

# Régularisation entropique des barycentres dans l'espace Wasserstein

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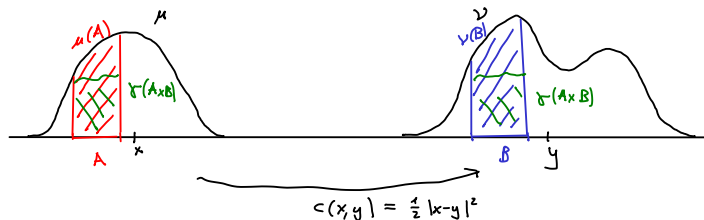
Joint work with Guillaume Carlier<sup>1</sup> and Alexey Kroshnin<sup>2</sup>

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# Optimal transport in a nutshell

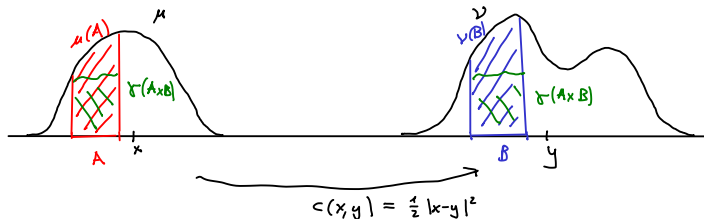


For  $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d) := \{\rho \in \mathcal{P}(\mathbb{R}^d) : \int_{\mathbb{R}^d} |x|^2 dx < \infty\}$  one seeks to optimize among all transport plans

$$\Pi(\mu, \nu) := \{\gamma \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d) : \pi_{1\#}\gamma = \mu, \pi_{2\#}\gamma = \nu\},$$

$$W_2^2(\mu, \nu) := \inf_{\gamma \in \Pi(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{1}{2} |x - y|^2 d\gamma(x, y),$$

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Kantorovich duality:

$$W_2^2(\mu, \nu) = \sup_{u(x) + v(y) \leq \frac{1}{2} |x - y|^2} \int u(x) d\mu(x) + \int v(y) d\nu(y)$$

# Optimal transport in a nutshell

Brenier's theorem:

If  $\mu \in \mathcal{P}_{\text{ac}}(\mathbb{R}^d)$ , then there is a  $\mu$ -a.e. **unique** transport map  $T$ , in the sense that the optimal transport plan  $\bar{\gamma}$  is of the form

$$\bar{\gamma} = (\text{Id}, T)_{\#}\mu,$$

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or in the form of Monge-Ampère equation

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$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{1}{2} |x - y|^2 d\bar{\gamma}(x, y) = \int_{\mathbb{R}^d} \frac{1}{2} |x - T(x)|^2 d\mu(x).$$

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Note that the right hand side corresponds to the original formulation by Monge.

Another important property is that  $W_2 : \mathcal{P}_2(\mathbb{R}^d) \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$  is a metric on  $\mathcal{P}_2(\mathbb{R}^d)$ , which makes  $\mathcal{P}_2(\mathbb{R}^d)$  Polish.

# On the Fréchet mean

A probabilistic perspective:

- For a random variable  $X$  in a Hilbert space  $H$  (with finite second moment) distributed according to  $P \in \mathcal{P}(H)$  its expectation  $\mathbb{E}[X]$  solves the following optimization problem

$$\inf_{c \in H} \mathbb{E}[\|X - c\|^2], \quad \text{respectively} \quad \inf_{c \in H} \int_H \|x - c\|^2 dP(x).$$



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- In particular for  $P = \sum_{i=1}^N p_i \delta_{\nu_i}$

$$\inf_{\rho \in \mathcal{P}_2(\mathbb{R}^d)} \sum_{i=1}^N p_i W_2^2(\rho, \nu_i),$$

which coincides with the Wasserstein barycenter introduced by Agueh and Carlier.

# Some motivation

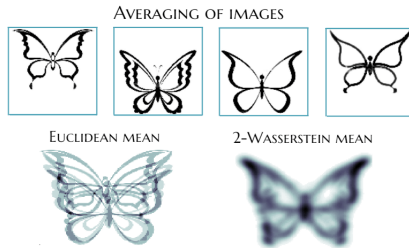


Figure: Taken from J. Ebert, V. Spokoyny and A. Suvorikova

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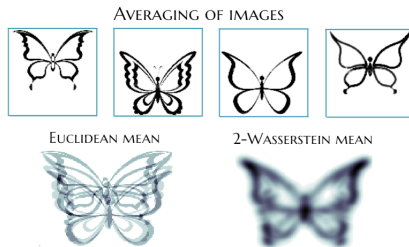


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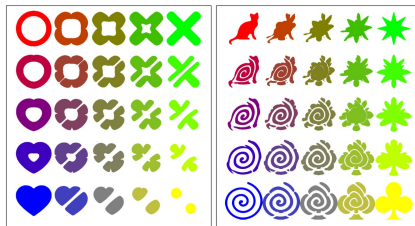


Figure: Taken from G. Peyré

# Entropically regularized Wasserstein barycenter

Problem: Discretization phenomena

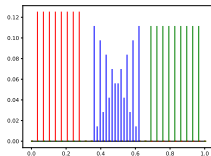


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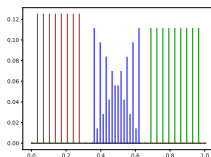


Figure: Taken from H. Lavenant

A way to fix this is to add a regularizing term, as introduced by Bigot, Cazelles and Papadakis.

For  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$ ,  $\Omega$  convex consider

$$\inf_{\rho \in \mathcal{P}_2(\mathbb{R}^d)} \int_{\mathcal{P}_2(\mathbb{R}^d)} W_2^2(\rho, \nu) dP(\nu) + \lambda \text{Ent}_\Omega(\rho) \quad (1)$$

where  $\text{Ent}_\Omega$  is defined for every  $\mu \in \mathcal{P}_2(\mathbb{R}^d)$  by

$$\text{Ent}_\Omega(\mu) = \begin{cases} \int_\Omega \rho \log \rho, & \text{if } \mu = \rho dx \text{ and } \int_\Omega \rho = 1, \\ +\infty, & \text{otherwise.} \end{cases}$$

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- Characterization:  $\bar{\rho} = \text{bar}_{\lambda,\Omega}(P)$  if and only if  $\bar{\rho}$  has a continuous density given by

$$\bar{\rho}(x) := \exp\left(-\frac{1}{2\lambda}|x|^2 + \frac{1}{\lambda} \int_{\mathcal{P}_2(\mathbb{R}^d)} \varphi_{\bar{\rho}}^{\nu}(x) \, dP(\nu)\right), \quad (2)$$

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- Regularity of  $\bar{\rho} := \text{bar}_{\lambda,\Omega}(P)$  from this representation:

$$\log(\bar{\rho}) \in L_{\text{loc}}^{\infty}(\Omega), \quad \bar{\rho} \in W_{\text{loc}}^{1,\infty}(\Omega) \text{ and } \nabla \bar{\rho} \in \text{BV}_{\text{loc}}(\Omega, \mathbb{R}^d).$$

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- Compare to (unregularized) barycenter:
  - Uniqueness only if  $P(\mathcal{P}_{\text{ac}}(\mathbb{R}^d)) > 0$ ,
  - Characterization by obstacle problem

$$\frac{1}{\lambda} \int_{\mathcal{P}_2(\mathbb{R}^d)} \varphi_{\bar{\rho}}^{\nu}(x) dP(\nu) \leq \frac{1}{2\lambda}|x|^2 + C \text{ with equality } \bar{\rho}\text{-a.e.}$$

## Further regularity estimates

- Bound on Fisher information:

$$\int_{\Omega} |\nabla \log(\bar{\rho})|^2 \bar{\rho} \leq \frac{1}{\lambda^2} \int_{\mathcal{P}_2(\mathbb{R}^d)} W^2(\bar{\rho}, \nu) dP(\nu).$$

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(where  $m_p(\nu) := \int_{\mathbb{R}^d} |x|^p d\nu(x)$ ). Then

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- The last two statements have also been shown for (unregularized) barycenters by Agueh & Carlier.

## More regular case

Assume now  $\Omega = B := B_R(0)$ ,  $R > 0$

$$P\left(\left\{\nu \in \mathcal{P}_{\text{ac}}(\overline{B}) : \|\nu\|_{C^{1,\alpha}(\overline{B})} + \|\log \nu\|_{L^\infty(\overline{B})} \leq C\right\}\right) = 1,$$

then

$$\varphi_{\bar{\rho}}^\nu \in C^{3,\alpha}(\overline{B}) \text{ for } P\text{-a.e. } \nu \quad \text{and} \quad \bar{\rho} \in C^{3,\alpha}(\overline{B}),$$

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In particular,  $\varphi_{\bar{\rho}}^\nu$  satisfies the Monge–Ampère equation in the classical sense

$$\det(D^2 \varphi_{\bar{\rho}}^\nu) \nu(\nabla \varphi_{\bar{\rho}}^\nu) = \bar{\rho} \text{ in } B$$

$$\nabla \varphi_{\bar{\rho}}^\nu(B) \subset B.$$

No higher regularity known for the (unregularized) barycenter due to free boundary aspect of optimality condition.

## Stochastic setting

Let now  $\nu_1, \nu_2, \dots$  be a i.i.d. sequence in  $\mathcal{P}_2(\mathbb{R}^d)$  distributed according to  $P$ . Define  $\bar{\rho} := \text{bar}_{\lambda, \Omega}(P)$  and the random variable

$$\bar{\rho}_n := \operatorname{argmin}_{\rho \in \mathcal{P}(\mathbb{R}^d)} \frac{1}{n} \sum_{i=1}^n W_2^2(\rho, \nu_i) + \lambda \operatorname{Ent}_{\Omega}(\rho). \quad (3)$$

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We obtain a Strong Law of Large Numbers. Namely if

- $\int_{\mathcal{P}_2(\mathbb{R}^d)} m_p(\nu) dP(\nu) < +\infty$  for  $p \geq 2$ , then a.s. (almost surely)

$$\begin{aligned} W_p(\bar{\rho}_n, \bar{\rho}) &\longrightarrow 0, \\ \bar{\rho}_n &\xrightarrow{W_{\text{loc}}^{1,q}(\Omega)} \bar{\rho} \quad \forall 1 \leq q < \infty, \\ \bar{\rho}_n^{1/p} &\xrightarrow{W^{1,p}(\Omega)} \bar{\rho}^{1/p}. \end{aligned}$$

- $P\left(\left\{\nu \in \mathcal{P}_{\text{ac}}(\bar{B}) : \|\nu\|_{C^{1,\alpha}(\bar{B})} + \|\log \nu\|_{L^\infty(\bar{B})} \leq C\right\}\right) = 1$ , then  $\bar{\rho}_n \xrightarrow{\text{a.s.}} \bar{\rho}$  in  $C^{3,\beta}(\bar{B})$  for any  $\beta \in (0, \alpha)$ .
- For (unregularized) barycenter LLN only w.r.t. convergence in  $W_2$  known.

# Central Limit Theorem

If  $P\left(\left\{\nu \in \mathcal{P}_{\text{ac}}(\overline{B}) : \|\nu\|_{C^{1,\alpha}(\overline{B})} + \|\log \nu\|_{L^\infty(\overline{B})} \leq C\right\}\right) = 1$ , The empirical barycenters satisfy a CLT in  $L^2_\diamond(B) := \{u \in L^2(B) : \int_B u dx = 0\}$ :

$$\sqrt{n}(\overline{\rho}_n - \overline{\rho}) \xrightarrow{d} \xi \sim \mathcal{N}(0, \Sigma),$$

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$$G: u \mapsto \lambda \frac{u}{\bar{\rho}} - \lambda \int_B \frac{u}{\bar{\rho}} - \mathbb{E}(\Phi^\nu)'(\bar{\rho}),$$

and where

$$\begin{aligned} \Phi^\nu : \mathcal{S} &\rightarrow \mathcal{M}, \\ \mu &\mapsto \varphi, \text{ where } \det(D^2\varphi) \nu(\nabla\varphi) = \mu, \\ &\quad \nabla\varphi(\bar{B}) = \bar{B}, \end{aligned}$$

with  $\mathcal{S} = \{\varrho \in \mathcal{P}_{\text{ac}}(\bar{B}) : \|\varrho\|_{C^{1,\alpha}(\bar{B})} + \|\log \varrho\|_{L^\infty(\bar{B})} < \infty\}$ ,  
 $\mathcal{M} = \{\varphi \in C^{3,\alpha}(\bar{B}) : \|\nabla\varphi\|^2 - R^2 = 0 \text{ on } \partial B, \int_B \varphi = 0\}$ .

# Central Limit Theorem: Idea of proof

Use a delta method: In our case, CLT in Hilbert spaces gives

$$\sqrt{n} \left( \frac{1}{n} \sum_{i=1}^n \varphi_{\bar{\rho}}^{\nu_i} - \mathbb{E}_P[\varphi_{\bar{\rho}}^{\nu}] \right) \xrightarrow{d} \mathcal{N}(0, \text{Var}_P(\varphi_{\bar{\rho}}^{\nu}))$$

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We want to rewrite this in the form  $G_n(\bar{\rho}_n - \bar{\rho})$ , where  $G_n$  are invertible operators which converges in a nice way to a suitable operator  $G$

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n \varphi_{\bar{\rho}}^{\nu_i} - \mathbb{E}_P[\varphi_{\bar{\rho}}^{\nu}] &= \frac{1}{n} \sum_{i=1}^n \varphi_{\bar{\rho}_n}^{\nu_i} - \mathbb{E}_P[\varphi_{\bar{\rho}}^{\nu}] - \frac{1}{n} \sum_{i=1}^n \left( \varphi_{\bar{\rho}_n}^{\nu_i} - \varphi_{\bar{\rho}}^{\nu_i} \right) \\ &= F(\bar{\rho}_n) - F(\bar{\rho}) - \frac{1}{n} \sum_{i=1}^n (\Phi^{\nu_i}(\bar{\rho}_n) - \Phi^{\nu_i}(\bar{\rho})) \\ &= \mathbf{G}_n(\bar{\rho}_n - \bar{\rho}) \end{aligned}$$

with  $F(\rho) = \lambda \log \rho + \frac{|\mathbf{x}|^2}{2} - f_B \left( \lambda \log \rho + \frac{|\mathbf{x}|^2}{2} \right)$ ,

$\mathbf{G}_n = \int_0^1 F'(\bar{\rho}_n^t) dt - \frac{1}{n} \sum_{i=1}^n \int_0^1 (\Phi^{\nu_i})'(\bar{\rho}_n^t) dt$  with  $\bar{\rho}_n^t = (1-t)\bar{\rho} + t\bar{\rho}_n$ .

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For  $\rho \in \mathcal{S} = \left\{ \varrho \in \mathcal{P}_{\text{ac}}(\bar{B}) : \|\varrho\|_{C^{1,\alpha}(\bar{B})} + \|\log \varrho\|_{L^\infty(\bar{B})} < \infty \right\}$

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- $\varphi := \Phi^\nu(\rho)$  is given by the solution of the Monge–Ampère equation

$$\begin{aligned} \det(D^2\varphi)\nu(\nabla\varphi) &= \bar{\rho} \text{ in } B \\ \nabla\varphi(B) &\subset B. \end{aligned}$$

So its derivative corresponds to linearizing this equation. We have enough regularity to conclude that  $\Phi^\nu$  is differentiable with  $(\Phi^\nu)'(\rho) : u \mapsto h$  where

$$\begin{aligned} \operatorname{div}(A_\nu \nabla h) &= u \text{ in } B, \\ \nabla\varphi \cdot \nabla h &= 0 \text{ on } \partial B, \end{aligned}$$

for  $A_\nu = \nu(\nabla\varphi) \det(D^2\varphi) (D^2\varphi)^{-1}$ .

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- Thanks to the regularity estimates

$$\bar{\rho}_n^t \in \left\{ \nu \in \mathcal{P}_{\text{ac}}(\mathbb{R}^d) : \nu(\bar{B}) = 1, \|\nu\|_{C^{1,\alpha}(\bar{B})} + \|\log \nu\|_{L^\infty(\bar{B})} \leq \tilde{C} \right\}$$

implying  $F'$  to be Hermitian, bounded and uniformly positive definite and  $(\Phi^\nu)'$  Hermitian, bounded and negative definite on  $L_\diamond^2(B)$ .

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- A version of Slutsky's theorem guarantees then that

$$\mathbf{G}_n^{-1} \sqrt{n} \mathbf{G}_n (\bar{\rho}_n - \bar{\rho}) \xrightarrow{d} \xi \sim \mathcal{N}(0, \Sigma).$$

# The End

Merci pour votre attention!