What distance to use between probabilities over probabilities?

Hugo Lavenant

Bocconi University

Optimal Transport Cargese Workshop

Cargèse (France), April 9, 2024

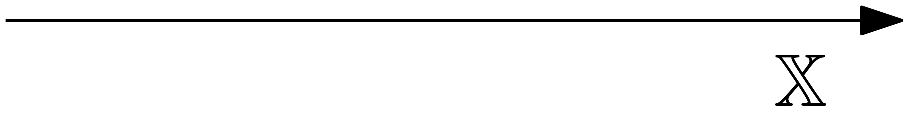
Joint work with

Marta Catalano (Luiss University)

Our article *Hierarchical Integral Probability Metrics: A distance on random probability measures with low sample complexity* is on arxiv!

Probabilities over Probabilities

$\mathbb{X}$ set (think subset of $\mathbb{R}^d$)



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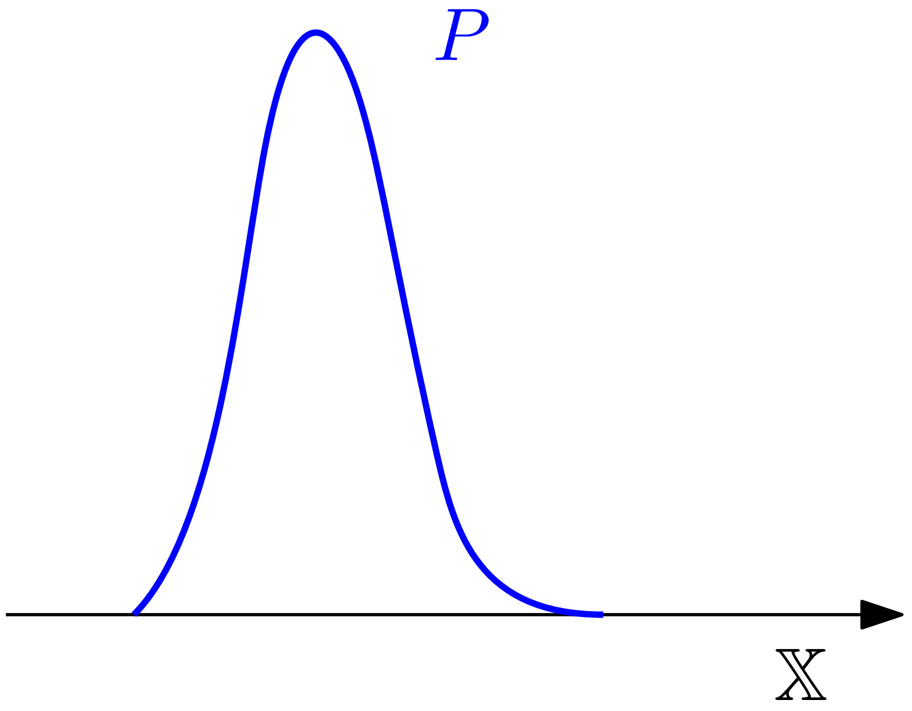

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Typical element P

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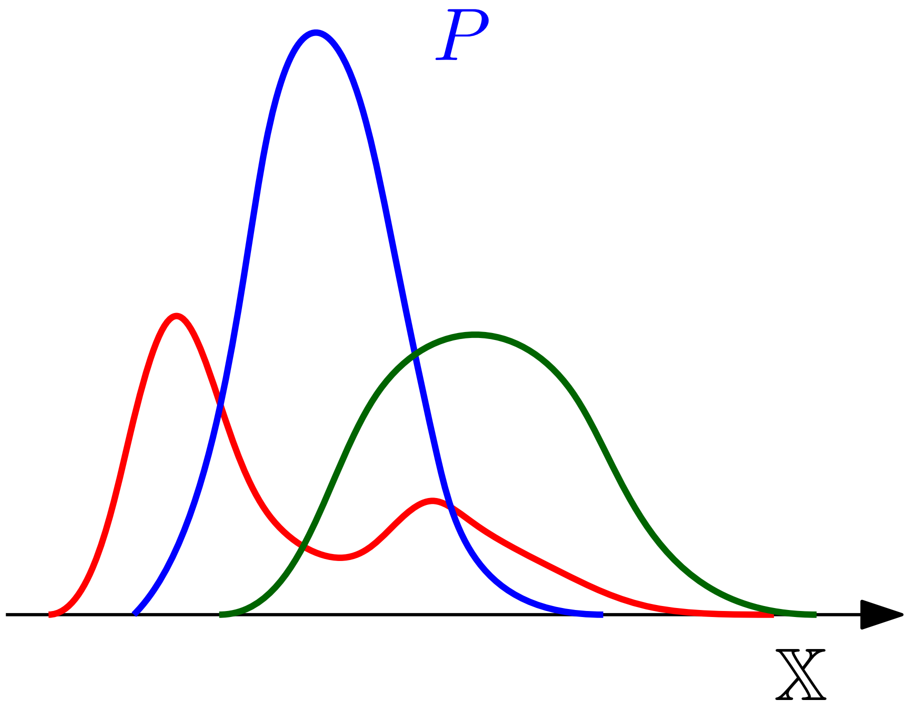

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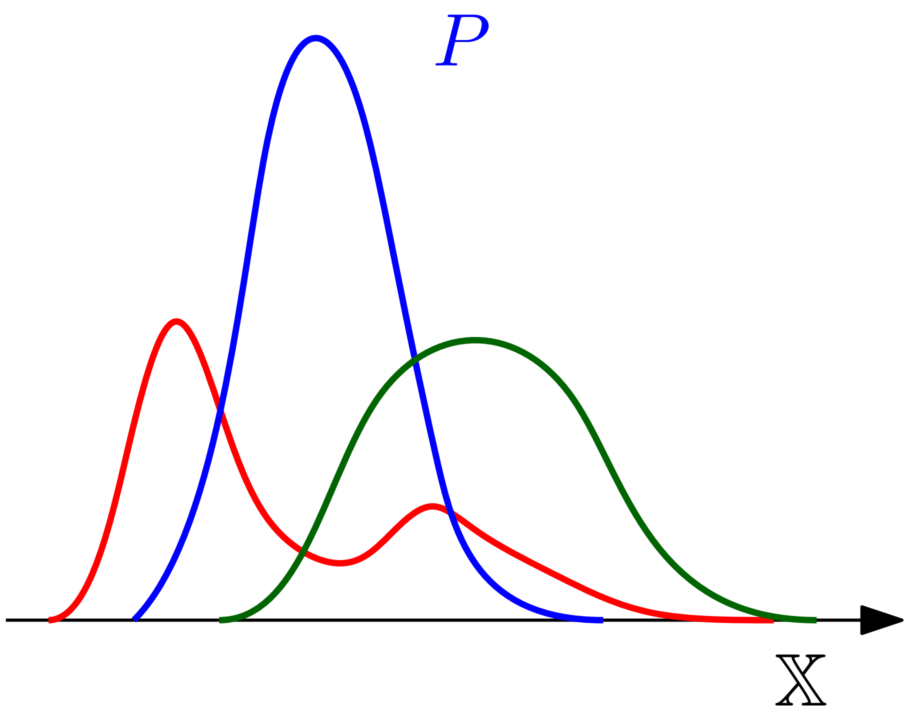

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What distance to put on the space $\mathcal{P}(\mathcal{P}(\mathbb{X}))$?

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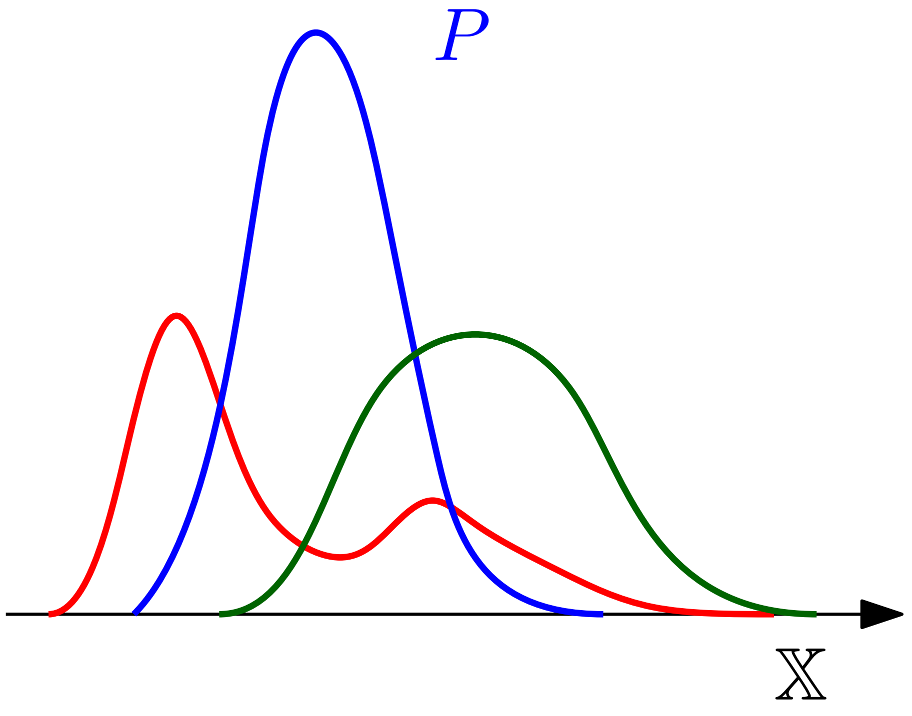

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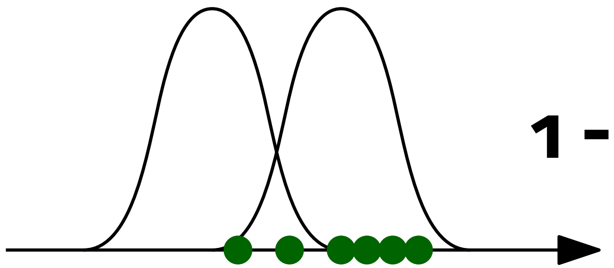
$\boxed{\text{What distance to put on the space } \mathcal{P}(\mathcal{P}(\mathbb{X}))\text{?}}$

Desiderata:

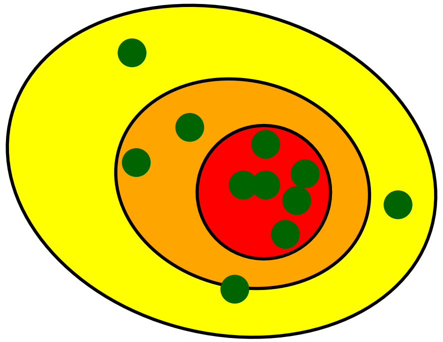
This talk

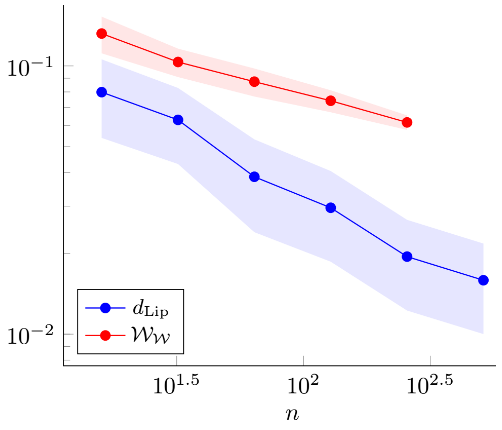
- Metrizing weak topology.
- Computation from samples: satistical and numerical complexity.
- Explicit formula, upper and lower bounds.



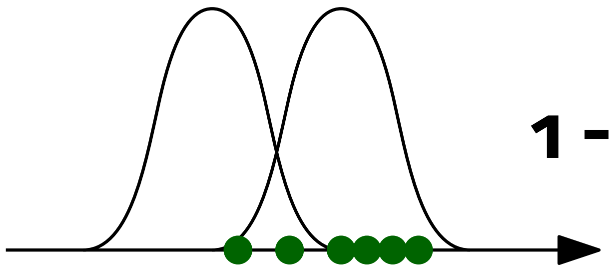
1 - Why? Bayesian Nonparametric Statistics

2 - Wasserstein over Wasserstein and its sample complexity





3 - A new distance with a better sample complexity



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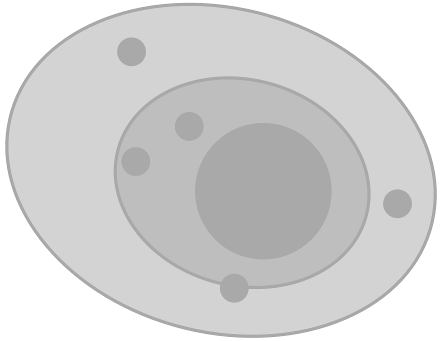

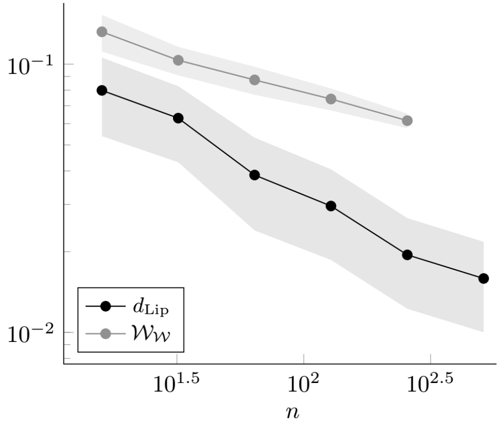

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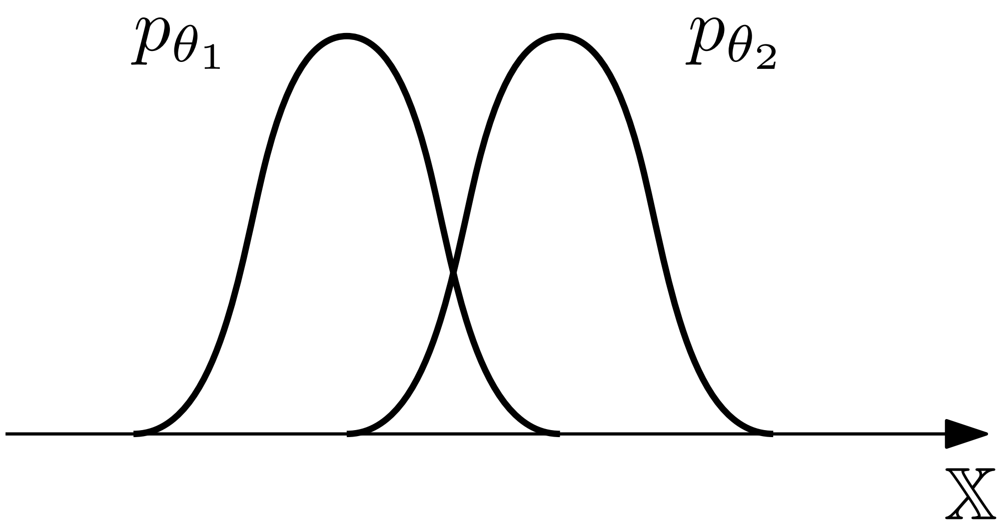
Bayesian (Nonparametric) Statistics

p_θ distributions over $\mathbb{X}$ indexed by $\theta \in \Theta$.

Goal: infer θ from data.



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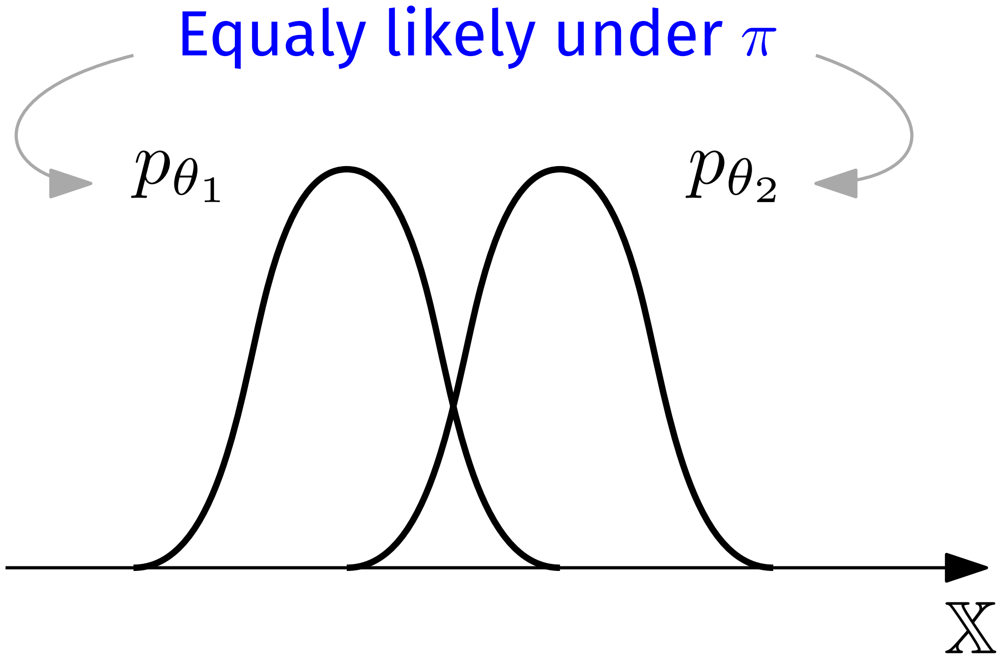
$$\theta \sim \pi$$

data in $\mathbb{X}$

$$X_1, \ldots, X_n | \theta \overset{\text{i.i.d.}}{\sim} p_\theta$$



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Inference gives posterior $\theta | X_1, \ldots, X_n$.

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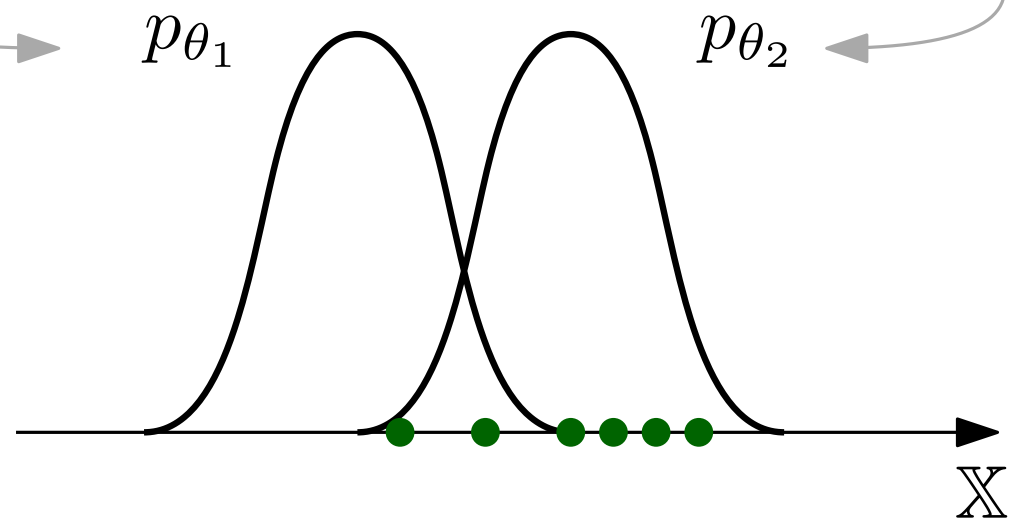

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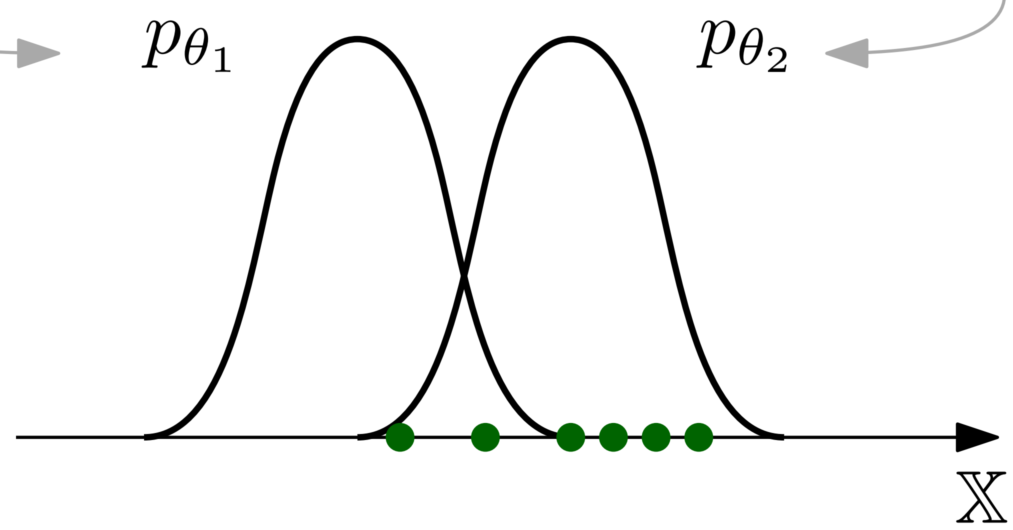

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Remark: p_θ with $\theta \sim \pi$ is a random probability: $\mathbb{Q} = (\theta \mapsto p_\theta)\#\pi$.

Bayesian NonParametrics: define directly $\mathbb{Q}$ (that is a random probability $\tilde{P}$) instead of p_θ and π.

Merging of opinions

Question. Different priors π^1, π^2 but same data $X_1, \ldots, X_n$.

Does the **distance** between the posteriors $\pi^1(\cdot|X_1, \ldots, X_n)$ and $\pi^2(\cdot|X_1, \ldots, X_n)$ converge to zero as $n \to +\infty$? At which rate in n?

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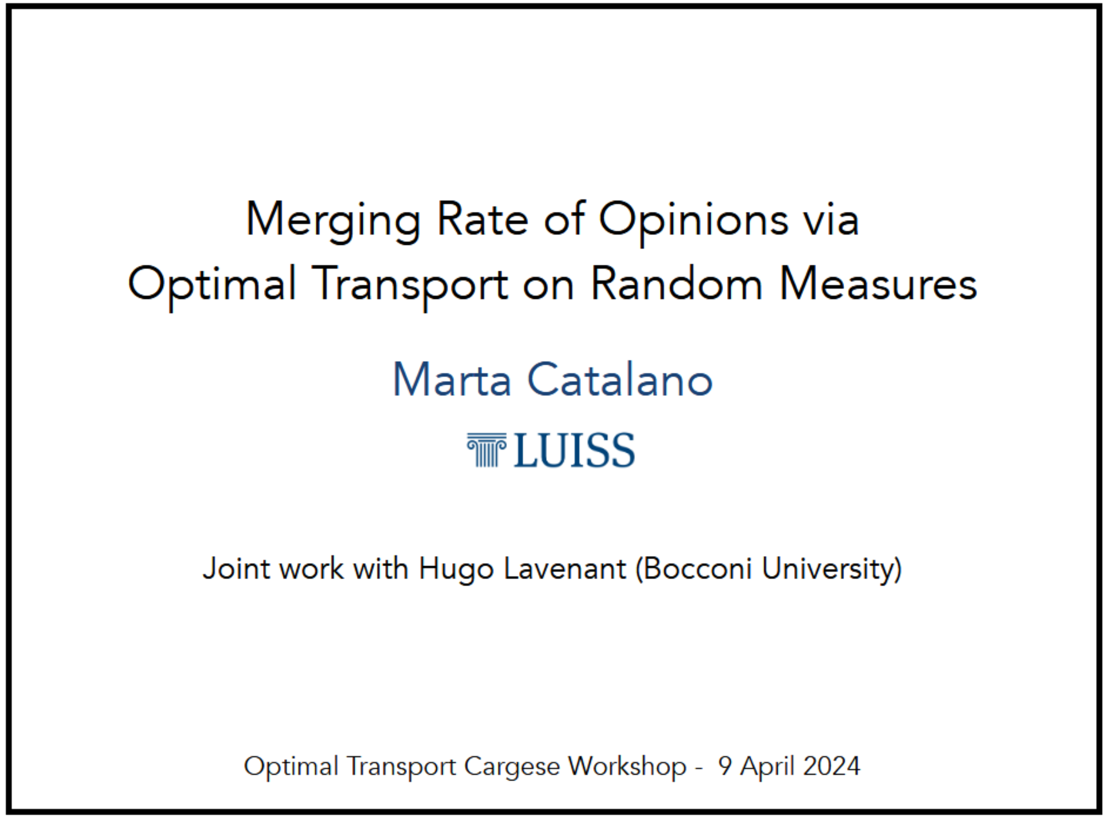
In Bayesian Nonparametrics, need for a distance between laws of random probabilities.

Blackwell & Dubins (1962). Merging of opinions with increasing information.
Catalano & Lavenant (2023). Merging Rate of Opinions via Optimal Transport on Random Measures.

Merging of opinions

Questi

Does t … and
$\pi^2(\cdot|X$ … e in n?


Merging Rate of Opinions via
Optimal Transport on Random Measures

Marta Catalano

LUISS

Joint work with Hugo Lavenant (Bocconi University)

Optimal Transport Cargese Workshop - 9 April 2024

More about this with Marta in a few minutes!

In Bayesian … f random
probabilitie

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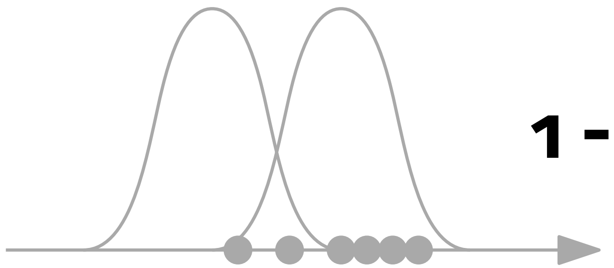

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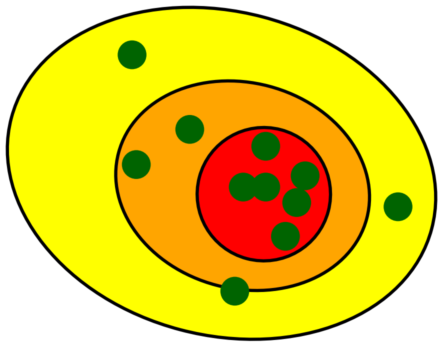

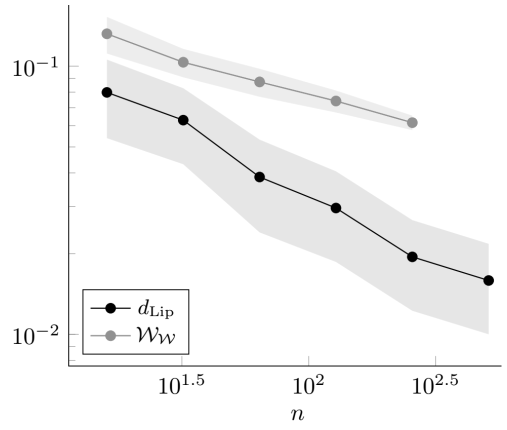

3 - A new distance with a better sample complexity

Wasserstein over Wasserstein distance

$\mathbb{X}$ metric space, $\mathcal{W}$ Wasserstein distance of order 1 on $\mathcal{P}(\mathbb{X})$.

Definition. If $\mathbb{Q}_1, \mathbb{Q}_2 \in \mathcal{P}(\mathcal{P}(\mathbb{X}))$, the "Wasserstein over Wasserstein" distance is:

$$\mathcal{W}_{\mathcal{W}}(\mathbb{Q}_1, \mathbb{Q}_2) = \inf_{\gamma \in \Gamma(\mathbb{Q}_1, \mathbb{Q}_2)} \mathbb{E}_{(\tilde{P}_1, \tilde{P}_2) \sim \gamma} \left[\mathcal{W}(\tilde{P}_1, \tilde{P}_2) \right].$$

Couplings between $\mathbb{Q}_1$ and $\mathbb{Q}_2$

Nguyen (2016). Borrowing strengh in hierarchical Bayes: Posterior concentration of the Dirichlet base measure.
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Couplings between $\mathbb{Q}_1$ and $\mathbb{Q}_2$

Weak convergence over weak convergence

Theorem. If $\mathbb{X}$ is bounded, then $\mathcal{W}_{\mathcal{W}}$ metrizes the weak convergence over $\mathcal{P}(\mathcal{P}(\mathbb{X}))$.

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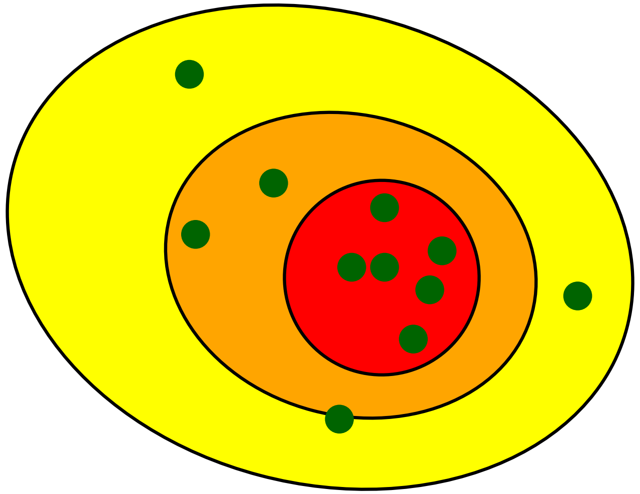
Sample complexity: reminder

- $P \in \mathcal{P}(\mathbb{X})$.
- $X_1, \dots X_n \overset{\text{i.i.d.}}{\sim} P$, build $\tilde{P}_{(n)} = \frac{1}{n}\sum_{i=1}^{n} \delta_{X_i}$.

How close is $\tilde{P}_{(n)}$ from P?

$X_i \in \mathbb{X}$ $\qquad$ $P \in \mathcal{P}(\mathbb{X})$



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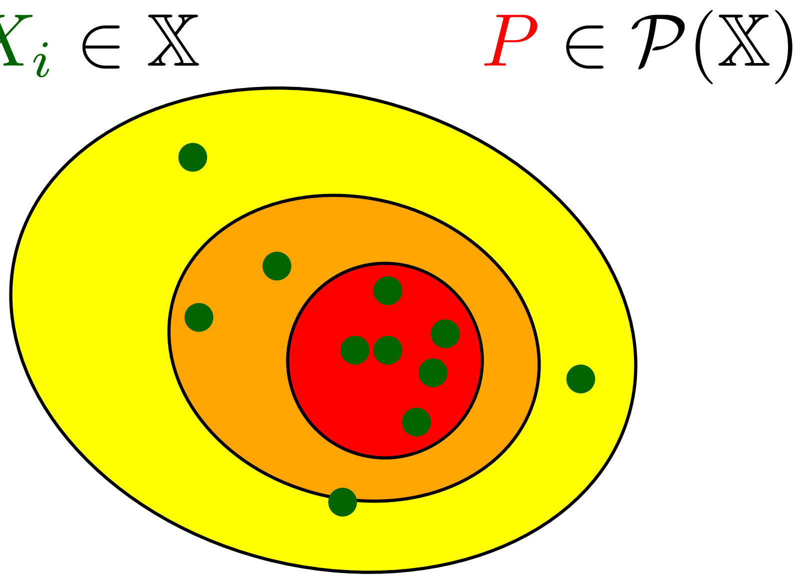

How close is $\tilde{P}_{(n)}$ from P?

Theorem. If P is "d-dimensional", then:

$$\mathbb{E}\left[\mathcal{W}(\tilde{P}_{(n)}, P)\right] \asymp \begin{cases} n^{-1/2} & \text{if } d = 1, \\ n^{-1/2} \log(n) & \text{if } d = 2, \\ n^{-1/d} & \text{if } d \geq 3. \end{cases}$$

Dudley (1969). The speed of mean Glivenko-Cantelli Convergence.
Weed & Bach (2019). Sharp asymptotic and finite-sample rates of convergence of empirical measures in Wasserstein distance.

Sample complexity for Wasserstein over Wasserstein

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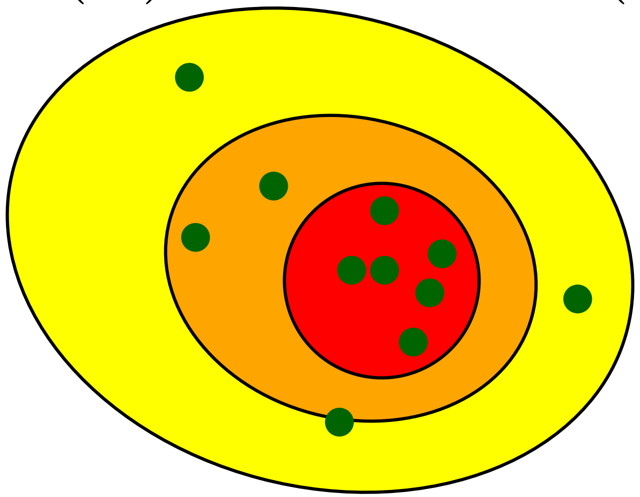

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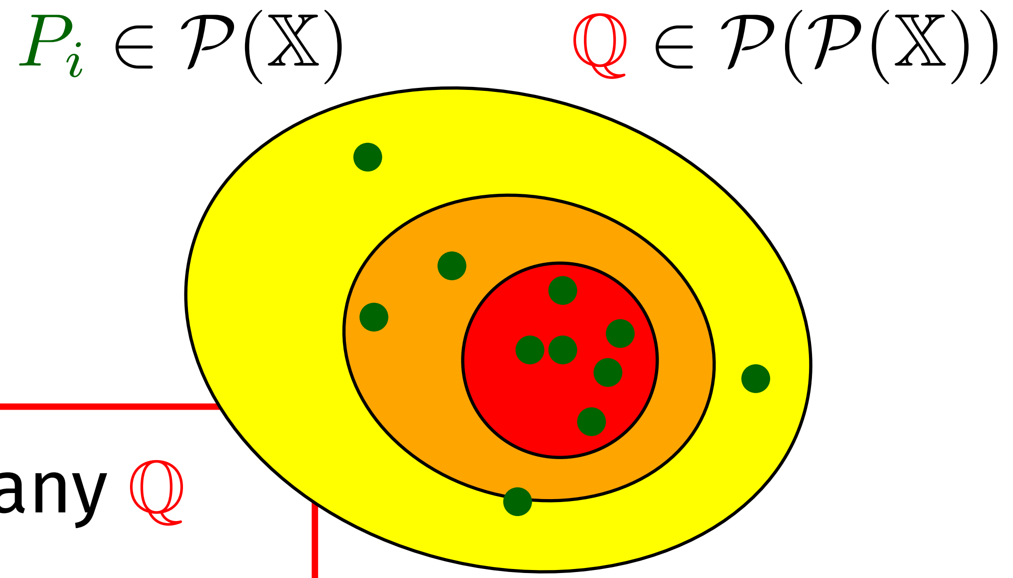

Theorem. Take $\mathbb{X} \subset \mathbb{R}^d$ bounded. Then for any $\mathbb{Q}$

$$\mathbb{E}\left[\mathcal{W}_{\mathcal{W}}\left(\tilde{\mathbb{Q}}_{(n)}, \mathbb{Q}\right)\right] \leq C_{\mathbb{X}} \frac{\log(\log(n))}{\log(n)},$$

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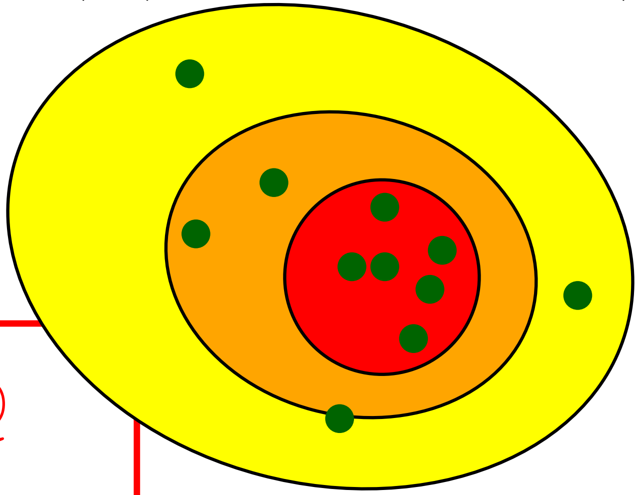

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and taking for $\mathbb{Q}$ a **Dirichlet process**, for any $\gamma > 0$,

$$\mathbb{E}\left[\mathcal{W}_{\mathcal{W}}\left(\tilde{\mathbb{Q}}_{(n)}, \mathbb{Q}\right)\right] \geq \frac{c_\gamma}{n^\gamma}.$$

What is this Dirichlet process giving a lower bound?

Parameters: base measure $P_0 \in \mathcal{P}(\mathbb{X})$ and concentration parameter $\alpha > 0$.

To draw $\tilde{P}$ according to a Dirichlet process:

Sethuraman (1994). A constructive definition of Dirichlet priors.

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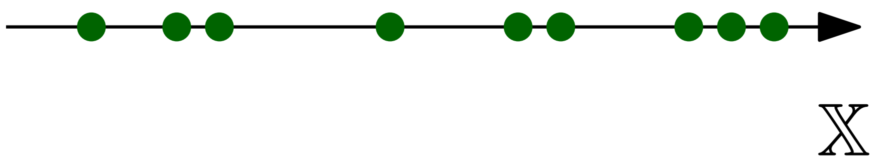

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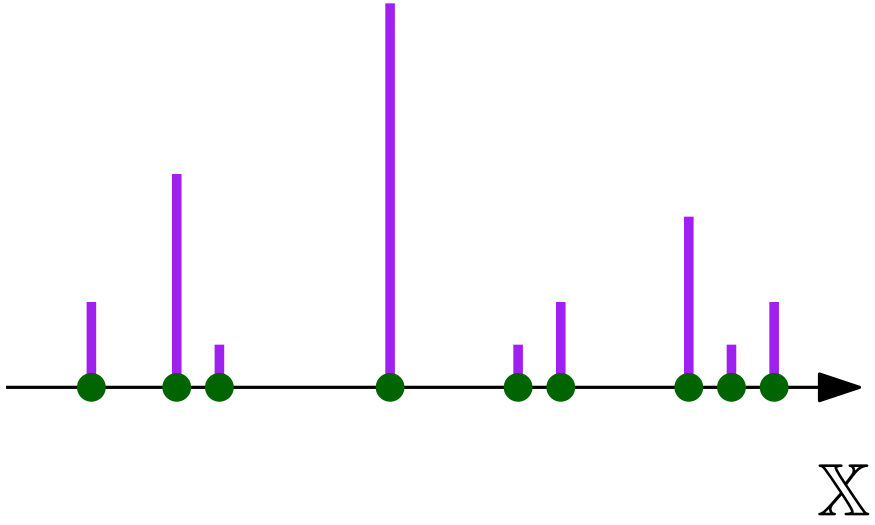
2. Draw independently weights $J_1, \dots, J_n, \dots$ which sum to 1 (law depending on α).
3. Define $\tilde{P} = \sum_{n=1}^{+\infty} J_n \delta_{X_n}$.



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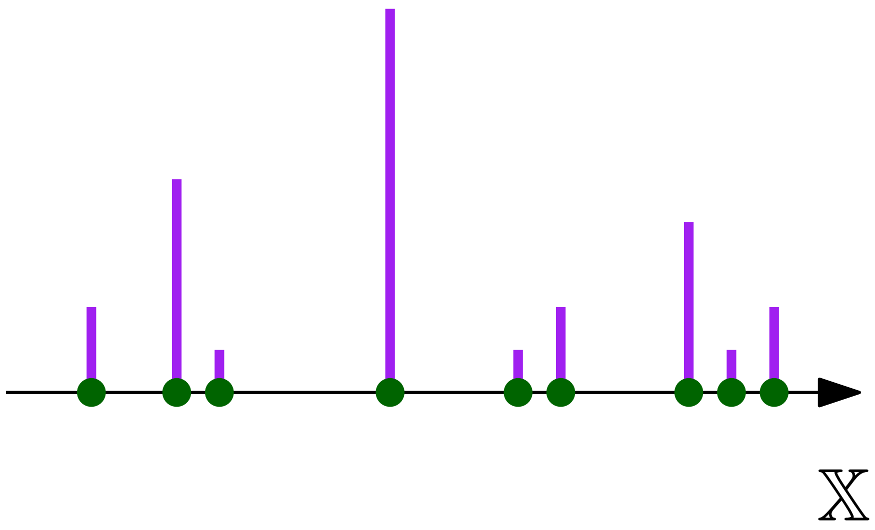

Remark. If the support of P_0 is $\mathbb{X}$, the topological support of the Dirichlet process is $\mathcal{P}(\mathbb{X})$.

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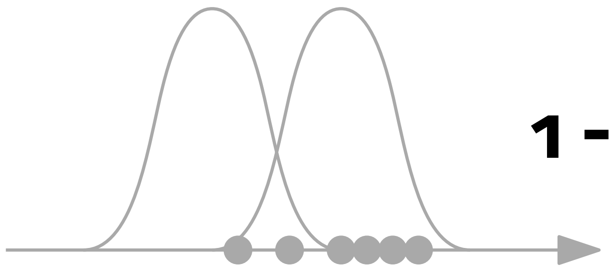

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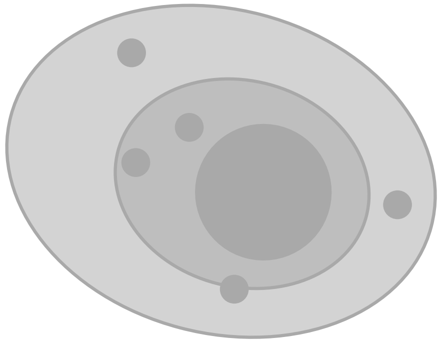

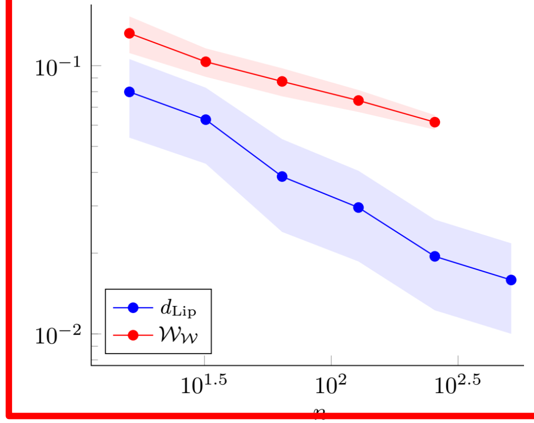

3 - A new distance with a better sample complexity

A new distance

$\mathbb{Q}_1, \mathbb{Q}_2 \in \mathcal{P}(\mathcal{P}(\mathbb{X}))$, recall:

$$\mathcal{W}_{\mathcal{W}}(\mathbb{Q}_1, \mathbb{Q}_2) = \inf_{\gamma \in \Gamma(\mathbb{Q}_1, \mathbb{Q}_2)} \sup_{f \in \mathrm{Lip}_1(\mathbb{X})} \mathbb{E}_{(\tilde{P}_1, \tilde{P}_2) \sim \gamma} \left[\left| \int_{\mathbb{X}} f \, \mathrm{d}\tilde{P}_1 - \int_{\mathbb{X}} f \, \mathrm{d}\tilde{P}_2 \right| \right].$$

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$$d_{\mathrm{Lip}}(\mathbb{Q}_1, \mathbb{Q}_2) = \sup_{f \in \mathrm{Lip}_1(\mathbb{X})} \inf_{\gamma \in \Gamma(\mathbb{Q}_1, \mathbb{Q}_2)} \mathbb{E}_{(\tilde{P}_1, \tilde{P}_2) \sim \gamma} \left[\left| \int_{\mathbb{X}} f \, \mathrm{d}\tilde{P}_1 - \int_{\mathbb{X}} f \, \mathrm{d}\tilde{P}_2 \right| \right]$$

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$$= \sup_{f \in \mathrm{Lip}_1(\mathbb{X})} \mathcal{W}\left(\int_{\mathbb{X}} f \, \mathrm{d}\tilde{P}_1, \int_{\mathbb{X}} f \, \mathrm{d}\tilde{P}_2 \right) \qquad \tilde{P}_1 \sim \mathbb{Q}_1, \ \tilde{P}_2 \sim \mathbb{Q}_2.$$

Idea. Project $\mathcal{P}(\mathbb{X})$ on $\mathbb{R}$ via $P \mapsto \int f \, \mathrm{d}P$ for $f \in \mathrm{Lip}_1(\mathbb{X})$, then measure Wasserstein distance of projections.

A new distance

Remark. Replace $\mathrm{Lip}_1(\mathbb{X})$ by $\mathcal{F}$ class of function $f : \mathbb{X} \to \mathbb{R}$ generating an *Integral Probability Metric*. We call the distance **Hierarchical IPM.**

Definition.

$$d_{\mathrm{Lip}}(\mathbb{Q}_1, \mathbb{Q}_2) = \sup_{f \in \mathrm{Lip}_1(\mathbb{X})} \inf_{\gamma \in \Gamma(\mathbb{Q}_1, \mathbb{Q}_2)} \mathbb{E}_{(\tilde{P}_1, \tilde{P}_2) \sim \gamma} \left[\left| \int_{\mathbb{X}} f \,\mathrm{d}\tilde{P}_1 - \int_{\mathbb{X}} f \,\mathrm{d}\tilde{P}_2 \right| \right]$$

$$= \sup_{f \in \mathrm{Lip}_1(\mathbb{X})} \mathcal{W}\left(\int_{\mathbb{X}} f \,\mathrm{d}\tilde{P}_1, \int_{\mathbb{X}} f \,\mathrm{d}\tilde{P}_2 \right) \qquad \tilde{P}_1 \sim \mathbb{Q}_1, \; \tilde{P}_2 \sim \mathbb{Q}_2.$$

Idea. Project $\mathcal{P}(\mathbb{X})$ on $\mathbb{R}$ via $P \mapsto \int f \,\mathrm{d}P$ for $f \in \mathrm{Lip}_1(\mathbb{X})$, then measure Wasserstein distance of projections.

Properties of this new distance

Theorem. There holds $d_{\mathrm{Lip}} \leq \mathcal{W}_{\mathcal{W}}$.
If $\mathbb{X}$ compact, d_{Lip} is a distance metrizing weak convergence over $\mathcal{P}(\mathcal{P}(\mathbb{X}))$.

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Theorem (sample complexity).

- $\mathbb{Q} \in \mathcal{P}(\mathcal{P}(\mathbb{X}))$ with $\mathbb{X}$ bounded subset of $\mathbb{R}^d$.
- $P_1, \dots P_n \overset{\text{i.i.d.}}{\sim} \mathbb{Q}$, build $\tilde{\mathbb{Q}}_{(n)} = \dfrac{1}{n} \sum_{i=1}^{n} \delta_{P_i}$.

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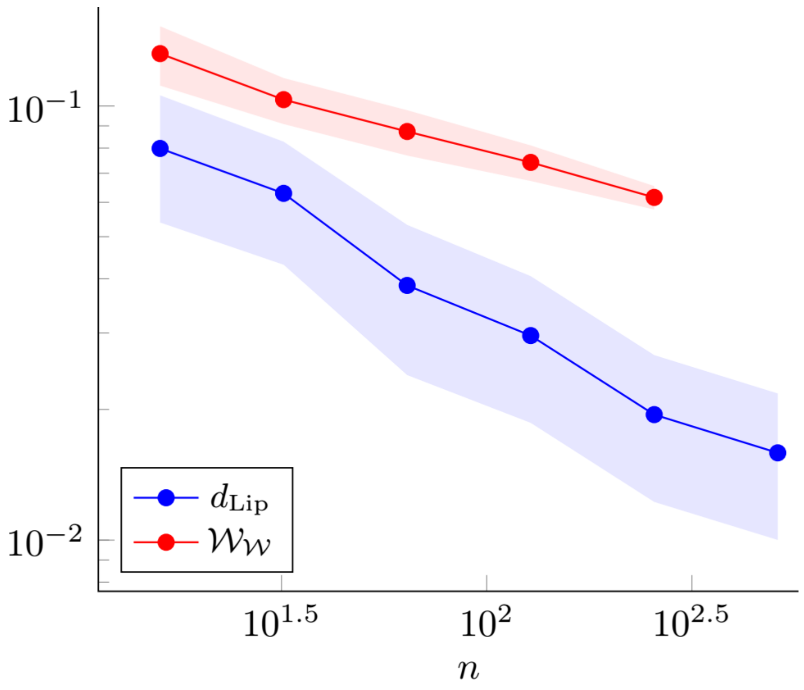
Then

$$\mathbb{E}\left[d_{\mathrm{Lip}}\left(\tilde{\mathbb{Q}}_{(n)}, \mathbb{Q}\right)\right] \lesssim \begin{cases} n^{-1/2} & \text{if } d = 1, \\ n^{-1/2}\log(n) & \text{if } d = 2, \\ n^{-1/d} & \text{if } d \geq 3. \end{cases}$$

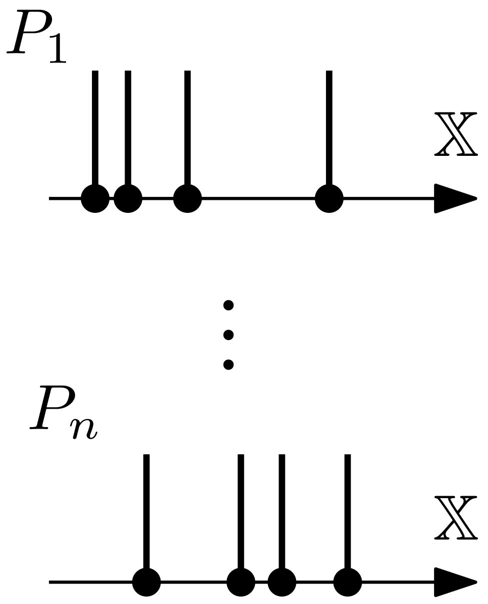
$d(\tilde{\mathbb{Q}}_{(n)}, \tilde{\mathbb{Q}}'_{(n)})$



Rate for *classical* Wasserstein distance in $\mathbb{R}^d$, $\ll \log(\log(n))/\log(n)$.

A word on Numerics

$$\mathbb{Q} = \frac{1}{n}\sum_{i=1}^{n} \delta_{P_i}$$ discrete



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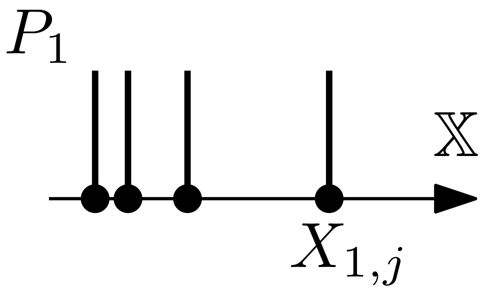
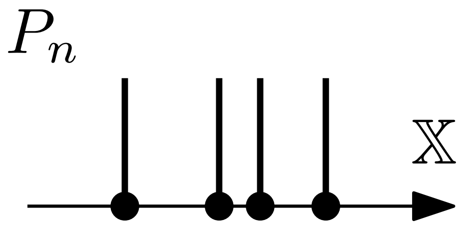


$$\rightsquigarrow \quad P_1 = \frac{1}{m}\sum_{j=1}^{m} \delta_{X_{1,j}} \text{ discrete}$$

$\vdots$



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Each element of $\mathcal{P}(\mathcal{P}(\mathbb{X}))$ is stored as a $n \times m$ array of atoms (and weights).

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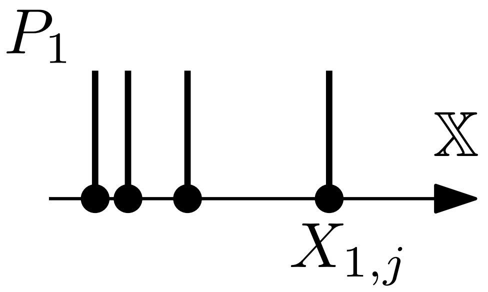

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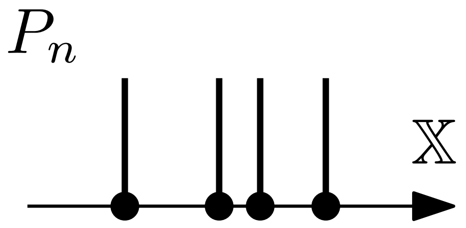

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Computing d_{Lip} is finding the supremum of $f \mapsto \mathcal{W}(\int f \, \mathrm{d}\tilde{P}_1, \int f \, \mathrm{d}\tilde{P}_2)$ among $\mathrm{Lip}_1(\mathbb{X})$.

Non convex, non concave. We propose a gradient ascent when $\mathbb{X} \subset \mathbb{R}$.

Thank you for your attention