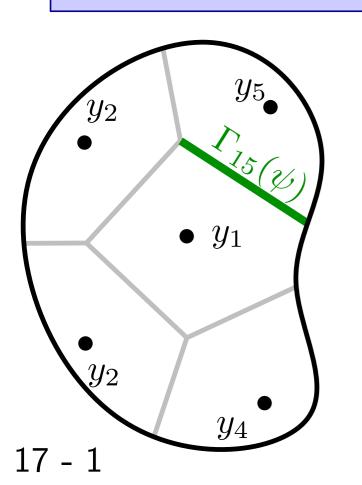
▶ Algorithm (Oliker–Prussner): coordinate-wise increment. Complexity: $O(N^3)$.

(Recall that $G_i(\psi) = \rho(V_i(\psi))$ and $\nabla \Phi = -(G_1, \dots, G_N)$)

Proposition: \blacktriangleright If $\rho \in \mathcal{C}^0(X)$ and $(y_i)_{1 \leq i \leq N}$ is generic, then $\Phi \in \mathcal{C}^2(\mathbb{R}^N)$ and

$$\forall i \neq j, \quad \frac{\partial G_i}{\partial \psi_j}(\psi) = \frac{1}{\|y_i - y_j\|} \int_{\Gamma_{ij}(\psi)} \rho(x) \, \mathrm{d} \, x \text{ where } \Gamma_{ij} = V_i(\psi) \cap V_j(\psi).$$

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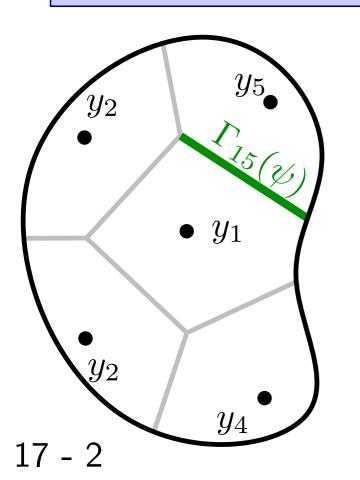
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Let
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▶ If $\Omega = \{\rho > 0\}$ is connected and $\psi \in E$, then $\mathrm{Ker}\mathrm{D}^2\Phi(\psi) = \mathbb{R}(1,\ldots,1)$.



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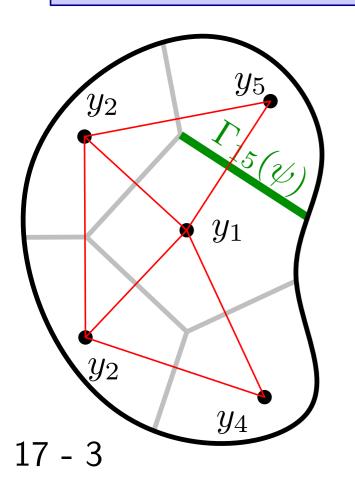
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Consider the matrix $L = DG(\psi)$ and the graph H: $(i,j) \in H \iff L_{ij} > 0$

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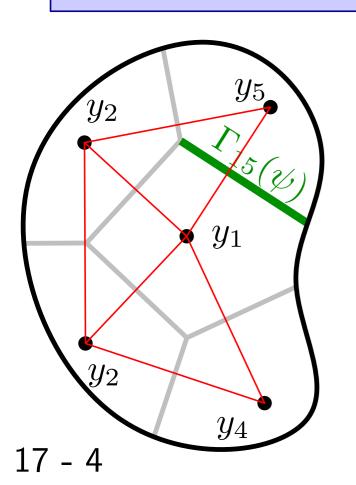
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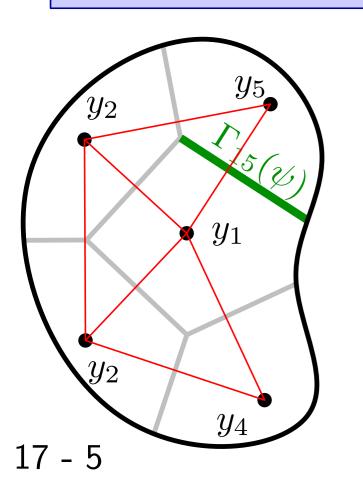
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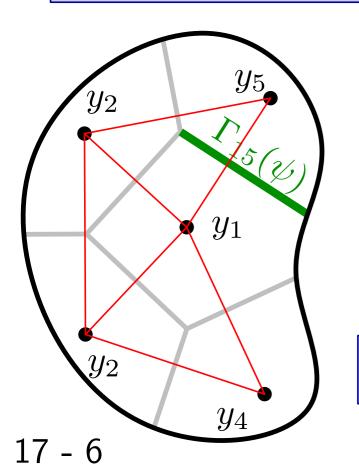
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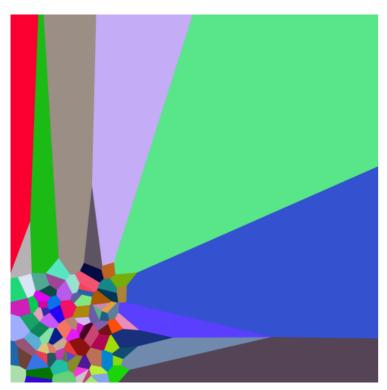
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Corollary: Global convergence of a damped Newton algorithm.

Source: $\rho = \text{uniform on } [0,1]^2$,

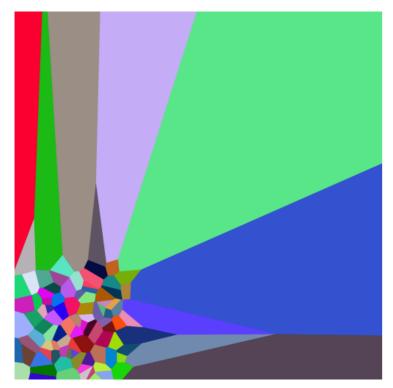
Target: $\mu = \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{y_i}$ with y_i uniform i.i.d. in $[0, \frac{1}{3}]^2$



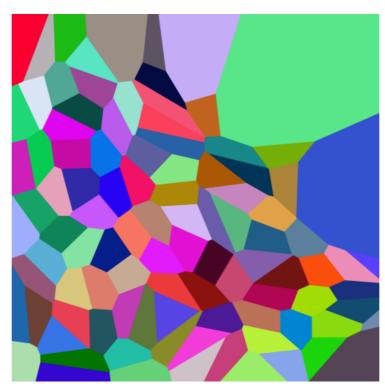
$$\psi_0 = \frac{1}{2} \| \cdot \|^2$$

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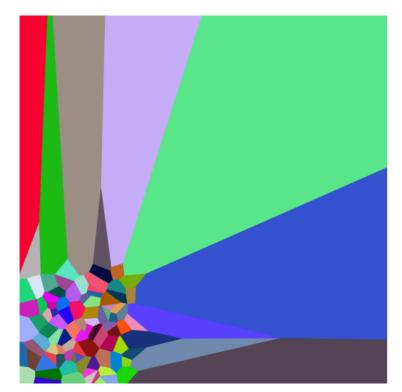


$$\psi_1 = \text{Newt}(\psi_0)$$

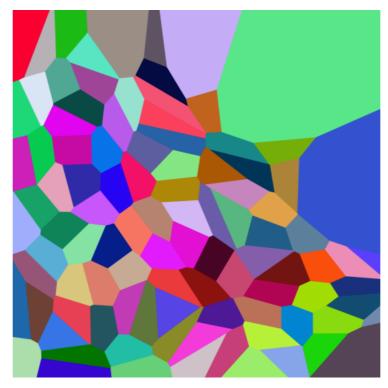
NB: The points do **not** move.

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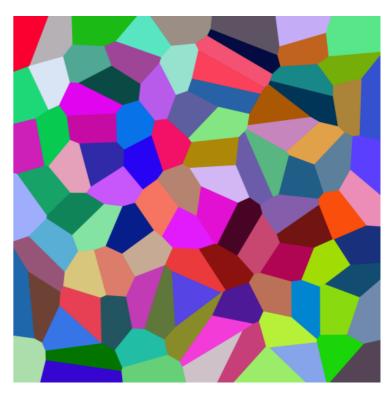
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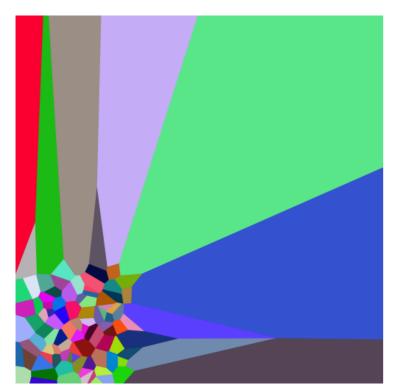


 $\psi_2 = \operatorname{Newt}(\psi_1)$

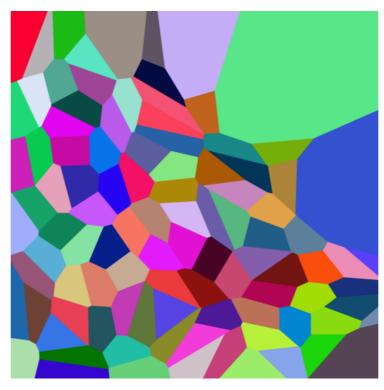
NB: The points do **not** move.

Source: $\rho = \text{uniform on } [0,1]^2$,

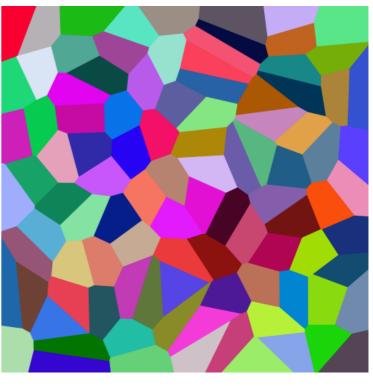
Target: $\mu = \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{y_i}$ with y_i uniform i.i.d. in $[0, \frac{1}{3}]^2$



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Convergence is *very* fast when $\operatorname{spt}(\rho)$ convex: 17 Newton iterations for $N \geq 10^7$ in 3D.

Thm (M., Delalande, Chazal '19): Let X convex compact with |X|=1 and $\rho=\mathrm{Leb}_X$, and let Y be compact. Then, there exists C s.t. for all $\mu,\nu\in\mathrm{Prob}(Y)$, $\|T_\mu-T_\nu\|_{\mathrm{L}^2(X)}\leq C\,\mathrm{W}_2(\mu,\nu)^{1/5}.$

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▶ We lose a little in the exponent to control the difference between OT maps...

A toy application

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We run the K-Means method on the transport plans, with K=20.

Each cluster $X^k \subseteq \{0,\ldots,M\}$ yields an average transport plan $S^k = \frac{1}{|X^k|} \sum_{\ell \in X} T^\ell$,

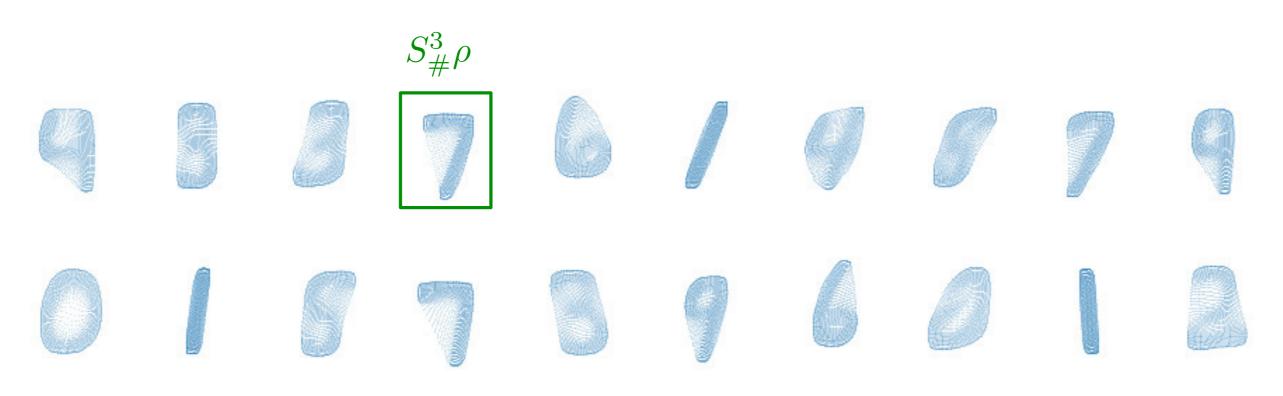
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Optimal transport can be used to embed of $\operatorname{Prob}(\mathbb{R}^d)$ into $L^2(\rho, \mathbb{R}^d)$, with possible applications in data analysis. Computations can be easily performed using

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Thank you for your attention!