

Statistical and algorithmic aspects of optimal quantization and sparse Wasserstein barycenters

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Example 1: Optimal quantization

μ
(Target Measure)

$$\frac{1}{N} \sum_{k=1}^N \delta_{y_k}$$

ν

$$\sum_{k=1}^N \pi_k \delta_{y_k}$$

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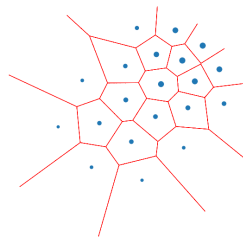
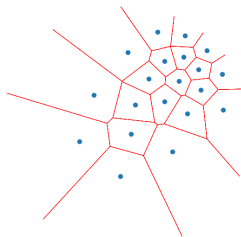
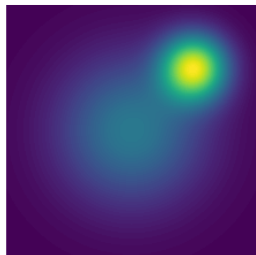


Figure: Optimal and uniform quantization of a Gaussian mixture

Simulations made using the library PyMongeAmpere by Quentin Mérigot.

Example 2: Empirical sparse Wasserstein barycenter

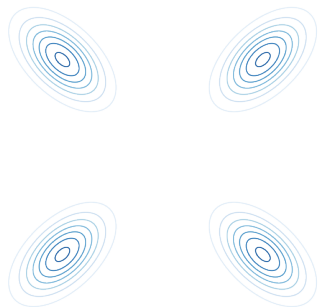


Figure: Wasserstein barycenter and its sample average approximation

Simulations made using the POT Library.

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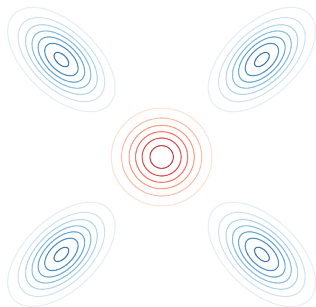


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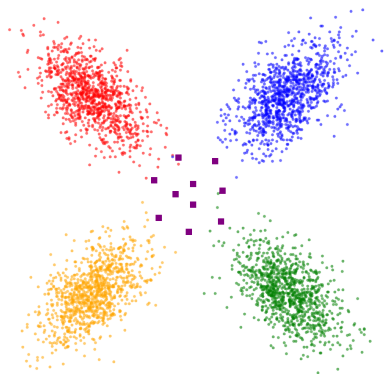
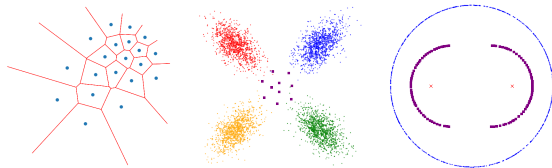


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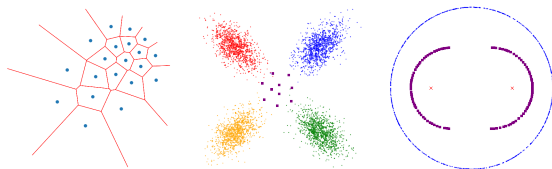
Example 3: Wasserstein geodesics

Connection between these examples



What do all these examples have in common?

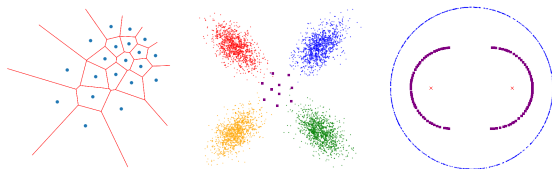
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They are all instances of problems of optimization of point clouds (seen as **probability measures**) and/or their probability weights.

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specifically, these examples aim at solving

$$\min_{(Y, \pi) \in A} \frac{1}{L} \sum_{\ell=1}^L \mathbb{D} \left(\mu^\ell, \sum_{i=1}^N \pi_i \delta_{y_i} \right)$$

where μ^1, \dots, μ^L are a collection of probability measures, A is a closed, non-empty subset of $(\mathbb{R}^d)^N \times \Delta_N$ and \mathbb{D} is a divergence between measures.

- Define a good notion of metric between arbitrary measures (**discrete** or **continuous**)

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- Study interesting sub cases of

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In particular

- 1 Algorithmic properties
- 2 Statistical properties.

Optimal transport

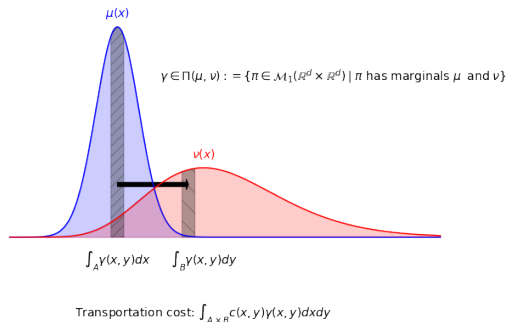
Optimal transport measures the minimal cost of transporting the target measure μ onto ν with **couplings** γ , according to a cost $c : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$.

$$\text{OT}_c(\mu, \nu) = \inf_{\gamma \in \Pi(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\gamma(x, y).$$

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Kantorovich duality:

$$\begin{aligned} \text{OT}_c(\mu, \nu) &= \inf_{\gamma \in \Pi(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\gamma(x, y) \\ &= \sup_{\substack{\varphi, \psi \in \mathcal{C}(\mathbb{R}^d) \\ \varphi \oplus \psi \leq c}} \int_{\mathbb{R}^d} \varphi d\mu + \int_{\mathbb{R}^d} \psi d\nu. \end{aligned}$$

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c-transform: $\varphi^c(x) := \inf_{y \in \mathbb{R}^d} c(x, y) - \psi(y).$

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c-transform: $\varphi^c(x) := \inf_{y \in \mathbb{R}^d} c(x, y) - \psi(y)$. Constraint $\varphi \oplus \psi \leq c$ is thus equivalent to $\psi \leq \varphi^c$.

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The quadratic cost

If $c(x, y) := \|x - y\|^p$, $p \geq 1$ then $W_p(\mu, \nu) := \text{OT}_c(\mu, \nu)^{1/p}$ is a **distance** over the probability space $\mathcal{M}_1(\mathbb{R}^d)$ called the **Wasserstein distance**.

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Moreover, if μ has density, then by Brenier's Theorem there exists a mapping $T: \mathbb{R}^d \rightarrow \mathbb{R}^d$ such that

$$\begin{aligned}\text{OT}_c(\mu, \nu) &= W_p^p(\mu, \nu) \\ &= \int_{\mathbb{R}^d} \|x - T(x)\|^p d\mu(x)\end{aligned}$$

T is called the **optimal transport map**.

The semi discrete setting

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where

$$L_i^c(Y, \varphi^*) = \{x \in \mathbb{R}^d \mid c(x, y_i) - \varphi_i^* \leq c(x, y_j) - \varphi_j^*, j \neq i\}.$$

The semi discrete setting

If $c(x, y) = \|x - y\|^p$, the power cells form a convex tessellation of \mathbb{R}^d and define the OT map $T = \sum_{i=1}^N y_i \mathbf{1}_{L_i(Y, \varphi^*)}$.

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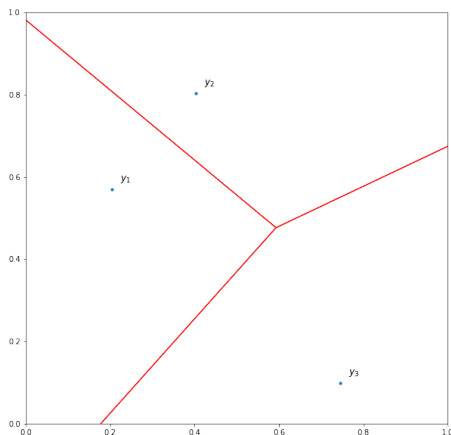


Figure: Example of semi-discrete OT between $\mu \sim \mathcal{U}_{[0,1]^2}$ and $\frac{1}{3}(\delta_{y_1} + \delta_{y_2} + \delta_{y_3})$.

Entropic Optimal transport

$$W_{\epsilon,p}(\mu, \nu) = \inf_{\gamma \in \Pi(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^p d\gamma(x, y) + \epsilon \text{KL}(\gamma, \mu \otimes \nu)$$

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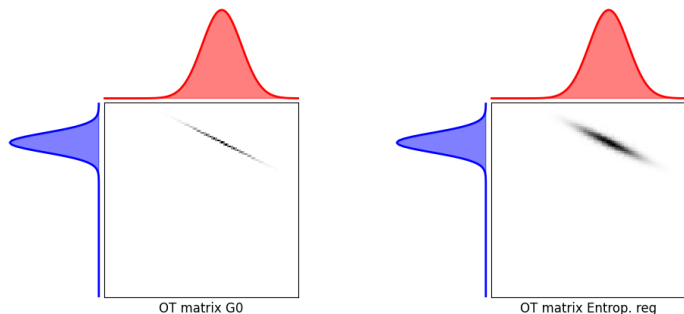


Figure: POT library example of a $W_{\epsilon,2}$ -transport plan

Wider because it penalizes couplings too far from the product measure

Sliced optimal transport

1-D optimal transport: if $\mu, \nu \in \mathcal{M}_1(\mathbb{R})$:

$$W_p^p(\mu, \nu) = \int_0^1 |F_\mu^{-1}(t) - F_\nu^{-1}(t)|^p dt$$

where F_α^{-1} denotes the **generalized inverse** of the c.d.f of α .

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$$SW_p^p(\mu, \nu) = \int_{\mathbb{S}^{d-1}} W_p^p(P_\theta \# \mu, P_\theta \# \nu) d\sigma(\theta), \sigma \sim \mathcal{U}_{\mathbb{S}^{d-1}}$$

$$\max\text{-}SW_p^p(\mu, \nu) = \max_{\theta \in \mathbb{S}^{d-1}} W_p^p(P_\theta \# \mu, P_\theta \# \nu).$$

Our object of study

Let $\mu^1, \dots, \mu^L \in \mathcal{M}_1(\mathbb{R}^d)$, we study

$$\min_{(Y, \pi) \in A} F_{\mathbb{D}} \left(\mu^1, \dots, \mu^L, \sum_{i=1}^N \pi_i \delta_{y_i} \right) := \frac{1}{L} \sum_{\ell=1}^L \mathbb{D} \left(\mu^\ell, \sum_{i=1}^N \pi_i \delta_{y_i} \right).$$

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A	$L = 1$	$L > 1$
$(\mathbb{R}^d)^N \times \Delta_N$	Optimal quantization	OT barycenter with sparse support
$(\mathbb{R}^d)^N \times \{\bar{\pi}\}$	Constrained quantization	Free support OT barycenter
$\{\bar{Y}\} \times \Delta_N$	-	Fixed support OT barycenter

The objective function

Focus on $\mathbb{D} = \mathcal{W}_p^p$ and $L = 1$

$$(Y, \pi) \mapsto \sup_{w \in \mathbb{R}^N} \int_{\mathbb{R}^d} \|x - y_i\|^p - w_i d\mu(x) + \sum_{i=1}^N w_i \pi_i$$

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In this section we provide such guarantees.

Uniform and optimal quantization

$$\min_{Y:=(y_1,\dots,y_N)} \frac{1}{2} W_2^2 \left(\mu, \frac{1}{N} \sum_{i=1}^N \delta_{y_i} \right) = \min_{Y:=(y_1,\dots,y_N)} F_N(Y)$$

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(Optimal Quantization)

Voronoi and Laguerre tessellation

- i'th Voronoi cell:

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Lloyd's algorithm¹: two equivalent formulations

Can be described in two ways

- 1 Choose an initial points cloud Y .

¹Lloyd, Stuart P. Least squares quantization in PCM, 1982.

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Which translates to

- UQ:

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Lloyd's algorithm¹: two equivalent formulations

Can be described in two ways

- 1 Choose an initial points cloud Y .
- 2 Construct either a Voronoï (OQ) or a Laguerre tessellation (UQ) of the support of μ .
- 3 Set the new points cloud as the barycenters of every cell.

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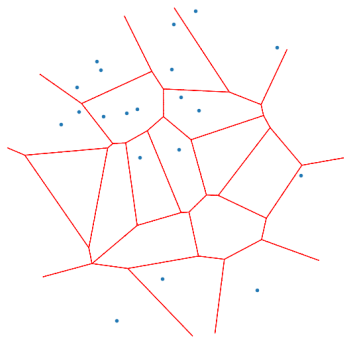
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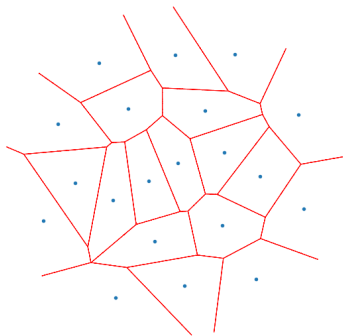
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Lloyd's algorithm for (Uniform Quantization): an example with $\mu \sim \mathcal{N}_{\mathbb{S}^1}(0_2, \sigma^2 I_2)$



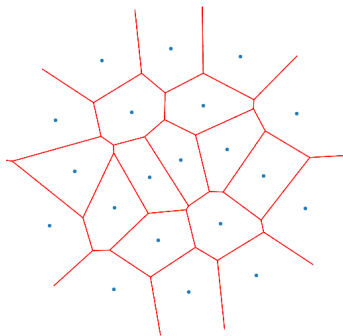
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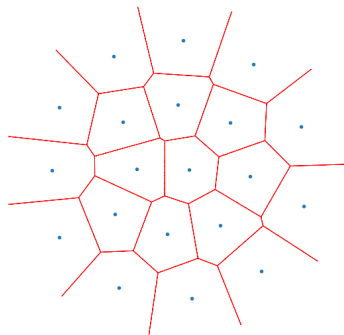
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Uniform Quantization

$$F_N(Y) = \max_{w \in \mathbb{R}^N} \frac{1}{2} \left\{ \int_{\mathbb{R}^d} (\min_{i=1, \dots, N} \|x - y_i\|^2 - w_i) f(x) dx + \frac{1}{N} \sum_{i=1}^N w_i \right\}$$

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Question:

What about $(Y_n)_{n \geq 1}$ and $(Z_n)_{n \geq 1}$?

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Remark

Convexity of $\text{Supp}(\mu)$ is not necessary for uniform quantization.

Convergence of gradient schemes in non-convex setting

- F_N and G_N both non convex.

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Kurdyka-Lojasiewicz Inequality

f verifies a KL inequality at x^* if there exists a neighborhood U of x^* , $c > 0$, $\eta > 0$ and a strictly increasing positive function $\Psi : [0, \eta[\rightarrow \mathbb{R}$ such that:

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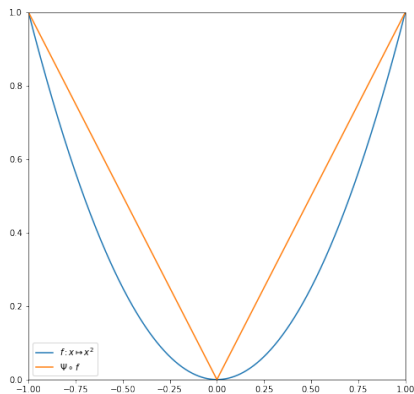
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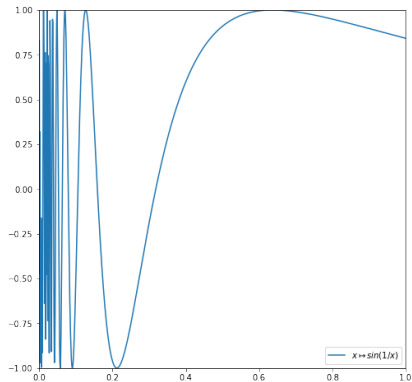
A function whose differential goes to zero can have infinitely many oscillations as it goes to 0. The KL property prevents that from happening.

KL inequality

A case where the function is KL... and another one where it is not (at 0).



$$f: x \mapsto x^2, \quad \Psi: x \mapsto \sqrt{|x|}$$



$$g: x \mapsto \sin 1/x.$$

Strong descent conditions

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A (very quick) overview on o-minimality

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Think of it as analytic functions restricted to a semi-algebraic compact subset

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Let μ be a continuous probability measure supported on a compact and convex subset of \mathbb{R}^d . Suppose its density is *globally subanalytic*. Then the iterates of Lloyd for both uniform and optimal quantization converge.

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Sparse optimal transport barycenters

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Empirical risk minimization:

For a general loss function L

$$\begin{aligned} \mathbb{E} \left[L(f_n(X)) - \min_{f \in \mathcal{F}} \mathbb{E}[L(f(X))] \right] &\leq 2 \mathbb{E} \left[\sup_{f \in \mathcal{F}} | \mathbb{P}_n L(f) - \mathbb{E}[L(f(X))] | \right] \\ &\lesssim \frac{\mathcal{C}(n)}{\sqrt{n}} \end{aligned}$$

where f_n is a minimizer of $\mathbb{P}_n L(f)$ and $\mathcal{C}(n)$ is a **measure of complexity** (Rademacher, VC dimension, log-entropy, ...)

The K-means as an empirical risk minimization scheme

It was shown¹⁰ that empirical optimal quantization (or **K-means**) behaves as

$$\mathbb{E} \left[D_2(\mu, Y_n) - \min_{Y \in \mathbb{B}_d(0,R)^N} D_2(\mu, Y) \right] \lesssim \sqrt{\frac{N \log(N)}{n}}$$

where $D_2(\mu, Y) = \int_{\mathbb{R}^d} \min_{i=1, \dots, N} \|x - y_i\|^2 d\mu(x)$.

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Question:

Does this result also hold for the more general problem

$$\min_{(Y, \pi) \in A} \frac{1}{L} \sum_{l=1}^L \mathbb{D} \left(\mu^l, \sum_{i=1}^N \pi_i \delta_{y_i} \right) \quad A \subset (\mathbb{R}^d)^N \times \Delta_N ?$$

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Let $\nu_n^* := \sum_{i=1}^N \pi_i^n \delta_{y_i^n}$ be a minimizer of $F_{\mathbb{D}}(\mu_n^1, \dots, \mu_n^L, \nu)$ over $A \subset (\mathbb{R}^d)^N \times \Delta_N$. Then

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Tightness of the bound

Lemma (Bartlett et.al, 2002)

Let $\mathbb{D} = W_2^2$, $n \in \mathbb{N}^*$ and $R > 0$. For any $N \in \mathbb{N}^*$ there exists $\mu \in \mathcal{M}_1(\mathbb{R}^d)$ and $\pi \in \Delta_N$ such that

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- Our bound is min-max optimal in n .
- But not optimal in N (depends heavily on the target measures).

Illustration of the convergence

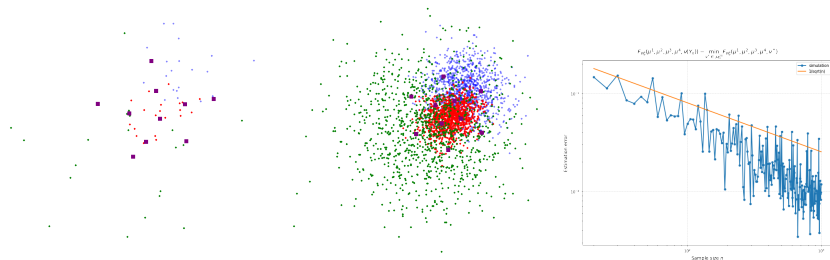


Figure: Empirical barycenter with increasing sample size.

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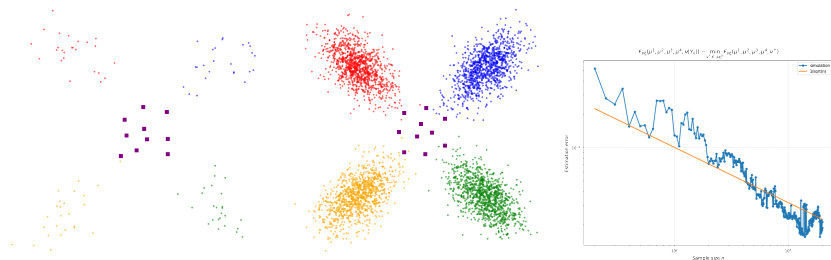


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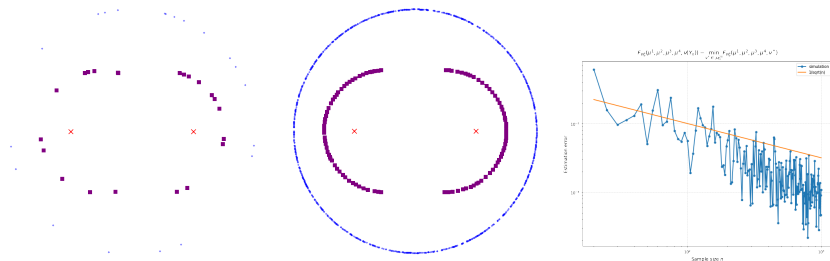


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Sketch of proof: generalization error

- Let $\nu_n^* := \sum_{i=1}^N \pi_i^n \delta_{y_i^n}$ be a minimizer of $F_{\mathbb{D}}(\mu_n^1, \dots, \mu_n^L, \nu(Y, \pi))$ over $A \subset (\mathbb{R}^d)^N \times \Delta_N$.
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(Generalization error)

Sketch of proof: control of the generalization error

For any fixed $(Y, \pi) \in (\mathbb{R}^d)^N \times \Delta_N$:

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Sketch of proof: Log-entropy

Taking the expectation on both sides

$$\mathbb{E} \left[\sup_{(Y, \pi)} \left\| \mathbb{F}_{\mathbb{D}} \left(\mu_n^1, \dots, \mu_n^L, \sum_{i=1}^N \pi_i \delta_{y_i} \right) - \mathbb{F}_{\mathbb{D}} \left(\mu^1, \dots, \mu^L, \sum_{i=1}^N \pi_i \delta_{y_i} \right) \right\| \right]$$

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Sketch of proof: Log-entropy

Taking the expectation on both sides

$$\begin{aligned} & \mathbb{E} \left[\sup_{(Y, \pi)} \left| F_{\mathbb{D}} \left(\mu_n^1, \dots, \mu_n^L, \sum_{i=1}^N \pi_i \delta_{y_i} \right) - F_{\mathbb{D}} \left(\mu^1, \dots, \mu^L, \sum_{i=1}^N \pi_i \delta_{y_i} \right) \right| \right] \\ & \leq \frac{1}{L} \sum_{\ell=1}^L \mathbb{E} \left[\sup_{(Y, \pi, w)} \left| \frac{1}{n} \sum_{i=1}^n f_{Y, w}(X_i^\ell) - \mathbb{E}_{X^\ell \sim \mu^\ell} [f_{Y, w}(X^\ell)] \right| \right] \\ & = \frac{1}{L} \sum_{\ell=1}^L \sup_{f \in \mathcal{F}_p} |\mathbb{P}_n^\ell(f) - \mathbb{E}_{X \sim \mu^\ell} [f(X)]| \\ & \leq \frac{C_1}{\sqrt{n}} \mathbb{E} \left[\int_0^{C_2} \sqrt{\log \left(2\mathcal{N}(\tau/2, \mathcal{F}_p, \|\cdot\|_{\mathbb{L}^2(\mu_n^\ell)}) \right)} d\tau \right] \end{aligned}$$

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Although non-convex, problems of points cloud optimization with **OT** losses have good rigidity properties under **definability** assumption on the target measures. This allows for good behavior of gradient sequences (such as **Lloyd's algorithms**).

Furthermore these problems have sample complexity $O(n^{-1/2})$, independent (exponentially) of the dimension. This rate is optimal in general.

Thank you for your attention!

Study of asymptotic behavior of $\mathbb{D}(\mu, \mu_n)$ and $\mathbb{D}(\mu, \nu_n)$ $\nu \neq \mu$.

¹¹On the rate of convergence in Wasserstein distance of the empirical measure, N.Fournier and A.Guillin. 2013

Study of asymptotic behavior of $\mathbb{D}(\mu, \mu_n)$ and $\mathbb{D}(\mu, \nu_n)$ $\nu \neq \mu$. In all generality it **depends on dimensionality**. For instance if μ 's support is compact¹¹:

$$\mathbb{E} [W_p(\mu_n, \mu)] \lesssim \begin{cases} n^{-1/d} & \text{if } d > 2p \\ n^{-1/2p} \log(n)^{1/p} & \text{if } d = 2p \\ n^{-1/2p} & \text{if } d < 2p \end{cases}$$

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and by triangle inequality this is **also true for** for $|W_p(\mu_n, \nu) - W_p(\mu, \nu)|$.

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Semi-discrete OT: fundamental $1/\sqrt{n}$ rate of convergence

Sharper results by investigating $\mathbb{D}(\mu_n, \nu)$ ($\mu \neq \nu$) insted. This is because the **sample complexity** of OT adapts to the "less complex" measure¹².

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Sharper results by investigating $\mathbb{D}(\mu_n, \nu)$ ($\mu \neq \nu$) instead. This is because the **sample complexity** of OT adapts to the "less complex" measure¹². In particular if ν is **discrete** then

$$\mathbb{E}[|W_p^p(\mu_n, \nu) - W_p^p(\mu, \nu)|] = O(1/\sqrt{n}).$$

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Statistical aspect of barycenters

Empirical Wasserstein barycenters are solutions of $\min_{\mu \in \mathcal{M}_1(\mathbb{R}^d)} \frac{1}{L} \sum_{l=1}^L W_p^p(\mu_n^l, \mu)$ with for all $l = 1, \dots, L$ μ_n^l **empirical measures** over i.i.d realizations of μ^l .

¹³Quantitative stability of barycenters in the Wasserstein space, G.Carlier, A.Delalande and Q.Méridot. 2022.

¹⁴Randomized Wasserstein barycenter computation: Resampling with statistical guarantees, F.Heinemann, A.Munk and Y.Zemel. 2023.

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$$\mathbb{E} \left[W_2^2(\mu_n^*, \mu^*) \right] \lesssim \begin{cases} n^{-1/12} & \text{if } d < 4 \\ n^{-1/12} \log(n)^{1/6} & \text{if } d = 4 \\ n^{-1/3d} & \text{if } d > 4. \end{cases}$$

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In the **discrete** setting we have¹⁴

$$\mathbb{E} \left[\frac{1}{L} \sum_{l=1}^L W_p^p(\mu^l, \nu_n) - \min_{\nu \in \mathcal{M}_1(\mathbb{R}^d)} \frac{1}{L} \sum_{l=1}^L W_p^p(\mu^l, \nu) \right] \lesssim \frac{1}{\sqrt{n}}.$$

Where ν_n is an empirical barycenter.

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