Linearization of the Wasserstein space & quantitative stability of optimal transport maps

Frédéric Chazal Alex Delalande Quentin Mérigot



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

p-Wasserstein distance between $\mu, \nu \in \operatorname{Prob}_p(\mathbb{R}^d)$: $W_p(\mu, \nu) = \left(\min_{\gamma \in \Gamma(\mu, \nu)} \|x - y\|^p \, \mathrm{d} \, \gamma(x, y)\right)^{1/p}.$ where $\Gamma(\mu, \nu) = \text{couplings between } \mu \text{ and } \nu \subseteq \operatorname{Prob}(\mathbb{R}^d \times \mathbb{R}^d).$

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but also: *k*-means algorithm, principal component analysis, etc. 3 - 6

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

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No such isometric embedding in higher dimension: $(Prob_p, W_p)$ is *curved*.

Proposition: The W₂ barycenter of $\mu_1, \ldots, \mu_N \in \operatorname{Prob}_2(\mathbb{R})$ and $\alpha_1, \ldots, \alpha_N \geq 0$ is

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Example: If $\mu_i = \frac{1}{N} \sum_j \delta_{x_i^j}$, with $x_i^1 \leq \ldots \leq x_i^N$ and $\alpha_i \geq 0$, the W₂ barycenter is

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In 1D, computing a W_2 barycenter between empirical measures \iff sorting the positions of the Dirac masses + averaging !

2. Linearized Wasserstein distance

[Wang, Slepcev, Basu, Ozolek, Rohde '13]

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- > T_{μ} is unique ρ -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: $\rho =$ 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



"Monge-Kantorovich depth of y_i " $\simeq ||T_{\mu}^{-1}(y_i)||$.

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Motivation 2: $\mu \mapsto T_{\mu} - \mathrm{id}$ as a logarithm









	Riemannian geometry	Optimal transport
point	$x \in M$	$\mu \in \operatorname{Prob}_2(\mathbb{R}^d)$
geodesic distance	$d_g(x,y)$	$\mathrm{W}_2(\mu, u)$
tangent space	$T_{ ho}M$	$\mathrm{T}_{\rho}\mathrm{Prob}_{2}(\mathbb{R}^{d}) \subseteq \mathrm{L}^{2}(\rho, X)$
exponential map	$\exp_{\rho} : \mathrm{T}_{\rho}M \to M$	$v \in \mathcal{T}_{\rho} \operatorname{Prob}_2(\mathbb{R}^d) \mapsto (\operatorname{id} + v)_{\neq}$
inverse exponential map	$\exp_{\rho}^{-1}(x) \in \mathcal{T}_{\rho}M$	$T_{\mu} - \mathrm{id} \in \mathrm{T}_{\rho}\mathrm{Prob}_2(X)$
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The map $\mu \in \operatorname{Prob}_2(\mathbb{R}^d) \to T_\mu \in L^2(X)$ is an injective map, with image the space of (square-integrable) gradients of convex functions on X.

Linearized OT framework \longrightarrow [Wang, Slepcev, Basu, Ozolek, Rohde '13]



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geodesic distance	$\mathrm{d}_g(x,y)$	$W_2(\mu, u)$
tangent space	$T_{ ho}M$	$\mathrm{T}_{\rho}\mathrm{Prob}_{2}(\mathbb{R}^{d}) \subseteq \mathrm{L}^{2}(\rho, X)$
exponential map	$\exp_{\rho} : \mathrm{T}_{\rho}M \to M$	$v \in \mathcal{T}_{\rho} \operatorname{Prob}_2(\mathbb{R}^d) \mapsto (\operatorname{id} + v)_{\neq}$
inverse exponential map	$\exp_{\rho}^{-1}(x) \in \mathcal{T}_{\rho}M$	$T_{\mu} - \mathrm{id} \in \mathrm{T}_{\rho}\mathrm{Prob}_2(X)$
distance in tangent space	$\ \exp_{\rho}^{-1}(x) - \exp_{\rho}^{-1}(y) \ _{g(x_0)}$	$ T_{\mu} - T_{\nu} _{\mathrm{L}^{2}(\rho)}$

The map $\mu \in \operatorname{Prob}_2(\mathbb{R}^d) \to T_\mu \in L^2(X)$ is an injective map, with image the space of (square-integrable) gradients of convex functions on X.

■ Linearized OT framework \longrightarrow [Wang, Slepcev, Basu, Ozolek, Rohde '13] ■ W_{2,ρ}(μ, ν) := $||T_{\mu} - T_{\nu}||_{L^{2}(\rho)} \longrightarrow$ [Ambrosio, Gigli, Savaré '04]



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Geometric embedding of $\operatorname{Prob}_2(\mathbb{R}^d)$ into the Hilbert space $L^2(\rho, \mathbb{R}^d)$.

Example: barycenter computation

► Barycenter in Wasserstein space: $\mu_1, \ldots, \mu_k \in \operatorname{Prob}_2(\mathbb{R}^d)$, $\alpha_1, \ldots, \alpha_k \ge 0$: $\mu := \arg \min_{1 \le i \le k} \sum_{1 \le i \le k} \alpha_i \operatorname{W}_2^2(\mu, \mu_i).$

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

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We run the K-Means method on the transport plans, with K = 20. Each cluster $X^k \subseteq \{0, \dots, M\}$ yields an *average transport plan* $S^k = \frac{1}{|X^k|} \sum_{\ell \in X} T^\ell$,

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2. Known properties of $\mu \mapsto T_{\mu}$.

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► The map $\mu \mapsto T_{\mu}$ is not better than $\frac{1}{2}$ -Hölder. Take $\rho = \frac{1}{\pi} \text{Leb}_{B(0,1)}$ on \mathbb{R}^2 , and let $\mu_{\theta} = \frac{1}{2}(\delta_{x_{\theta}} + \delta_{x_{\theta+\pi}})$, with $x_{\theta} = (\cos(\theta), \sin(\theta))$. Then $T_{\mu_{\theta}}(x) = \begin{cases} x_{\theta} & \langle x_{\theta} | x \rangle \ge 0 \\ x_{\theta+\pi} & \text{if not} \end{cases}$, so that $\|T_{\mu_{\theta}} - T_{\mu_{\theta+\delta}}\|_{L^{2}(\rho)}^{2} \ge C\delta$ Since on the other hand, $W_2(\mu_{\theta}, \mu_{\theta+\delta}) \leq C\delta$, x_{θ} $\|T_{\mu_{\theta}} - T_{\mu_{\theta+\delta}}\|_{\mathrm{L}^{2}(\rho)} \geq C \operatorname{W}_{2}(\mu_{\theta}, \mu_{\theta+\delta})^{1/2}$ $x_{\theta+\pi}$ 13 - 6

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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- > The hypothesis that T_{μ} is Lipschitz is practically restricting:
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 - 2) it can be proven only under very strong conditions on the data:
 - e.g. if ρ, μ are absolutely continuous on smooth uniformly convex sets, with C^{α} densities bounded from above and below, then T_{μ} is $C^{1,\alpha}$.

Theorem (Berman '18): Assume that ρ is the Lebesgue measure on X, and $\mu, \nu \in \operatorname{Prob}(Y)$ with X convex compact and Y compact. Then,

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▶ By [Andoni, Naor, Neiman '18], the space (Prob₂(ℝ^d), W₂) does not admit a bi-Hölder embedding into any L^p space when d ≥ 3.

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

Thm: Let X be convex compact and ρ a density on X with $\|\log(\rho)\|_{\infty} < +\infty$ Let Y be compact. Then, $\forall \mu, \nu \in \operatorname{Prob}(Y), \|T_{\mu} - T_{\nu}\|_{L^{2}(X)} \leq C \operatorname{W}_{2}(\mu, \nu)^{1/6}.$

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► 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.

Semidiscrete OT for $c(x, y) = -\langle x | y \rangle$

• Let $\rho, \nu \in \operatorname{Prob}_1^{\operatorname{ac}}(\mathbb{R}^d)$ and $\Gamma(\rho, \mu) = \operatorname{couplings}$ between ρ, μ ,

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$$\mathsf{Legendre-Fenchel transform:}$$

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• Let $\mu = \sum_{1 \le i \le N} \mu_i \delta_{y_i}$ and $\psi_i = \psi(y_i)$. Then, $\psi^*|_{V_i(\psi)} := \langle \cdot | y_i \rangle - \psi_i$ where $V_i(\psi) = \{x \mid \forall j, \ \langle x | y_i \rangle - \psi_i \ge \langle x | y_j \rangle - \psi_j\}$





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• Let $\mu = \sum_{1 \le i \le N} \mu_i \delta_{y_i}$ and $\psi_i = \psi(y_i)$. Then, $\psi^*|_{V_i(\psi)} := \langle \cdot | y_i \rangle - \psi_i$ where $V_i(\psi) = \{x \mid \forall j, \ \langle x | y_i \rangle - \psi_i \ge \langle x | y_j \rangle - \psi_j\}$



18 - 6 Thus, $\mathcal{T}(\rho,\mu) = \min_{\psi \in \mathbb{R}^N} \sum_i \int_{V_i(\psi)} \langle x | y_i \rangle - \psi_i \, \mathrm{d} \, \rho(x) + \sum_i \mu_i \psi_i$

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Hölder-stability of optimal transport maps \simeq strong concavity of Φ .

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

• Consider the matrix $L = DG(\psi)$ and the graph H:

$$(i,j) \in \mathbf{H} \iff L_{ij} > 0$$

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Thm: Let X be convex compact and ρ a density on X with $\|\log(\rho)\|_{\infty} < +\infty$ Let Y be compact. Then, $\forall \mu, \nu \in \operatorname{Prob}(Y), \|T_{\mu} - T_{\nu}\|_{L^{2}(X)} \leq C \operatorname{W}_{2}(\mu, \nu)^{1/6}.$

[M., Delalande, Chazal '19; Delalande, M. '21]

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Combining a) and b) we get $\|\psi^1 - \psi^0\|_{L^2(\mu^0)}^2 \lesssim |\langle \mu^1 - \mu^0 | \psi^1 - \psi^0 \rangle|$

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b) Control of μ_t : Brunn-Minkowski's inequality implies $\mu^t \ge (1-t)^d \mu^0$. Combining a) and b) we get $\|\psi^1 - \psi^0\|_{L^2(\mu^0)}^2 \le |\langle \mu^1 - \mu^0 | \psi^1 - \psi^0 \rangle|$ (Kantorovich-Rubinstein) $\le \operatorname{Lip}(\psi^1 - \psi^0) \operatorname{W}_1(\mu^0, \mu_1)$

Thm: Let X be convex compact and ρ a density on X with $\|\log(\rho)\|_{\infty} < +\infty$ Let Y be compact. Then, $\forall \mu, \nu \in \operatorname{Prob}(Y), \|T_{\mu} - T_{\nu}\|_{L^{2}(X)} \leq C \operatorname{W}_{2}(\mu, \nu)^{1/6}.$

[M., Delalande, Chazal '19; Delalande, M. '21]

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► We lose a little in the exponent to control the difference between OT maps... 21 - 9

Theorem Let $\mu^0, \mu^1 \in \operatorname{Prob}_2(\mathbb{R}^d)$, ϕ^k the Brenier potential from $\rho \in \operatorname{Prob}^{\operatorname{ac}}(X)$ to μ^k , where X is convex and ρ is bounded from above and below. Assume that (i) $\forall k \in \{0,1\}, \forall x, y \in X, |\phi^k(x) - \phi^k(y)| \leq C_H ||x - y||^{\alpha}$ (ii) $M_4(\mu^k) \leq M$.

Then, $W_2(\mu^0, \mu^1) \le ||T_{\mu^1} - T_{\mu^0}||_{L^2(\rho)} \le C(d, X, \rho, C_H, M) W_1(\mu^0, \mu^1)^{\frac{1}{2(11-8\alpha)}}$.

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- ▶ When $\alpha = 1$, we recover the exponent of the compact case: $2(11 8\alpha) = 6$.
- ► By Morrey's inequality, (i) holds when $M_p(\mu^k) < +\infty$ for p > d. Indeed, $M_p(\mu^k) = \int \|y\|^p \,\mathrm{d}\,\mu^k(y) = \int \|\nabla\phi^k\|^p \,\mathrm{d}\,\rho < +\infty \Longrightarrow \phi^k \in W^{1,p}(X) \subseteq \mathcal{C}^{1-\frac{d}{p}}(X)$

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 In particular, this result applies to sub-exponential or sub-Gaussian measures.
- ▶ By [Andoni, Naor, Neiman '18], the space $(\operatorname{Prob}_2(\mathbb{R}^d), W_2)$ does not admit a bi-Hölder embedding into any L^p space when $d \ge 3$.

Summary

Optimal transport plans can be used to embed of $\operatorname{Prob}_2(\mathbb{R}^d)$ into $L^2(\rho, \mathbb{R}^d)$, while preserving some of its metric geometry, with applications in data analysis.

https://github.com/sd-ot

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Open questions/current work:

- ▶ optimal Hölder exponent for $\mu \mapsto T_{\mu}$ in the compact case?
- what happens for other cost functions?
- ► is there a bi-Hölder embedding of $\{\mu \in \operatorname{Prob}_2(\mathbb{R}^d) \mid M_2(\mu) \leq R\}$ into $L^2(\rho)$?

Thank you for your attention!