Displacement functional and absolute continuity of Wasserstein barycenters

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February 5, 2024, GT CalVa

Definitions

see the blackboard ☛

Barycenters

- Notion of mean for probability measures μ on metric spaces (E, d)
- Always exist in proper spaces (metric spaces whose bounded closed sets are compact)

Wasserstein spaces $(\mathcal{W}(E), W)$

- Metric spaces for optimal transport between probability measures on a Polish space (a complete and separable metric space)
- Wasserstein spaces are Polish spaces.

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Define $W(\mu, E) := \inf_{x \in E} W(\mu, \delta_x)$.

z is a barycenter of $\mu \in \mathcal{W}(E)$ iff $W(\mu, \delta_z) = W(\mu, E)$

Wasserstein barycenters

Definition

Given a Polish space (E, d), the Wasserstein space $(\mathcal{W}(E), W)$ is also Polish, over which we can construct the Wasserstein space $(\mathcal{W}(\mathcal{W}(E)), \mathbb{W})$.
Barycenters $\overline{\mu}$ of measures $\mathbb{P} \in \mathcal{W}(\mathcal{W}(E))$ are called Wasserstein barycenters.

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Remark

By definition, $\mathbb{P}$ is a probability measure on $\mathcal{W}(E)$, its barycenter $\overline{\mu}$ is thus a probability measure on E.

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Example (Displacement interpolation)

Consider the earth surface (E, d) with two uniform measures μ, ν supported on two regions. We simulate the barycenter of $\frac{1}{2}\delta_\mu + \frac{1}{2}\delta_\nu$ by discrete points.

🇫🇷 $+$ 🇨🇳 $\xrightarrow{\texttt{barycenter}}$ 🦙 (llama)

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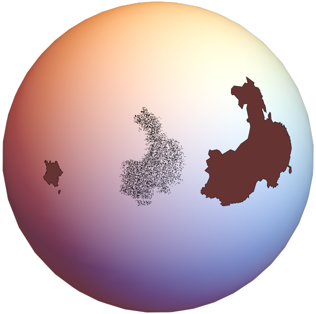
Existence [Le Gouic and Loubes, 2017]

Assuming that (E, d) is a proper space, Wasserstein barycenters in $\mathcal{W}(E)$ always exist.



Structure of Wasserstein barycenters

Fix a proper space (E, d) and n positive real numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$ such that $\sum_{i=1}^n \lambda_i = 1$. Given n measures $\mu_1, \mu_2, \ldots, \mu_n$, one can construct a barycenter $\overline{\mu}$ of $\sum_{i=1}^n \lambda_i \delta_{\mu_i}$ as follows.

Construction of $\overline{\mu} := B_{\#}\gamma$

1. Let $B : E^n \to E$ be a measurable map `(barycenter selection map)` sending $(x_1, x_2, \ldots, x_n)$ to a barycenter of $\sum_{i=1}^n \lambda_i \, \delta_{x_i}$.
2. Let γ be a measure `(multi-marginal optimal transport plan)` on E^n s.t.

$$\int_{E^n} W(\sum_{i=1}^n \lambda_i \, \delta_{x_i}, E)^2 \, \mathrm{d}\, \gamma(x_1, \ldots, x_n) = \inf_{\theta \in \Theta} \int_{E^n} W(\sum_{i=1}^n \lambda_i \, \delta_{x_i}, E)^2 \, \mathrm{d}\, \theta(x_1, \ldots, x_n),$$

where Θ is the set of measures on E^n with marginals $\mu_1, \mu_2, \ldots, \mu_n$ and $\gamma \in \Theta$.

Corollary: $(B, \mathrm{proj}_i)_{\#}\gamma$ is an optimal transport plan between $\overline{\mu}$ and μ_i.

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Properties of Wasserstein barycenter

Consistency [Le Gouic and Loubes, 2017]

Let (E, d) be proper space. Given a sequence of measures $\mathbb{P}_j \in \mathcal{W}(\mathcal{W}(E))$ with barycenters $\overline{\mu}_j$, if $\mathbb{W}(\mathbb{P}_j, \mathbb{P}) \to 0$, then $\overline{\mu}_j$ converges to a barycenter of $\mathbb{P}$ up to extracting a subsequence.

Remark

Construction for finitely many measures + consistency $\implies$ general existence.

Indeed, we rely on the consistency to investigate general barycenters.

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Uniqueness [Kim and Pass, 2017]

Let (M, d) be a Riemannian manifold. If $\mathbb{P} \in \mathcal{W}(\mathcal{W}(M))$ gives mass to the set of absolutely continuous measures, then it has a unique barycenter.

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Absolute continuity [Agueh and Carlier, 2011]

Let $\mu_1, \mu_2, \ldots, \mu_n$ be n probability measures on $\mathbb{R}^m$. If μ_1 is absolutely continuous with bounded density function, then the unique barycenter of $\sum_{i=1}^n \lambda_i \, \delta_{\mu_i}$ is also absolutely continuous.

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Uniqueness [Kim and Pass, 2017]

Let (M, d) be a Riemannian manifold. If $\mathbb{P} \in \mathcal{W}(\mathcal{W}(M))$ gives mass to the set of absolutely continuous measures, then it has a unique barycenter.

Absolute continuity [Kim and Pass, 2017]

Let (M, d) be a compact Riemannian manifold. If $\mathbb{P} \in \mathcal{W}(\mathcal{W}(M))$ gives mass to a set of absolutely continuous measures with uniformly bounded density functions, then its unique barycenter is absolutely continuous.

How to prove absolute continuity

`(a.c stands for absolutely continuous)`

Absolute continuity and compactness [Kim and Pass, 2017]

Let (M, d) be a compact manifold. If $\mathbb{P} \in \mathcal{W}(\mathcal{W}(M))$ gives mass to a set of a.c measures with uniformly bounded density functions, then its barycenter is a.c.

Absolute continuity and Ricci curvature bound [Ma, 2023]

Let (M, d) be a complete manifold with a lower Ricci curvature bound.
If $\mathbb{P} \in \mathcal{W}(\mathcal{W}(M))$ gives mass to the set of a.c measures, then its barycenter $\overline{\mu}$ is a.c.

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Sketch of proof, when $\mathbb{P} = \sum_{i=1}^{n} \lambda_i \delta_{\mu_i}$ and each μ_i has compact support

Similar to the case of displacement interpolation: locally Lipschitz + compactness

1. When μ_1 is a.c and μ_i's for $2 \leq i \leq n$ are Dirac measures, the optimal transport map from $\overline{\mu}$ to μ_1 is locally Lipschitz. (See details later)
2. Apply a divide-and-conquer (conditional measure) argument for the case when $\mu_i, 2 \leq i \leq n$ are discrete measures to retain the Lipschitz estimate.
3. Compactness and Rauch comparison theorem imply a uniform Lipschitz estimate for approximating sequences of general $\mu_i, i \leq 2 \leq n$.

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Pass to the general case of $\mathbb{P}$ by consistency

Hessian equality for Wasserstein barycenters: let $\overline{\mu}$ be the unique a.c barycenter of $\sum_{i=1}^{n} \lambda_i \delta_{\mu_i}$ and let $\exp(-\nabla \phi_i)$ be the optimal transport map between $\overline{\mu}$ and μ_i, then

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$$\sum_{i=1}^{n} \lambda_i \operatorname{Hess} \phi_i \geq 0.$$

Approach of [Kim and Pass, 2017]: plug Monge-Ampère equations into the above inequality and bound the density of $\overline{\mu}$ by a uniform upper bound of those of μ_i's.

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Our approach [Ma, 2023]: define a novel class of displacement functionals exploiting the equality, and bound them from above with the help of Souslin space theory.

Absolute continuity of Wasserstein barycenters of finitely many measures

Fix $\mathbb{P} = \sum_{i=1}^n \lambda_i \, \delta_{\mu_i}$, where μ_1 is a.c with compact support and $\mu_i = \delta_{x_i}$ for $i \geq 2$.
Its unique barycenter is $\overline{\mu} = B_{\#}\gamma$, where B is a measurable barycenter selection map and $\gamma = \mu_1 \otimes \delta_{x_2} \otimes \cdots \delta_{x_n}$ is the unique coupling of its marginals.

c-conjugating formulation of B

1. Define $c(x,y) := \frac{1}{2} d(x,y)^2$ and $g(y) := -\frac{1}{\lambda_1} \sum_{i=2}^n \lambda_i \, c(x_i, y)$
2. Given $x_1 \in M$, z is a barycenter of $\nu := \sum_{i=1}^n \lambda_i \, \delta_{x_i}$

$$\iff z \quad \text{reaches the infimum of} \quad 2\lambda_1 \inf_{y \in M} \{c(x_1, y) - g(y)\}$$

3. Define $X = \operatorname{supp}(\mu_1)$ and Y the set of barycenters of ν when x_1 runs through X. The map g is smooth on Y [Kim and Pass, 2015]. Set $F := \exp(-\nabla g)$.

$$z \in Y \text{ and } x_1 = F(z) \iff x_1 \in X \text{ and } z \text{ is a barycenter of } \nu$$

Conclusion: $F_{\#}\overline{\mu} = \mu_1$. Since F is Lipschitz, $\overline{\mu}$ is a.c.

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Displacement functionals for Wasserstein barycenters

Assumptions and notation for the functional $\mathcal{G} : f \cdot \mathrm{Vol} \mapsto \int_M G(f)\,\mathrm{d}\,\mathrm{Vol}$

1. M, m-dimensional manifold with lower Ricci curvature bound $-K \leq 0$.
2. $\mu_i, 1 \leq i \leq n$, compactly supported measures which are a.c for indices $1 \leq i \leq k$.
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Define $\Lambda := \sum_{i=1}^{k} \lambda_i$, then

$$\mathcal{G}(\overline{\mu}) := \int_M G(f)\,\mathrm{d}\,\mathrm{Vol} \leq \sum_{i=1}^{k} \frac{\lambda_i}{\Lambda} \int_M G(g_i)\,\mathrm{d}\,\mathrm{Vol} + \frac{L_H K}{2\Lambda} \mathbb{W}(\mathbb{P}, \delta_{\overline{\mu}})^2 + \frac{L_H}{2\Lambda}(m^2 + 2m)\,.$$

Displacement functionals for Wasserstein barycenters

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Special case: curvature-dimension condition

Take $G(x) := x \log x$, $n = k = 2$, $\Lambda = L_H = 1$. Set $\lambda = \lambda_1$ and $\mathrm{Ent} = \mathcal{G}$, then

$$\mathrm{Ent}(\overline{\mu}) \leq \lambda \, \mathrm{Ent}(\mu_1) + (1-\lambda)\, \mathrm{Ent}(\mu_2) + \frac{K}{2} \lambda(1-\lambda)\, W(\mu_1, \mu_2)^2 + \frac{m^2}{2} + m\,.$$

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Difference from classical displacement functionals

Gradient flow theory `(first-order)` and displacement convexity `(second-order)` gives that

$$\mathcal{G}(\mu_i) \geq \mathcal{G}(\overline{\mu}) + \int_M \Delta\phi_i \, H'(\log f)\,\mathrm{d}\,\overline{\mu} - \frac{L_H\,K}{2} W_2(\overline{\mu}, \mu_i)^2, \quad 1 \leq i \leq k.$$

Preservation of absolute continuity when passing to the limit

Reminder of the problem setting

We approximate a general measure $\mathbb{P} \in \mathcal{W}(\mathcal{W}(M))$ with $\mathbb{P}_j$. After proving that the barycenter $\overline{\mu}_j$ of $\mathbb{P}_j$ is a.c, how to show that the barycenter $\overline{\mu} = \lim \overline{\mu}_j$ of $\mathbb{P}$ is also a.c?

Use displacement functionals $\mathcal{G}$ admitting finite values only for a.c measures

1. Assume G is in addition super-linear and convex, then $\mathcal{G}$ is lower semi-continuous;
2. Bound $\{\mathcal{G}(\overline{\mu}_j)\}_{j \geq 1}$ from above, for which we use the displacement inequality;
3. By choosing the sequence $\mathbb{P}_j$ properly, it reduces to show that $\mathbb{P}$ gives mass to a $\mathrm{B}(G, L)$ set, the set of a.c measures whose values under $\mathcal{G}$ are bounded by $L > 0$;
4. Compact sets w.r.t. the $\sigma(L^1, L^\infty)$ topology are $B(G, L)$ sets;
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Justifications for the generalized displacement functionals

$$\mathcal{G}(\overline{\mu}) \leq \sum_{i=1}^{k} \frac{\lambda_i}{\Lambda} \mathcal{G}(\mu_i) + \frac{L_H K}{2\Lambda} \mathbb{W}(\mathbb{P}, \delta_{\overline{\mu}})^2 + \frac{L_H}{2\Lambda}(m^2 + 2m)$$

Step 1, change of variables

Denote by F_i the optimal transport map from $\overline{\mu}$ to μ_i, by $\mathrm{Jac}\, F_i$ the Jacobian of F_i.
Since $f = g(F_i)\,\mathrm{Jac}\, F_i$, $\quad \mathcal{G}(\mu_i) = \int_M H(\log f + l_i)\,\mathrm{d}\,\overline{\mu}$, where $l_i := -\log \mathrm{Jac}\, F_i$.

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Step 4, integrate and apply the Hessian equality

The Hessian equality $\sum_{i=1}^{n} \lambda_i\, \mathrm{Hess}_x\, \phi_i = 0$ implies $\sum_{i=1}^{n} \lambda_i\, \Delta\phi_i(x) = 0$.