Régularisation entropique des barycentres dans l'espace de Wasserstein

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Joint work with Guillaume Carlier[1] and Alexey Kroshnin[2]

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Optimal transport in a nutshell

For $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d) := \left\{\rho \in \mathcal{P}(\mathbb{R}^d) : \int_{\mathbb{R}^d} |x|^2 dx < \infty\right\}$ one seeks to optimize among all transport plans
$\Pi(\mu, \nu) := \left\{\gamma \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d) : \ \pi_{1\#}\gamma = \mu, \ \pi_{2\#}\gamma = \nu\right\},$

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

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Brenier's theorem:
If $\mu \in \mathcal{P}_{\mathrm{ac}}(\mathbb{R}^d)$, then there is a μ-a.e. **unique** transport map T, in the sense that the optimal transport plan $\bar{\gamma}$ is of the form

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

and it is the gradient of a convex function φ_μ^ν, which we call Brenier potential.

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and it is the gradient of a convex function φ_μ^ν, which we call Brenier potential. Equivalently we have

$$\nabla \varphi_{\mu\,\#}^{\nu} \mu = \nu,$$

or in the form of Monge-Ampère equation

$$\det(D^2 \varphi_\mu^\nu) \nu(\nabla \varphi_\mu^\nu) = \mu,\ \nabla \varphi_\mu^\nu(\mathrm{supp}\mu) \subset \mathrm{supp}\nu.$$

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

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

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- This motivates the definition of Fréchet mean, which generalizes the notion of mean for metric spaces. In particular, on $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ a Fréchet mean of $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$ is a minimizer of

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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

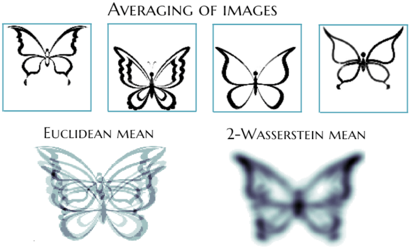

Figure: Taken from J. Ebert, V. Spokoiny and A. Suvorikova

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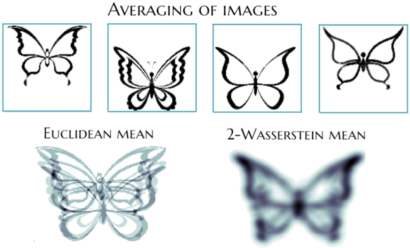

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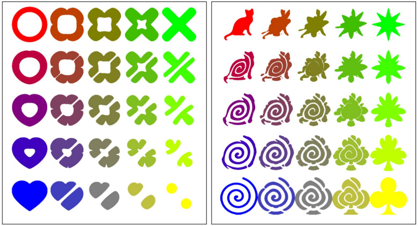

Figure: Taken from G. Peyré

Wasserstein barycenter on discretized space

Problem: Discretization phenomena
Given discretizations on a uniform grid of two uniform measures (red and green)

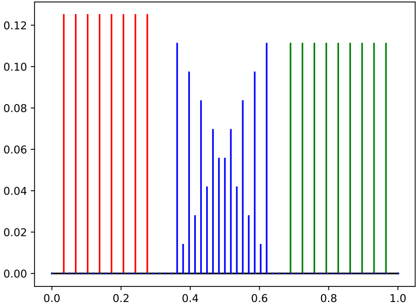

Figure: Taken from H. Lavenant

The true barycenter is given in blue (without being constraint on being on a grid)

Entropically regularized Wasserstein barycenter

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

For $P \in \mathcal{P}_2\left(\mathcal{P}_2(\mathbb{R}^d)\right)$, Ω open, convex consider

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

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

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

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- $\mathsf{bar}_{\lambda,\Omega}(P)$ is absolutely continuous and $\mathrm{supp}(\mathsf{bar}_{\lambda,\Omega}(P)) = \overline{\Omega}$
- Characterization: $\overline{\rho} = \mathsf{bar}_{\lambda,\Omega}(P)$ if and only if $\overline{\rho}$ has a continuous density given by

$$\overline{\rho}(x) \coloneqq \exp\Big(-\frac{1}{2\lambda}|x|^2 + \frac{1}{\lambda}\int_{\mathcal{P}_2(\mathbb{R}^d)} \varphi_{\overline{\rho}}^{\nu}(x)\,\mathrm{d}P(\nu)\Big), \tag{2}$$

  where $\varphi_{\overline{\rho}}^{\nu}$ denote the Brenier potentials from $\overline{\rho}$ to ν (properly normalized).

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  where $\varphi_{\overline{\rho}}^{\nu}$ denote the Brenier potentials from $\overline{\rho}$ to ν (properly normalized).
- Regularity of $\overline{\rho} := \mathrm{bar}_{\lambda,\Omega}(P)$ from this representation:

$$\log(\overline{\rho}) \in L^{\infty}_{\mathrm{loc}}(\Omega),\ \overline{\rho} \in W^{1,\infty}_{\mathrm{loc}}(\Omega) \text{ and } \nabla\overline{\rho} \in \mathrm{BV}_{\mathrm{loc}}(\Omega, \mathbb{R}^d).$$

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

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

Further regularity estimates

- Bound on Fisher information:

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

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- Further moment estimates: For $p \geq 2$ assume that

$$\int_{\mathcal{P}_2(\mathbb{R}^d)} m_p(\nu) \, \mathrm{d}P(\nu) < +\infty$$

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

$$m_p(\overline{\rho}) \leq C(p) \left(\int_{\mathcal{P}_2(\mathbb{R}^d)} m_p(\nu) \, \mathrm{d}P(\nu) \right) + C(d,p)(\lambda)^{(d+p)/2}.$$

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- The last statement has also been shown for (unregularized) barycenters by Agueh & Carlier. (displacement convexity argument)

Maximum principle

Let Ω be convex. If $P(\{\nu \in \mathcal{P}_2(\mathbb{R}^d) : \nu(\Omega) = 1\}) = 1$, then for $\overline{\rho} := \mathrm{bar}_{\lambda,\Omega}(P)$

$$\|\overline{\rho}\|_{L^\infty(\mathbb{R}^d)} \leq \left(\int_{\mathcal{P}_2(\mathbb{R}^d)} \|\nu\|_{L^\infty(\mathbb{R}^d)}^{-1/d} \, \mathrm{d}P(\nu) \right)^{-d}.$$

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In particular, if

$$P\left(\{\nu \in L^\infty(\mathbb{R}^d),\ \nu \leq C\}\right) = \alpha > 0,$$

then the inequality becomes

$$\|\overline{\rho}\|_{L^\infty(\mathbb{R}^d)} \leq \frac{C}{\alpha^d}.$$

The L^∞ has also been shown for (unregularized) barycenters by Agueh & Carlier for $\alpha = 1$ and generalized for $0 < \alpha < 1$ by Kim & Pass.

More regular case

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

$$P\Big(\Big\{\nu \in \mathcal{P}_{\mathrm{ac}}(\overline{B}) : \|\nu\|_{C^{1,\alpha}(\overline{B})} + \|\log \nu\|_{L^\infty(\overline{B})} \le C\Big\}\Big) = 1,$$

then

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

and there is a constant $K > 0$ such that

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$$\left\|\varphi_{\bar\rho}^{\nu}\right\|_{C^{3,\alpha}(\overline{B})} \le K \text{ for } P\text{-a.e. } \nu.$$

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

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

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We obtain a Strong Law of Large Numbers. Namely if

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

$$W_p(\overline{\boldsymbol{\rho}}_{\boldsymbol{n}}, \overline{\rho}) \longrightarrow 0,$$

$$\overline{\boldsymbol{\rho}}_{\boldsymbol{n}} \xrightarrow{W^{1,q}_{\mathrm{loc}}(\Omega)} \overline{\rho} \quad \forall 1 \leq q < \infty,$$

$$\overline{\boldsymbol{\rho}}_{\boldsymbol{n}}^{\,1/p} \xrightarrow{W^{1,p}(\Omega)} \overline{\rho}^{1/p}.$$

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

Central Limit Theorem

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

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

with covariance operator $\Sigma = G^{-1}\,\mathrm{Var}_P(\varphi^{\nu}_{\overline{\rho}})G^{-1}$

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$$G\colon\, u \mapsto \lambda \frac{u}{\overline{\rho}} - \lambda \fint_B \frac{u}{\overline{\rho}} - \mathbb{E}(\Phi^\nu)'(\overline{\rho}),$$

and where

$$\begin{array}{rcl} \Phi^\nu : \mathcal{S} & \to & \mathcal{M}, \\ \mu & \mapsto & \varphi, \text{ where } \det\left(D^2\varphi\right)\nu(\nabla\varphi) = \mu, \\ & & \qquad\qquad\qquad\qquad\quad \nabla\varphi(\bar{B}) = \bar{B}, \end{array}$$

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

Central Limit Theorem: Idea of proof

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

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

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

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

with $F(\rho) = \lambda \log\rho + \frac{|x|^2}{2} - ⨏_B\left(\lambda\log\rho + \frac{|x|^2}{2}\right)$,
$\boldsymbol{G_n} = \int_0^1 F'(\boldsymbol{\overline{\rho}_n^t})\,\mathrm{d}t - \frac{1}{n}\sum_{i=1}^{n}\int_0^1(\Phi^{\boldsymbol{\nu_i}})'(\boldsymbol{\overline{\rho}_n^t})\,\mathrm{d}t$ with $\boldsymbol{\overline{\rho}_n^t} = (1-t)\overline{\rho} + t\boldsymbol{\overline{\rho}_n}$.

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- F is differentiable with

$$F'(\rho)\colon u \mapsto \lambda \frac{u}{\rho} - \lambda \fint_B \frac{u}{\rho}.$$

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

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

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

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

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

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- A version of Słutsky's theorem guarantees then that

$${\boldsymbol{G_n}}^{-1}\sqrt{n}\boldsymbol{G_n}\left(\overline{\rho}_n - \overline{\rho}\right) \xrightarrow{d} \xi \sim \mathcal{N}(0, \Sigma).$$

The End

Thank you for your attention!