Regularity of Wasserstein barycenters

Dissertation defense

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Application background: motivations behind Wasserstein barycenters

Barycenter (center of mass)

Barycenter z_μ averages points in a metric space (E, d) according to the probability measure μ on E, in the sense that

$$\int_E d(z_\mu, y)^2 \,\mathrm{d}\,\mu(y) = \inf_{x \in E} \int_E d(x, y)^2 \,\mathrm{d}\,\mu(y).$$

Wasserstein barycenters: averaging measures

1. $(E, d) \to (\mathcal{W}_2(E), d_W)$
2. $\mu \to \mathbb{P}$ and $z_\mu \to \mu_{\mathbb{P}}$

$\mathcal{W}_2(E)$ is the set of probability measures on E with finite second-order moments, including $\mu_{\mathbb{P}}$.

Geometric Awareness

- Structure via base metric space
- Feature-preserving after averaging: e.g. Gaussians remain Gaussian

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Example: $\mu_{\mathbb{P}}$ of $\mathbb{P} := \frac{1}{2}\delta_{\nu_1} + \frac{1}{2}\delta_{\nu_2}$

Consider the earth surface (E, d) with uniform measures ν_1, ν_2 supported on two regions.

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

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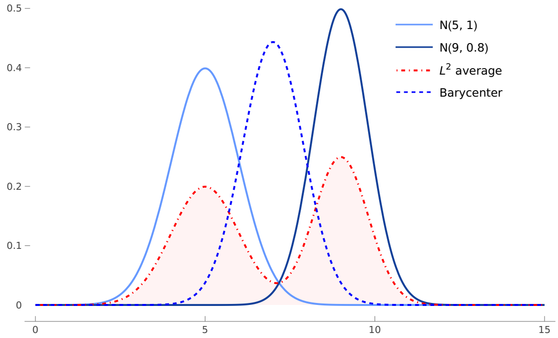
Example: averaging Gaussian data

Two sensors returning estimates $\mathcal{N}(5,1)$ and $\mathcal{N}(9,0.8)$, then averaged in two different ways.



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Absolute continuity

Singularity

Example: coloring a cat with brush or pen

Gradient with brush

hue values change continuously $\implies$ absolute continuity

Tattoo with pen

curves have zero area $\implies$ singularity

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`[Contributions of the thesis]`

1. lower Ricci curvature bound suffices
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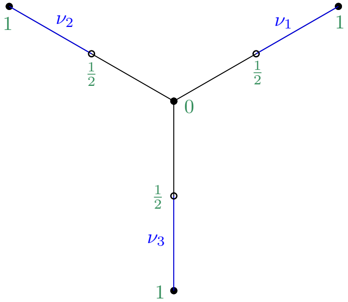

Example: singularity at the branching point

$$\mathbb{P} := \tfrac{1}{3}\delta_{\nu_1} + \tfrac{1}{3}\delta_{\nu_2} + \tfrac{1}{3}\delta_{\nu_3} \implies \mu_{\mathbb{P}} = \delta_0$$

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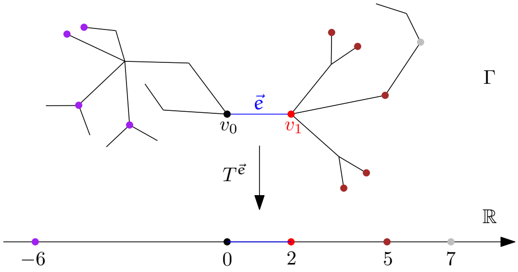

Reduction: flatten w.r.t. a fixed edge $\vec{e}$

Localization: looping over all edges

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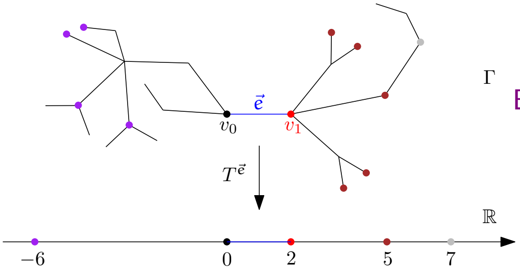

Example: being singular is a rigid property

$\mu_{\mathbb{P}} \in \mathcal{W}_2(\mathbb{R})$ is singular $\implies$ $\mathbb{P}$-almost every ν is singular

Before the thesis: known properties of Wasserstein barycenters

`proper: bounded + closed` $\implies$ `compact`

`a.c. = absolutely continuous`

Existence, uniqueness, and consistency

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Thesis result on absolute continuity of Wasserstein barycenters

[J. Ma, 2023]
Let (M, d_g) be a complete Riemannian manifold with a lower Ricci curvature bound. If a measure $\mathbb{P} \in \mathcal{W}_2(\mathcal{W}_2(M))$ assigns positive mass to the set of a.c. probability measures, then its unique barycenter $\mu_{\mathbb{P}}$ is also a.c..

Improvements compared to the previous work

[Eliminate technical assumption]
a.c. ~~with uniformly bounded density functions~~

[No obscure dependency on compactness]
confirm the impact of lower Ricci curvature bound on the regularity of barycenters

Difficulty: control $\mu_{\mathbb{P}}$ via approximation

$$\mathbb{P} = \sum_{i=1}^{n} \lambda_i \delta_{\nu_i} \implies \mu_{\mathbb{P}} \text{ can be constructed.}$$

However, when $\mathbb{P}$ is not finitely supported, its barycenter $\mu_{\mathbb{P}}$ is only accessible via consistency: as a limit of constructable barycenters $\mu_{\mathbb{P}_j}$ with $\mathbb{P}_j$ finitely supported.

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Displacement functionals defined for a.c. measures

[(M, d_{g})]: m-dimensional, with lower Ricci curvature bound 0 `(for simplicity)`.

[$\mathbb{P}$]: $\mathbb{P} = \sum_{j=1}^{n} \lambda_j \, \delta_{\nu_j}$, each $\mathrm{supp}(\nu_j)$ is compact, $\{\nu_i\}_{1 \le i \le k}$ are a.c., $\Lambda := \sum_{i=1}^{k} \lambda_i$.

[$\mathcal{G}$]: $\mathcal{G}(f \cdot \mathrm{Vol}) = \int_M G(f) \, \mathrm{d}\,\mathrm{Vol}$, G satisfies certain properties (defining $L_G > 0$).

$$\mathcal{G}(\mu_{\mathbb{P}}) \le \sum_{i=1}^{k} \frac{\lambda_i}{\Lambda} \mathcal{G}(\nu_i) + \frac{L_G}{2\Lambda}(m^2 + 2m).$$

Background: synthetic lower Ricci curvature bound 0

Consider the entropy functional Ent with $G(x) := x \log x$ and $n = k = 2$.

(M, d_{g}) has lower Ricci curvature bound 0 iff:

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According to the previous inequality

$$\mathcal{G}(\mu_{\mathbb{P}}) \leq \sum_{i=1}^{k} \frac{\lambda_i}{\Lambda} \mathcal{G}(\nu_i) + \frac{L_G}{2\Lambda}(m^2 + 2m),$$

if $\{\nu_i\}_{1 \leq i \leq k} \subset \mathrm{B}(G, L)$, then $\mu_{\mathbb{P}} \in \mathrm{B}(G, L')$.

Properties imposed on G

a. function $H(x) := e^{-x}\, G(e^x)$ has positive and continuous derivative bounded from above by L_G

b. continuous, convex, positive with $G(0) = 0$

c. $\lim_{x \to \infty} \frac{G(x)}{x} = +\infty$

d. increasing

Bound $\mathcal{G}$ in approximation

$\Downarrow$

$\mu_{\mathbb{P}}$ belongs to some $\mathrm{B}(G, L')$ set and is thus is a.c..

Compactness in $\sigma(L^1, L^\infty)$

$\Downarrow$

$\Longleftarrow$ $\mathbb{P}$ assigns positive mass to a $\mathrm{B}(G, L)$ set.

Souslin space theory

$\Downarrow$

$\Longleftarrow$ $\mathbb{P}$ assigns positive mass to a compact set F w.r.t. $\sigma(L^1, L^\infty)$.

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$$\mathcal{G}(\mu_{\mathbb{P}}) \leq \sum_{i=1}^{k} \frac{\lambda_i}{\Lambda} \mathcal{G}(\nu_i) + \frac{L_G}{2\Lambda}(m^2 + 2m),$$

if $\{\nu_i\}_{1 \leq i \leq k} \subset \mathrm{B}(G, L)$, then $\mu_{\mathbb{P}} \in \mathrm{B}(G, L')$.

Properties imposed on G

a. function $H(x) := e^{-x}\, G(e^x)$ has positive and continuous derivative bounded from above by L_G

b. continuous, convex, positive with $G(0) = 0$

c. $\lim_{x \to \infty} \frac{G(x)}{x} = +\infty$

d. increasing

Bound $\mathcal{G}$ in approximation		Compactness in $\sigma(L^1, L^\infty)$		Souslin space theory
$\Downarrow$		$\Downarrow$		$\Downarrow$
$\mu_{\mathbb{P}}$ belongs to some $\mathrm{B}(G, L')$ set and is thus is a.c..	$\Longleftarrow$	$\mathbb{P}$ assigns positive mass to a $\mathrm{B}(G, L)$ set.	$\Longleftarrow$	$\mathbb{P}$ assigns positive mass to a compact set F w.r.t. $\sigma(L^1, L^\infty)$.

Three steps to prove $\mathbb{P}(\text{a.c. measures}) > 0 \implies \mu_{\mathbb{P}}$ is a.c.

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Bound $\mathcal{G}$ in approximation

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Compactness in $\sigma(L^1, L^\infty)$

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`Dunford-Pettis theorem`

`de la Vallée Poussin criterion`

If F is weakly compact, then it is uniformly integrable, and thus contained in a $\mathrm{B}(G, L)$ set.

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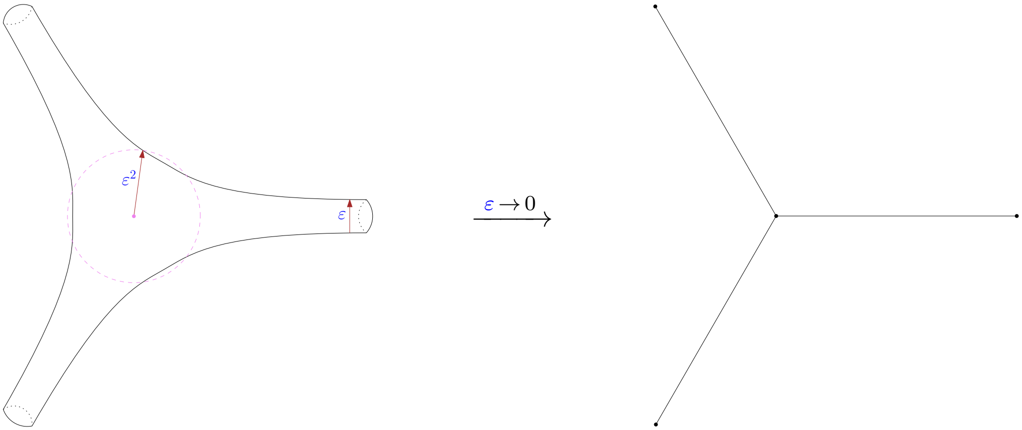
Souslin space theory

$\mathbb{P}$ is a Radon measure w.r.t. the $\sigma(L^1, L^\infty)$ topology.

Shifting focus: manifolds $\longrightarrow$ metric trees



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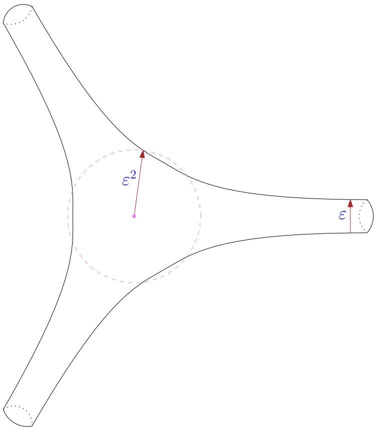
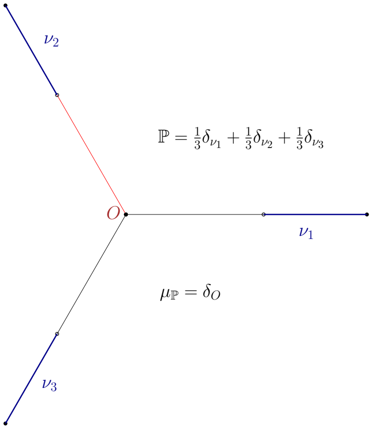
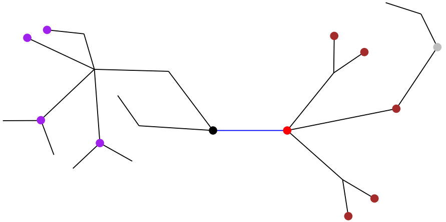


$\xrightarrow{\varepsilon \to 0}$



Reduction Technique: flatten the tree to solve optimal transport problems



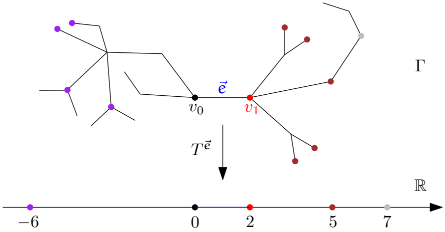
[Metric tree $\Gamma = (\mathcal{V}, \mathcal{E}, d_l)$]

Metric d_l is induced by length function $l : \mathcal{E} \to \mathbb{R}$.

Γ is a proper and geodesic metric space.

Reduction Technique: flatten the tree to solve optimal transport problems

Reduction map $T^{\vec{e}} : \Gamma \to \mathbb{R}$ associated to $\vec{e}$



[Flatten via the reduction map $T^{\vec{e}}$]

$T^{\vec{e}}$ is continuous. $T^{\vec{e}}(\vec{e}) = [0, l(\vec{e})]$.

For $x \in \vec{e}, y \in \Gamma$, $d_l(x, y) = |\,T^{\vec{e}}(x) - T^{\vec{e}}(y)|$.

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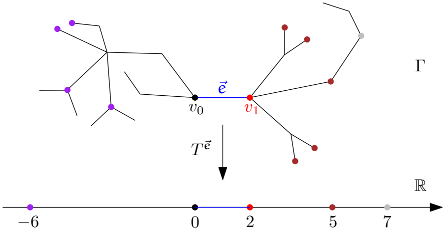

Reduction preserves Wasserstein distances

For $\mu, \nu \in \mathcal{W}_2(\Gamma)$, if $\mathrm{supp}(\mu) \subset \vec{e}$, then

$$d_W(\mu, \nu) = d_W(\mathcal{T}(\mu), \mathcal{T}(\nu)),$$

where $\mathcal{T} : \mathcal{W}_2(\Gamma) \to \mathcal{W}_2(\mathbb{R})$ is the induced push-forward map: $\mathcal{T}(\mu) := T^{\vec{e}}{}_{\#}\mu$.

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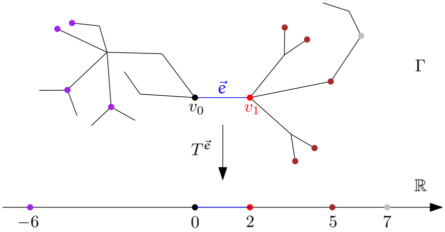

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Idea of its proof: recover optimal transports between from $\mathbb{R}$ to Γ via $\nu = \sum_{e \in \mathcal{E}} \lambda_e \nu_e$.

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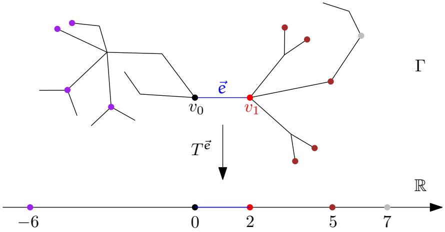

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Properties: 1. $\mathcal{T}(\nu)$ is a.c. $\Leftrightarrow$ ν is a.c.;
2. if $\mathcal{T}(\nu)$ is singular, then so is ν.

Localization Technique: extending known results of barycenters

Restriction property of Wasserstein barycenters

Assume the base metric space (E, d) is proper.
For any decomposition of a given barycenter

$$\mu_{\mathbb{P}} = \lambda\, \mu^1 + (1-\lambda)\mu^2,$$

there exist continuous maps F^i such that

1. $\lambda\, F^1(\nu) + (1-\lambda)F^2(\nu) = \nu$;
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`[Preserved properties of` $\mathbb{P}$`]`

For any reference measure η on E, if $\mathbb{P}$ assigns full (or positive) mass to measures a.c. w.r.t. η, then so do the measures $\mathbb{Q}^1$ and $\mathbb{Q}^2$.

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A lemma using reduction technique

Fix an oriented edge $\vec{e}$ of a metric tree Γ.
If a barycenter $\mu_{\mathbb{P}}(\mathring{e}) = 1$, then $\mathcal{T}(\mu_{\mathbb{P}})$ is the unique barycenter of $\mathcal{T}_{\#}\mathbb{P}$.

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Application: almost absolute continuity on Γ

If $\mathbb{P}(\text{a.c. measures}) > 0$, then $\mu_{\mathbb{P}}|_{\mathring{e}}$ is a.c. for any barycenter $\mu_{\mathbb{P}}$ and any edge $\vec{e}$.

Therefore, if $\mu_{\mathbb{P}}$ is not a.c., then its singular part is a sum of Dirac measures at vertices.

Wasserstein barycenters on $\mathbb{R}$: rigid properties

Rigid properties of barycenters on $\mathbb{R}$

A measure property $\mathcal{Q}$ is *rigid* if

$\mu_{\mathbb{P}}$ satisfies $\mathcal{Q} \implies \mathbb{P}$-almost every ν satisfies $\mathcal{Q}$.

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Properties proven to be rigid

a. being not a.c.
b. having compact support
c. being a Dirac measure
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[Quantile functions]

1. For $0 < t < 1$, f_μ^{-1} is defined by

$$f_\mu^{-1}(t) := \inf_x \{x \in \mathbb{R} \mid f_\mu(x) > t\}.$$

2. $f_\mu^{-1}(0)$, $f_\mu^{-1}(1)$: defined as one-sided limits.

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$$f_{\mu}^{-1}(0) = \inf \operatorname{supp}(\mu)$$
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$$\mu = \delta_x \iff f_\mu^{-1} \equiv x$$

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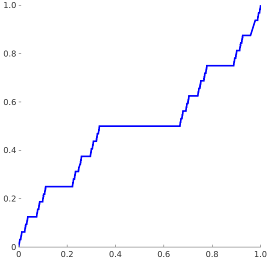

$$\mathrm{ArcLength}(f_\mu) = \|\operatorname{Leb}^1|_{[0,1]} + \mathrm{i}\,\mu\|_{\mathrm{TV}} = 2$$

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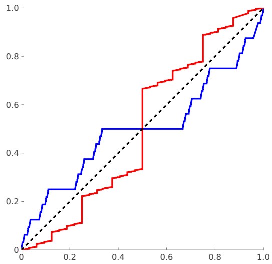

$\mathrm{ArcLength}(f_\mu) = 2 = \mathrm{ArcLength}(f_\mu^{-1})$

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[Quantile functions]

f_{μ}^{-1} is singular iff

$$V_0^1\left(f_{\mu}^{-1} - \mathrm{Id}\right) = V_0^1\left(f_{\mu}^{-1} + \mathrm{Id}\right).$$

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Explicit formula for barycenters

$$f_{\mu_{\mathbb{P}}}^{-1}(t) = \int_{\mathcal{W}_2(\mathbb{R})} f_\nu^{-1}(t)\,\mathrm{d}\,\mathbb{P}(\nu)$$

[Quantile functions]

f_μ^{-1} is singular iff

$$V_0^1\left(f_\mu^{-1} - \mathrm{Id}\right) = V_0^1\left(f_\mu^{-1} + \mathrm{Id}\right).$$

Properties proven to be rigid

a. being not a.c.

b. having compact support

c. being a Dirac measure

d. being singular

e. being supported in a negligible set

$$\begin{aligned} V_0^1\left(f_{\mu_{\mathbb{P}}}^{-1} - \mathrm{Id}\right) &\le \int_{\mathcal{W}_2(\mathbb{R})} V_0^1\left(f_\nu^{-1} - \mathrm{Id}\right)\mathrm{d}\,\mathbb{P}(\nu) \\ &\le \int_{\mathcal{W}_2(\mathbb{R})} V_0^1\left(f_\nu^{-1}\right) + V_0^1\left(\mathrm{Id}\right)\mathrm{d}\,\mathbb{P}(\nu) \end{aligned}$$

Wasserstein barycenters on $\mathbb{R}$: rigid properties

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&\leq \int_{\mathcal{W}_2(\mathbb{R})} V_0^1\left(f_\nu^{-1}\right) + V_0^1\left(\mathrm{Id}\right)\mathrm{d}\,\mathbb{P}(\nu) \\
&= \int_{\mathcal{W}_2(\mathbb{R})} f_\nu^{-1}(1) - f_\nu^{-1}(0) + 1\,\mathrm{d}\,\mathbb{P}(\nu) \\
&= f_{\mu_{\mathbb{P}}}^{-1}(1) - f_{\mu_{\mathbb{P}}}^{-1}(0) + 1 \\
&= V_0^1\left(f_{\mu_{\mathbb{P}}}^{-1} + \mathrm{Id}\right)
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Future research directions

1. Extending displacement functional arguments to metric measure spaces
2. Quantitative estimates for barycenter densities

3. Necessity of curvature bounds and the role of branching
4. Generalizing reduction techniques to metric graphs

Example: non-uniqueness of Wasserstein barycenters on metric trees