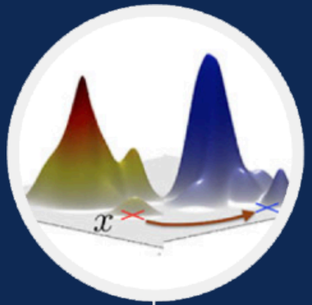
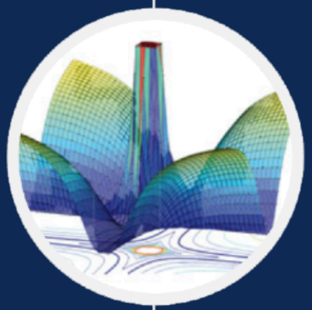
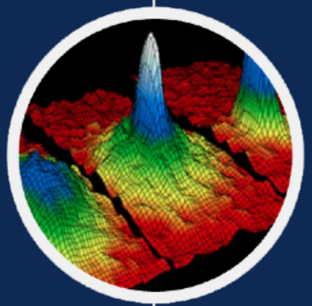
A crash-course on

Entropic Regularized Optimal Transport







Simone Di Marino

Department of Mathematics
Machine Learning Genoa Center
University of Genoa

Augusto Gerolin

Department of Mathematical and Statistics
Dep. of Chemistry and Biomolecular Sciences
University of Ottawa

uOttawa

Chaires de recherche du Canada — Canada Research Chairs

Canada

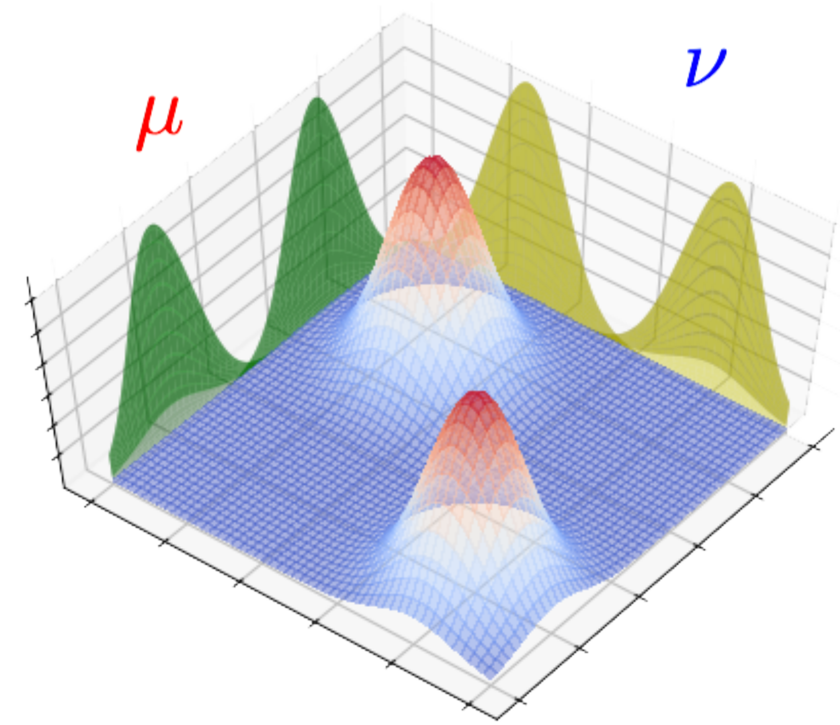
School *Mathematics of Machine Learning*
Centro De Giorgi, Pisa - 9-16th January 2023

PACE

Monge-Kantorovich formulation
of Optimal Transport

Data: $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$

$c(x,y) = |x-y|^2$



<u>Problem</u>: *Find the best coupling* γ between μ and ν.

$$\min \left\{ \int_{\mathbb{R}^d \times \mathbb{R}^d} |x-y|^2 d\gamma(x,y) : \gamma \in \Pi(\mu,\nu) \right\}$$

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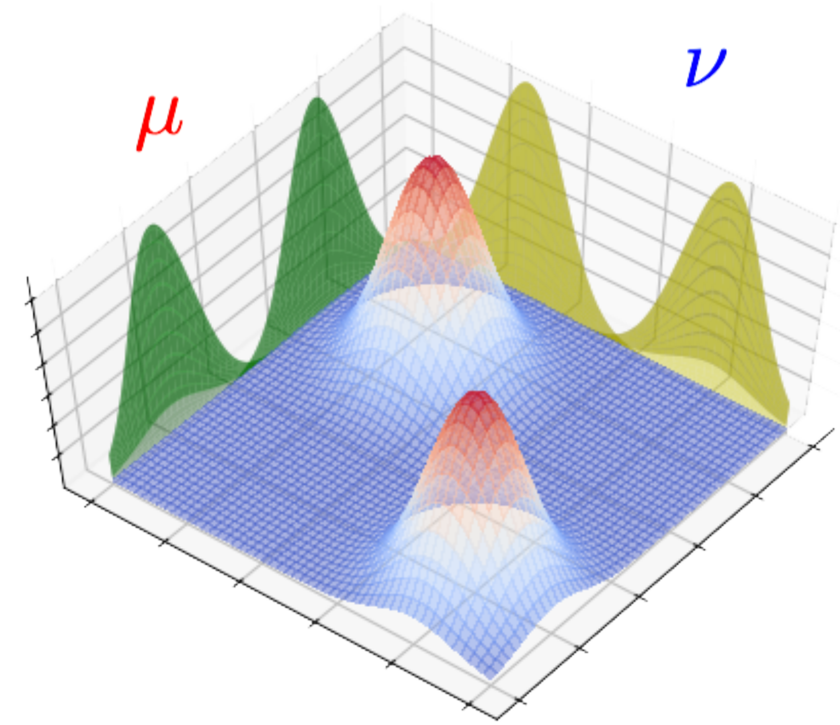

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γ is a probability in $\mathbb{R}^d \times \mathbb{R}^d$

such that $(e_1)_\sharp\gamma = \mu$ and $(e_2)_\sharp\gamma = \nu$

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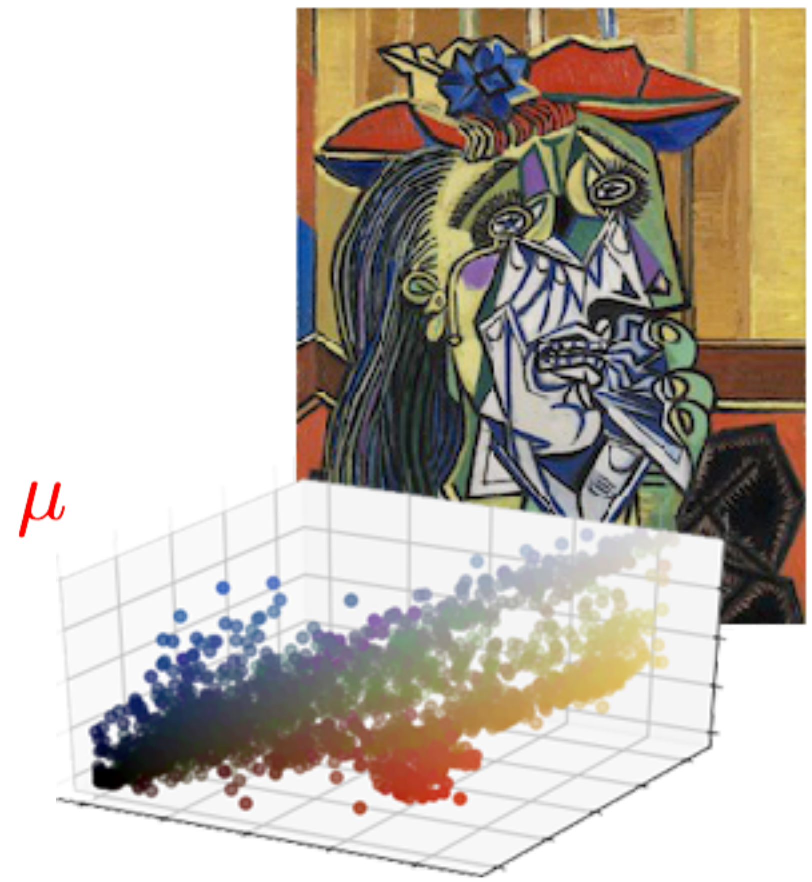

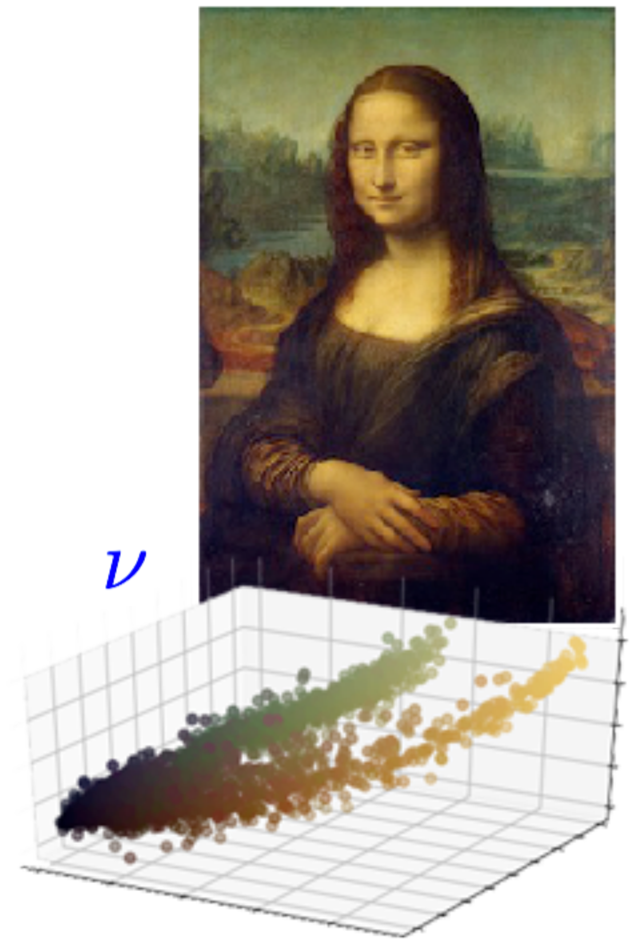

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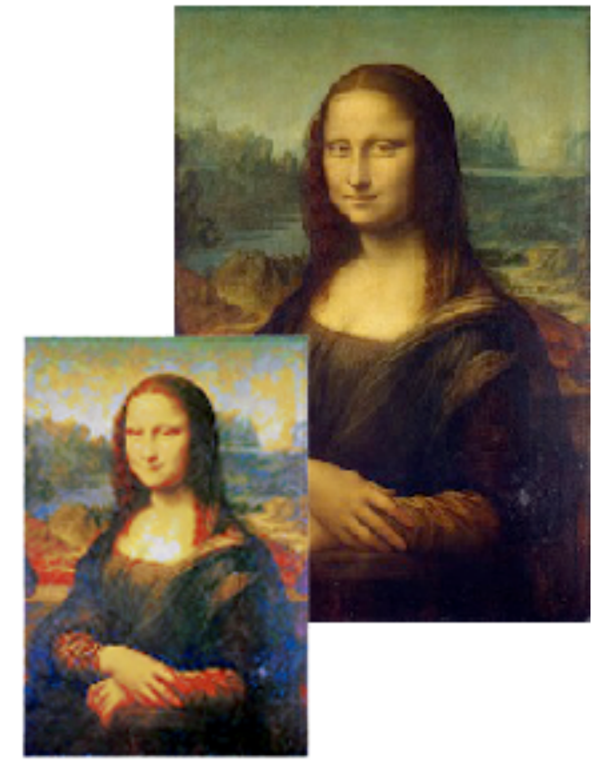

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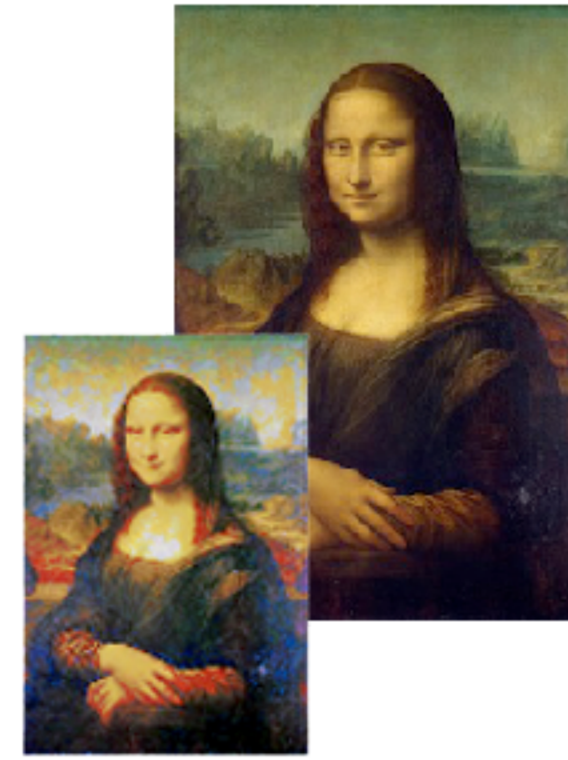

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$$W_2^2(\mu,\nu) = \min \left\{ \int_{\mathbb{R}^d \times \mathbb{R}^d} |x-y|^2 d\gamma(x,y) : \gamma \in \Pi(\mu,\nu) \right\}$$

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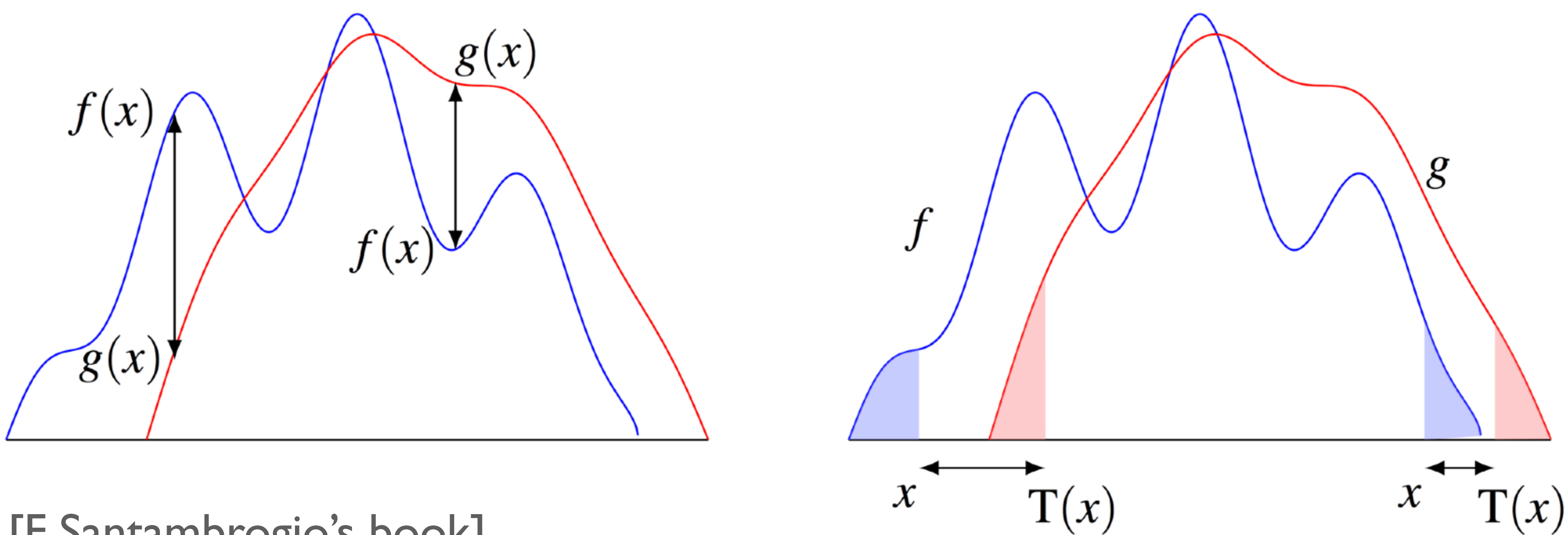
Why Optimal Transport?

It is define the Wasserstein distance on the space of probability measures.

$$W_2^2(\mu,\nu) = \min\left\{ \int_{\mathbb{R}^d\times\mathbb{R}^d} |x-y|^2 d\gamma(x,y) : \gamma\in\Pi(\mu,\nu)\right\}$$



[F. Santambrogio's book]

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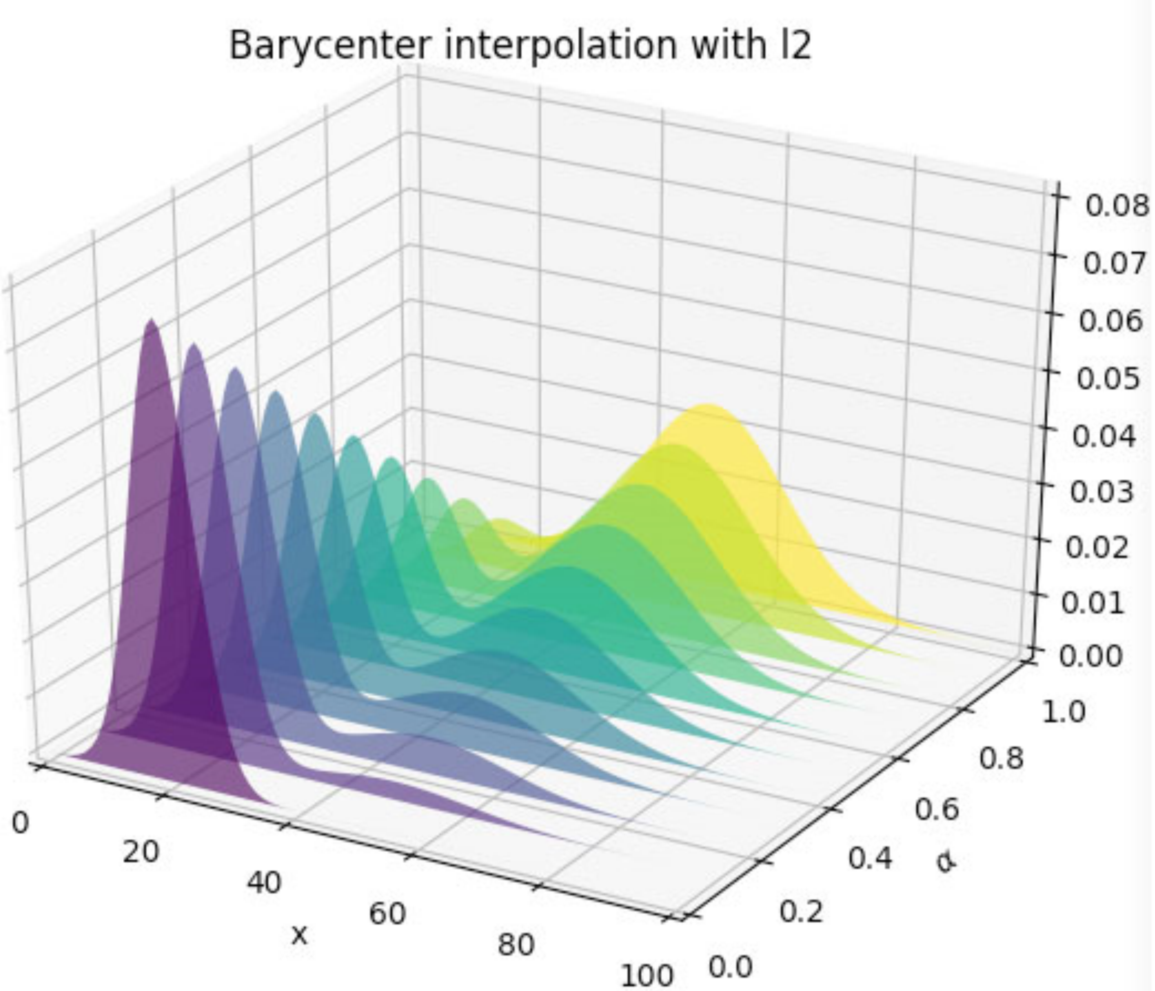

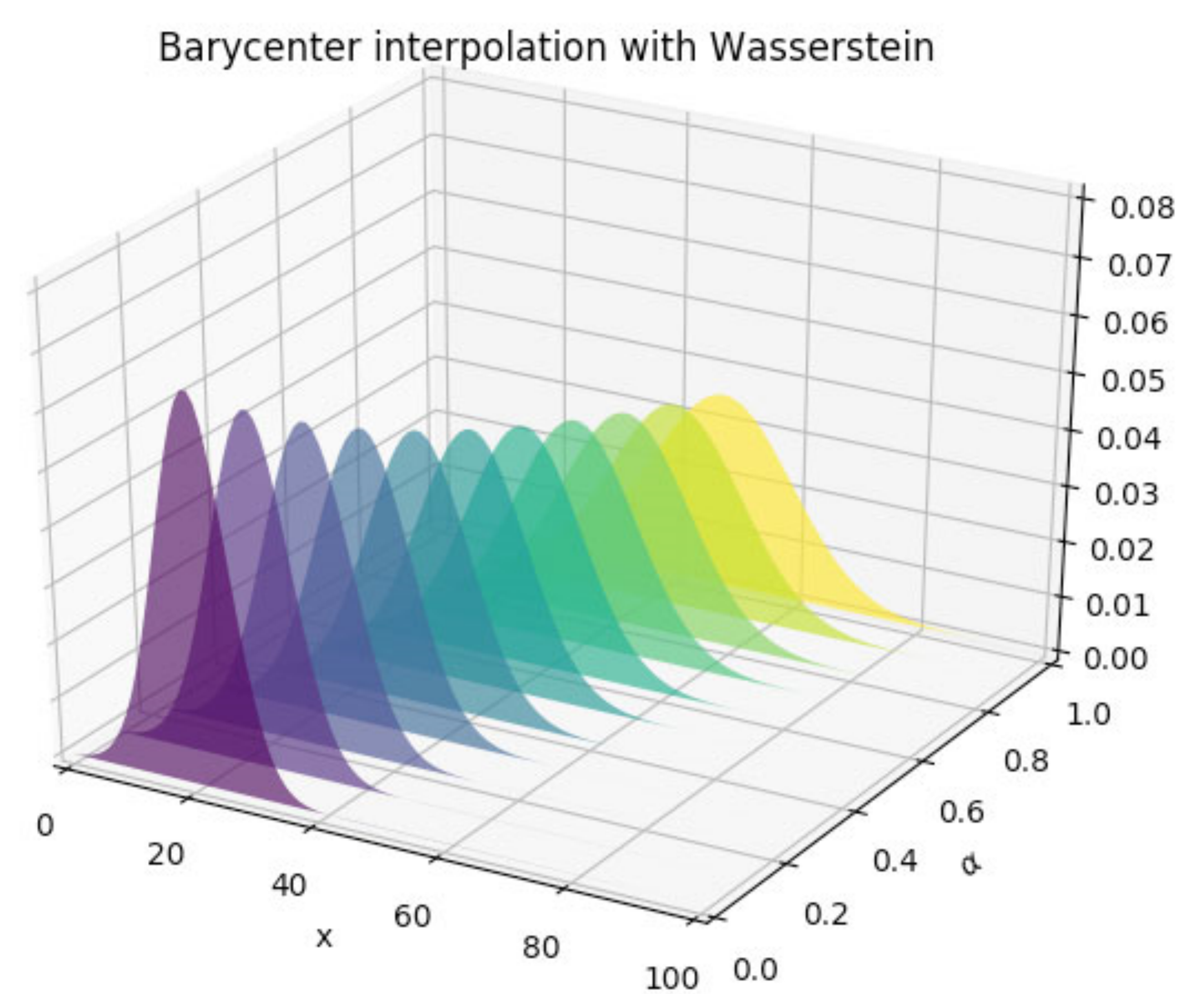

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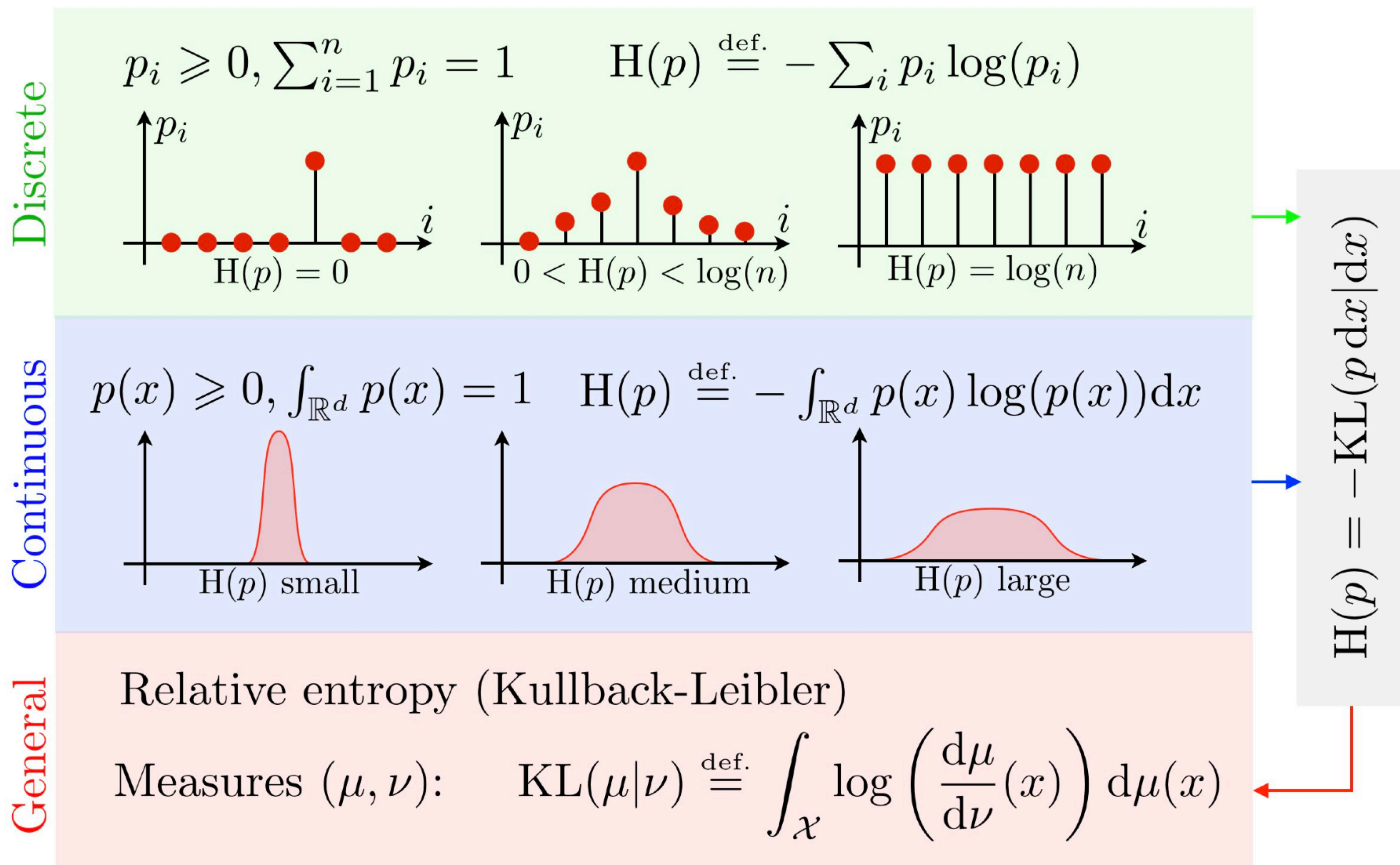
Relative Entropy between probability measures

[*Gabriel Péyre, Twitter*]



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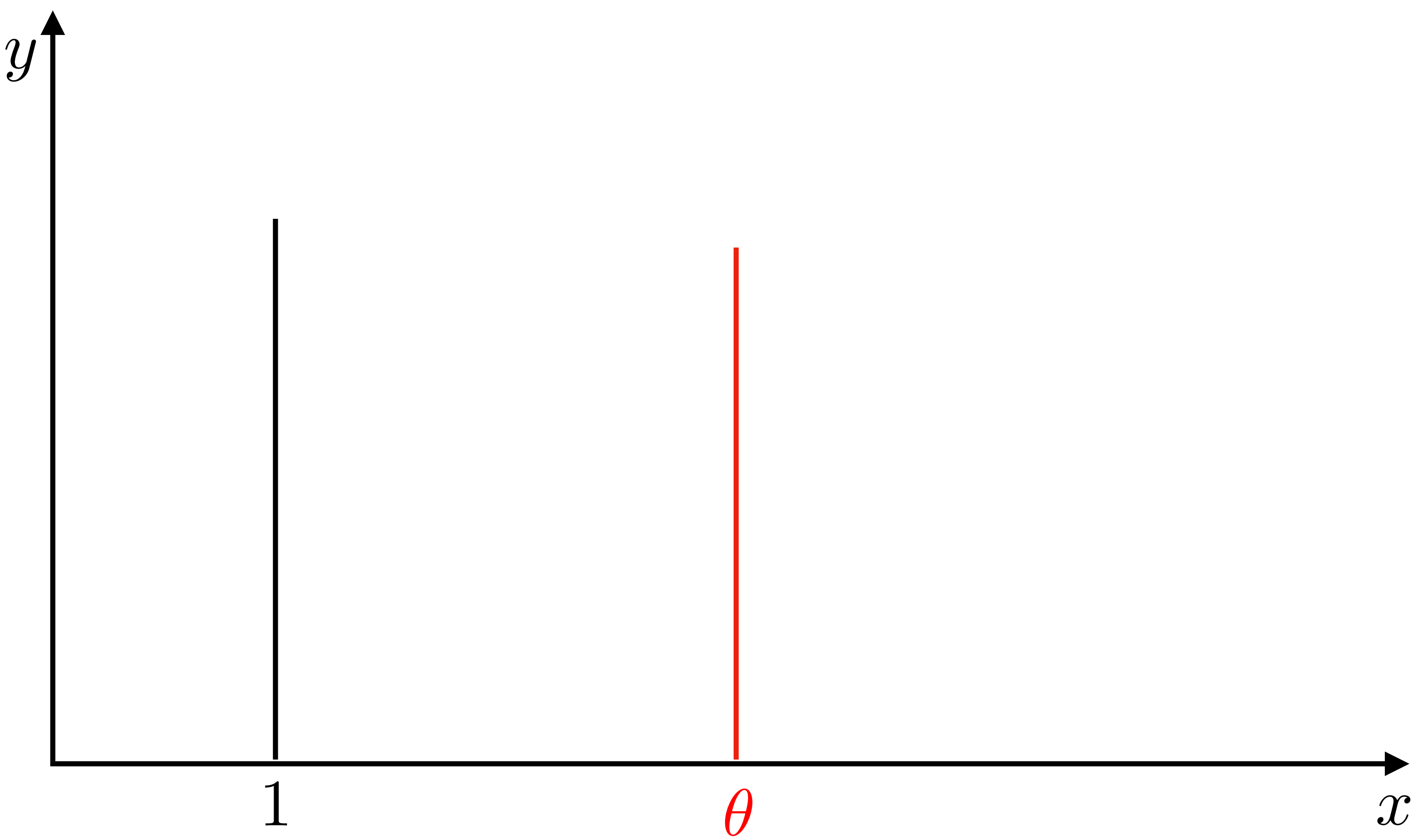
An enlightening example



$$P_0(x) = \begin{cases} 1 & \text{if } x = 1 \\ 0 & \text{otherwise} \end{cases} \qquad P_\theta(x) = \begin{cases} 1 & \text{if } x = \theta \\ 0 & \text{otherwise} \end{cases}$$

Kullback-Leibler divergence

$$\mathrm{KL}(\mathrm{P}_0|\mathrm{P}_\theta) = \begin{cases} 0 & \text{if } \theta = 0 \\ \infty & \text{otherwise} \end{cases}$$

Jensen–Shannon divergence

$$\mathrm{JSD}(\mathrm{P}_0|\mathrm{P}_\theta) = \begin{cases} 0 & \text{if } \theta = 0 \\ \log 2 & \text{otherwise.} \end{cases}$$

[Ian Goodfellow et al, Generative Adversarial Nets, 2014]
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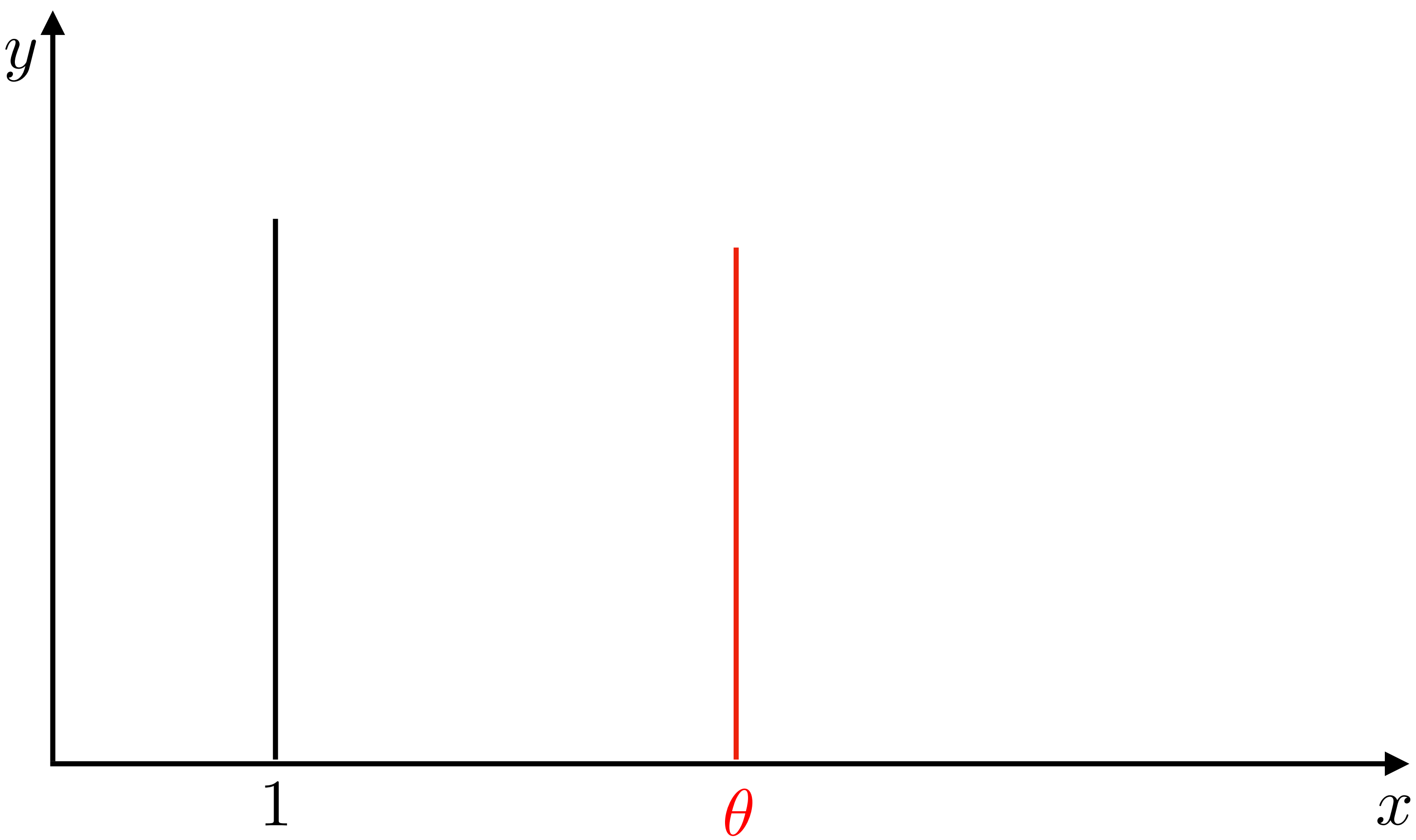

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2-Wasserstein distance

$$W_2^2(P_0, P_\theta) = |\theta|^2$$

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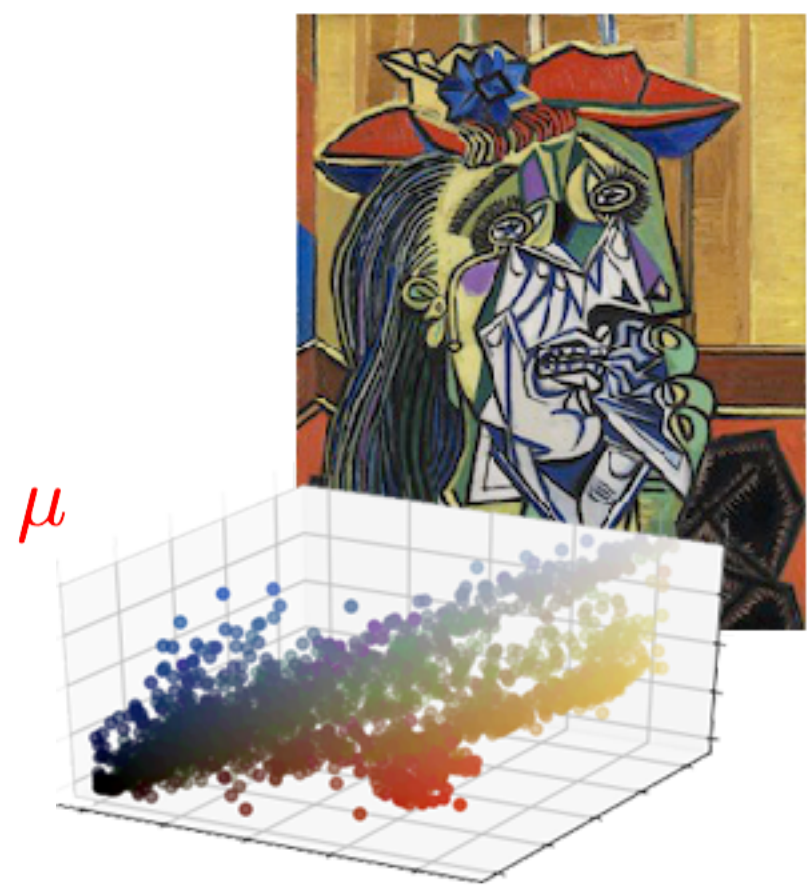

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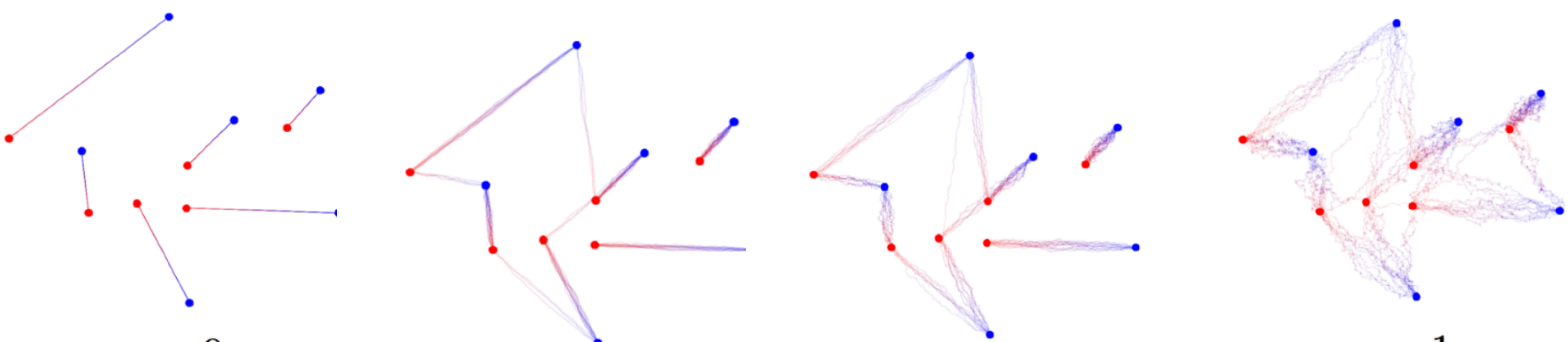
Shannon entropy regularized Optimal Transport

$$\mathrm{OT}_\varepsilon(\rho_1,\rho_2) = \min_{\gamma\in\Pi(\rho_1,\rho_2)} \varepsilon \int_{X\times Y} \gamma \log\left(\frac{\gamma}{e^{-c/\varepsilon}}\right) d(\rho_1\otimes\rho_2) \qquad \varepsilon > 0$$

$$= \min_{\gamma\in\Pi(\rho_1,\rho_2)} \int_{X\times Y} c(x,y)d\gamma(x,y) + \varepsilon \int_{X\times Y} \gamma(x,y)\log\gamma(x,y)d\left(\rho_1\otimes\rho_2\right).$$

After the works of I. Czisar, L. Ruschendorf, J. M. Borwein, A. S. Lewis and R. D. Nussbaum, C. Léonard, T. Georgiou, Y. Chen, M. Pavon, N. Gigli and L. Tamanini …

There exists a unique minimizer γ^ε *(strictly convex)* $\gamma^\varepsilon(x,y) = a^\varepsilon(x)b^\varepsilon(y)e^{-c(x,y)/\varepsilon}$



$\varepsilon = 0$ $\quad \varepsilon = .05$ $\quad \varepsilon = 0.2$ $\quad \varepsilon = 1$

[Gabriel Péyre, Twitter] $c(x,y) = |x-y|^2$

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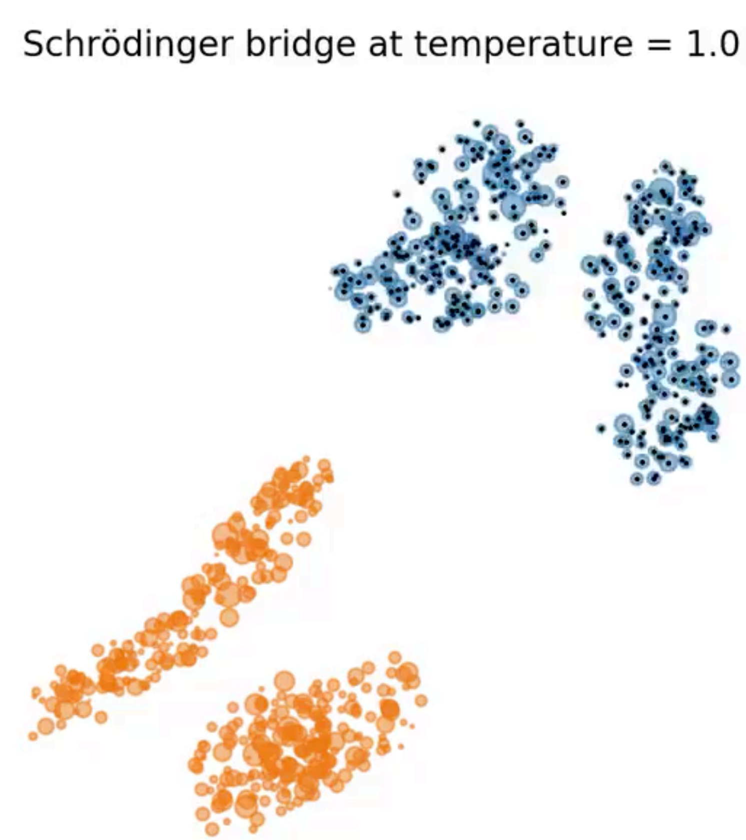

[Lénaïc Chizat, Twitter] $c(x,y) = |x-y|^2$

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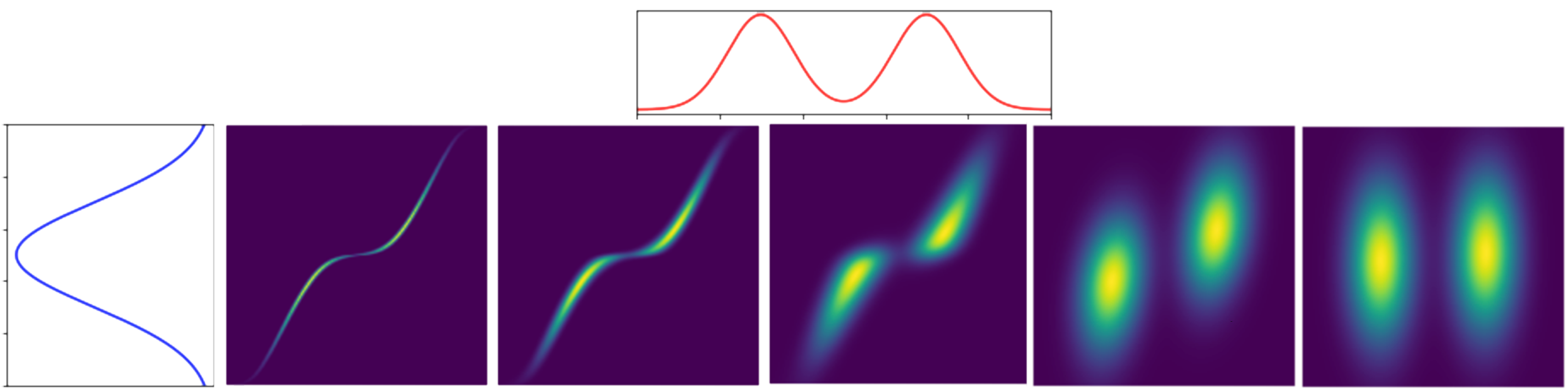

$c(x,y) = |x-y|^2$ $\quad\varepsilon$ *increases*

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If and only if solves the Schrödinger system

[E. Schrödinger, 1932]

$$\begin{cases} a^\varepsilon(x)\displaystyle\int_Y b^\varepsilon(y)e^{-c(x,y)/\varepsilon}d\rho_2(y) = 1 \\ b^\varepsilon(y)\displaystyle\int_X a^\varepsilon(y)e^{-c(x,y)/\varepsilon}d\rho_1(x) = 1 \end{cases}$$

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Explicit solutions when $c(x,y) = |x-y|^2$ *and* ρ_1, ρ_2 *are (multi-dimensional) Gaussians.*

[AG, Grossi, Gori-Giorgi, 2019]
[Mallasto, AG, Mihn, 2020]
[del Barrio, Loubes, 2020]
[Janati, Muzellec, Peyré, Cuturi, 2020]

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Computed numerically via Sinkhorn algorithm…

Sinkhorn algorithm

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The algorithm: $a^0(x) = b^0(y) = 1$

Define the sequences (iteratively) $(a^n)_{n\in\mathbb{N}}$ and $(b^n)_{n\in\mathbb{N}}$ by

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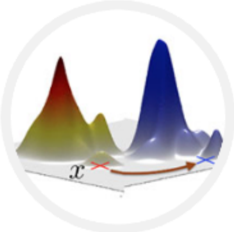

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Theoretical guarantees of convergence

[R. Sinkhorn, 1964]
[J. Franklin and J. Lorenz, 1989]
[L. Ruschendorf, 1995]
[Y. Chen, T. Georgiou and M. Pavon, 2016]

Approximates OT distances in near-linear time

[J. Altschuler, J. Weed, P. Rigollet, 2017]

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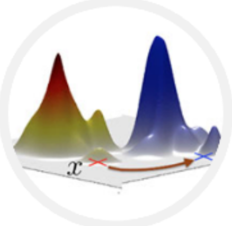

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Martin Idel (2016)

A review of matrix scaling and Sinkhorn's normal form for matrices and positive maps

Probabilistic / Large Deviations / Stochastic control

Cristian Léonard (2013)
Y. Chen, T. Georgiou and M. Pavon (2020)

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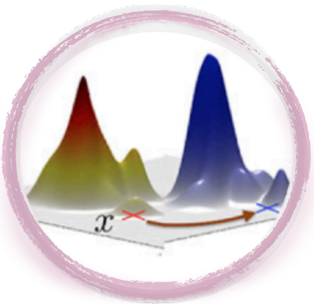
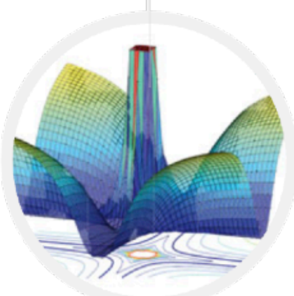
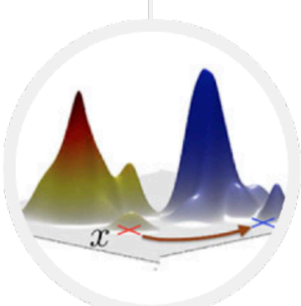
Outline



Duality approach for the Shannon Entropy-Regularized Optimal Transport



Convergence proof of the Sinkhorn algorithm (variational)



Applications

Shannon Entropy-Regularized Optimal Transport

A duality approach

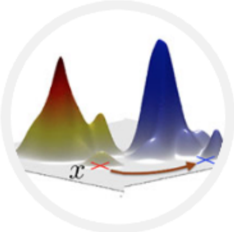
Setting: Let (X, d_X), (Y, d_Y) be Polish spaces, $c : X \times Y \to \mathbb{R}$ be a Borel bounded cost, $\rho_1 \in \mathcal{P}(X)$, $\rho_2 \in \mathcal{P}(Y)$ be probability measures and $\varepsilon > 0$ be a positive number.

Dual functional Let $u \in L^{\exp}_{\varepsilon}(\rho_1), v \in L^{\exp}_{\varepsilon}(\rho_2)$

$$D_\varepsilon(u,v) = \int_X u(x) d\rho_1(x) + \int_Y v(y) d\rho_2(y) - \varepsilon \int_{X\times Y} e^{\frac{u(x)+v(y)-c(x,y)}{\varepsilon}} d(\rho_1 \otimes \rho_2).$$

Dual (Kantorovich) problem: $\sup\left\{ D_\varepsilon(u,v) \ : \ u \in L^{\exp}_{\varepsilon}(\rho_1), v \in L^{\exp}_{\varepsilon}(\rho_2) \right\}.$

where $L^{\exp}_{\varepsilon}(X,\rho_1) = \left\{ u : X \to [-\infty, \infty[: u \text{ is a measurable function in } (X,\rho_1) \text{ and } 0 < \int_X e^{u/\varepsilon}\, d\rho_1 < \infty \right\}.$



Shannon Entropy-Regularized Optimal Transport

A duality approach

Setting: Let (X, d_X), (Y, d_Y) be Polish spaces, $c : X \times Y \to \mathbb{R}$ be a Borel bounded cost, $\rho_1 \in \mathcal{P}(X)$, $\rho_2 \in \mathcal{P}(Y)$ be probability measures and $\varepsilon > 0$ be a positive number.

Dual functional Let $u \in L^{\exp}_{\varepsilon}(\rho_1), v \in L^{\exp}_{\varepsilon}(\rho_2)$

$$D_\varepsilon(u, v) = \int_X u(x) d\rho_1(x) + \int_Y v(y) d\rho_2(y) - \varepsilon \int_{X \times Y} e^{\frac{u(x)+v(y)-c(x,y)}{\varepsilon}} d(\rho_1 \otimes \rho_2).$$

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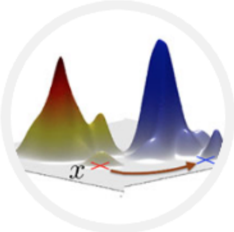
Lemma: Let (X, d_X), (Y, d_Y) be Polish spaces, $c : X \times Y \to \mathbb{R}$ be a Borel bounded cost, $\rho_1 \in \mathcal{P}(X)$, $\rho_2 \in \mathcal{P}(Y)$ be probability measures. Then

$$D_\varepsilon(u, u^{(c,\varepsilon)}) \geq D_\varepsilon(u, v) \qquad \forall v \in L^{\exp}_\varepsilon(\rho_2),$$
$$D_\varepsilon(u, u^{(c,\varepsilon)}) = D_\varepsilon(u, v) \text{ if and only if } v = u^{(c,\varepsilon)}.$$

In particular we can say that $u^{(c,\varepsilon)} \in \operatorname{argmax}\{D_\varepsilon(u, v) \ : \ v \in L^{\exp}_\varepsilon(\rho_2)\}$.

Proof idea:



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Shannon Entropy-Regularized Optimal Transport

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&= \int_X u(x) d\rho_1(x) + \int_Y v(y) d\rho_2(y) - \varepsilon \int_Y e^{\frac{v(y)}{\varepsilon}} \left(\int_X e^{\frac{u(x)-c(x,y)}{\varepsilon}} d\rho_1 \right) d\rho_2, \\
&= \int_X u(x) d\rho_1(x) + \int_Y v(y) - \varepsilon e^{\frac{v(y)-u^{(c,\varepsilon)}(y)}{\epsilon}} d\rho_2(y).
\end{aligned}$$

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&= \int_X u(x) d\rho_1(x) + \int_Y v(y) d\rho_2(y) - \varepsilon \int_Y e^{\frac{v(y)}{\varepsilon}} \left(\int_X e^{\frac{u(x)-c(x,y)}{\varepsilon}} d\rho_1 \right) d\rho_2, \\
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Therefore, for any $v \in L^{\exp}_\varepsilon(\rho_1)$, $D_\varepsilon(u, v) \leq D_\varepsilon(u, u^{(c,\varepsilon)})$, since the function $g(t) = t - \varepsilon e^{(t-a)/\varepsilon}$ is strictly concave and attains its maximum in $t = a$.

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Proposition: Let (X,d_X), (Y,d_Y) be Polish spaces, $u \in L^{\exp}_{\varepsilon}(\rho_1), v \in L^{\exp}_{\varepsilon}(\rho_2)$ and $\varepsilon > 0$. $c : X \times Y \to \mathbb{R}$ be a Borel bounded cost,

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Also, for the lower bound we have

$$u^{(c,\varepsilon)}(y) = -\varepsilon \log\left(\int_X e^{\frac{u(x)-c(x,y)}{\varepsilon}} d\rho_1\right) \geq -\|c\|_\infty - \varepsilon \log\left(\int_X e^{\frac{u(x)}{\varepsilon}} d\rho_1\right).$$

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Shannon Entropy-Regularized Optimal Transport

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Proof idea: Let us prove (ii), i.e. $u^{(c,\varepsilon)} \in L^{\infty}(\rho_2)$.

$$\int_Y e^{\frac{u^{(c,\varepsilon)}(y)}{\varepsilon}} d\rho_2(y) \leq \int_Y e^{\|c\|_\infty/\varepsilon}\left(\int_X e^{\frac{u(x)}{\varepsilon}} d\rho_1(x)\right)^{-1} d\rho_2(y) < +\infty.$$

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Proposition:

(i) if c is L-Lipschitz, then $u^{(c,\varepsilon)}$ is L-Lipschitz;

(ii) if $|c| \leq M$ then $\operatorname{osc}(u^{(c,\varepsilon)}) \leq 2M$.

(iii) if $|c| \leq M$, then $u^{(c,\varepsilon)} : L^\infty(\rho_1) \to L^p(\rho_2)$ is a 1-Lip. compact operator.

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$$|u^{(c,\varepsilon)}(y_1) - u^{(c,\varepsilon)}(y_2)| = \varepsilon \log\left(\int_X e^{\frac{u(x)-c(x,y_2)}{\varepsilon}}\, d\rho_1\right) - \varepsilon \log\left(\int_X e^{\frac{u(x)-c(x,y_1)}{\varepsilon}}\, d\rho_1\right)$$

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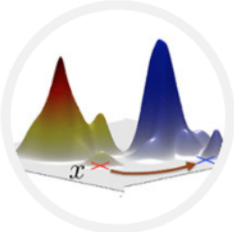

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&= \varepsilon \log\left(\int_X e^{\frac{u(x)-c(x,y_1)+c(x,y_1)-c(x,y_2)}{\varepsilon}} d\rho_1\right) - \varepsilon \log\left(\int_X e^{\frac{u(x)-c(x,y_1)}{\varepsilon}} d\rho_1\right) \\
&\leq \varepsilon \log\left(e^{\frac{Ld(y_1,y_2)}{\varepsilon}} \int_X e^{\frac{u(x)-c(x,y_1)}{\varepsilon}} d\rho_1\right) - \varepsilon \log\left(\int_X e^{\frac{u(x)-c(x,y_1)}{\varepsilon}} d\rho_1\right) \\
&= Ld(y_1, y_2)
\end{aligned}$$

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Shannon Entropy-Regularized Optimal Transport

A duality approach

Theorem (S. Di Marino & AG, 2020)

The supremum

$$\sup\left\{D_\varepsilon(u,v)\ :\ u\in L^{\exp}_\varepsilon(\rho_1), v\in L^{\exp}_\varepsilon(\rho_2)\right\}$$

is attained for a unique couple (u_0,v_0) (up to the trivial tranformation$(u,v)\mapsto(u+a,v-a)$).
In particular we have $u_0\in L^\infty(\rho_1)$ and $v_0\in L^\infty(\rho_2)$;

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Lemma

There exist $u^*\in L^{\exp}_\varepsilon(\rho_1)$ and $v^*\in L^{\exp}_\varepsilon(\rho_2)$ such that $D_\varepsilon(u,v)\le D_\varepsilon(u^*,v^*)$ with $\|v^*\|_\infty,\|u^*\|_\infty\le 3\|c\|_\infty/2$.
Moreover, there exist $a\in\mathbb{R}$ such that $u^*=(v+a)^{(c,\varepsilon)}$ and $v^*=(u^*)^{(c,\varepsilon)}$.

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Moreover, there exist $a\in\mathbb{R}$ such that $u^*=(v+a)^{(c,\varepsilon)}$ and $v^*=(u^*)^{(c,\varepsilon)}$.

Proof idea: Let $(u_n)_{n\in\mathbb{N}}\subset L^{\exp}_\varepsilon(\rho_1)$ and $(v_n)_{n\in\mathbb{N}}\subset L^{\exp}_\varepsilon(\rho_2)$ be maximizing sequences.
We can suppose that $u_n\in L^\infty(\rho_1)$, $v_n\in L^\infty(\rho_2)$ and $\|u_n\|_\infty,\|v_n\|_\infty\leq\frac{3}{2}\|c\|_\infty$.
By Banach-Alaoglu theorem there exists subsequences $u_{n_k}\rightharpoonup\overline{u}$ and $v_{n_k}\rightharpoonup\overline{v}$.

Then,

$$\sup_{u,v}D_\varepsilon(u,v)=\lim_{n\to\infty}D_\varepsilon(u_n,v_n)\leq\lim_{n\to\infty}\left\{\int_X u_n d\rho_1+\int_Y v_n d\rho_2\right\}-\varepsilon\liminf_{n\to\infty}\left\{\int_{X\times Y}e^{\frac{u_n+v_n-c}{\varepsilon}}d(\rho_1\otimes\rho_2)\right\}$$

$$\leq\int_X\overline{u}d\rho_1+\int_Y\overline{v}d\rho_2-\varepsilon\int_{X\times Y}e^{\frac{\overline{u}+\overline{v}-c}{\varepsilon}}d(\rho_1\otimes\rho_2)=D(\overline{u},\overline{v}).$$

Shannon Entropy-Regularized Optimal Transport

A duality approach

Shannon Entropy-Regularized Optimal Transport

A duality approach

Theorem (S. Di Marino & AG, 2020)

Let $\varepsilon > 0$ be a positive number, (X, d_X) and (Y, d_Y) be Polish metric spaces, $c : X \times Y \to \mathbb{R}$ be a cost function (not necessarily bounded), $\rho_1 \in \mathcal{P}(X)$, $\rho_2 \in \mathcal{P}(Y)$ be probability measures. Then for every $\gamma \in \Pi(\rho_1, \rho_2)$, $u \in L^{\exp}_{\varepsilon}(\rho_1)$ and $v \in L^{\exp}_{\varepsilon}(\rho_2)$

$$\varepsilon \mathrm{KL}(\gamma | e^{-c/\varepsilon}) \geq D_{\varepsilon}(u, v) + \varepsilon, \qquad \text{with equality iff } \gamma = e^{\frac{u+v-c}{\varepsilon}}.$$

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$$\varepsilon \mathrm{KL}(\gamma | e^{-c/\varepsilon}) \geq D_{\varepsilon}(u, v) + \varepsilon, \qquad \text{with equality iff } \gamma = e^{\frac{u+v-c}{\varepsilon}}.$$

Proof idea:

$$\begin{aligned}
\varepsilon \mathrm{KL}(\gamma | e^{-c/\varepsilon}) &= \int_{X \times Y} c d\gamma + \varepsilon \int_{X \times Y} \gamma \log \gamma d\left(\rho_1 \otimes \rho_2\right) \\
&= \int_{X \times Y} (c + \varepsilon \log \gamma - u - v) \cdot \gamma d\rho_1 \otimes \rho_2 + \int_X u d\rho_1 + \int_Y v d\rho_2
\end{aligned}$$

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Proof idea:

$$\begin{aligned}
\varepsilon \mathrm{KL}(\gamma | e^{-c/\varepsilon}) &= \int_{X\times Y} c\, d\gamma + \varepsilon \int_{X\times Y} \gamma \log \gamma\, d\left(\rho_1 \otimes \rho_2\right) \\
&= \int_{X\times Y} (c + \varepsilon \log \gamma - u - v) \cdot \gamma\, d\rho_1 \otimes \rho_2 + \int_X u\, d\rho_1 + \int_Y v\, d\rho_2 \\
&= \int_X u\, d\rho_1 + \int_Y v\, d\rho_2 + \int_{X\times Y} (\varepsilon \log \gamma + c - u - v) \cdot \gamma\, d\left(\rho_1 \otimes \rho_2\right) \\
&\geq \int_X u\, d\rho_1 + \int_Y v\, d\rho_2 - \varepsilon \int_{X\times Y} e^{\frac{u+v-c}{\varepsilon}}\, d\left(\rho_1 \otimes \rho_2\right) + \varepsilon \\
&= D_\varepsilon(u, v) + \varepsilon,
\end{aligned}$$

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&= \int_{X\times Y} (c + \varepsilon \log \gamma - u - v) \cdot \gamma d\rho_1 \otimes \rho_2 + \int_X u d\rho_1 + \int_Y v d\rho_2 \\
&= \int_X u d\rho_1 + \int_Y v d\rho_2 + \int_{X\times Y} (\varepsilon \log \gamma + c - u - v) \cdot \gamma d\left(\rho_1 \otimes \rho_2\right) \\
&\geq \int_X u d\rho_1 + \int_Y v d\rho_2 - \varepsilon \int_{X\times Y} e^{\frac{u+v-c}{\varepsilon}} d\left(\rho_1 \otimes \rho_2\right) + \varepsilon \\
&= D_\varepsilon(u, v) + \varepsilon,
\end{aligned}$$

$ts + \varepsilon t \ln t - \varepsilon \geq -\varepsilon e^{-s/\varepsilon}$
with equality if $t = e^{-s/\varepsilon}$

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Shannon Entropy-Regularized Optimal Transport

A duality approach

Theorem (S. Di Marino & AG, 2020)

The following are equivalent:

1. *(Maximizers)* u^* and v^* are maximizing potentials for dual problem;
2. *(Maximality condition)* $\mathcal{F}_1^{(c,\varepsilon)}(u^*) = v^*$ and $\mathcal{F}_2^{(c,\varepsilon)}(v^*) = u^*$;
3. *(Schrödinger system)* let $\gamma^* = e^{(u^*(x)+v^*(y)-c(x,y))/\varepsilon} \cdot \rho_1 \otimes \rho_2$, then $\gamma^* \in \Pi(\rho_1, \rho_2)$;
4. *(Duality attainement)* $\mathrm{OT}_\varepsilon(\rho_1, \rho_2) = D_\varepsilon(u^*, v^*) + \varepsilon$.

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Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

Shannon Entropy-Regularized Optimal Transport

A duality approach

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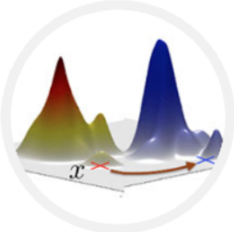
4. *(Duality attainement)* $\mathrm{OT}_\varepsilon(\rho_1, \rho_2) = D_\varepsilon(u^*, v^*) + \varepsilon$.

Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

$$1 \implies 2$$



Shannon Entropy-Regularized Optimal Transport

A duality approach

Theorem (S. Di Marino & AG, 2020)

The following are equivalent:

1. *(Maximizers)* u^* and v^* are maximizing potentials for dual problem;
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4. *(Duality attainement)* $\mathrm{OT}_\varepsilon(\rho_1, \rho_2) = D_\varepsilon(u^*, v^*) + \varepsilon$.

Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

$1 \implies 2$

We have $D_\varepsilon(u^*, (u^*)^{(c,\varepsilon)}) \geq D_\varepsilon(u^*, v^*)$;

However, by the maximality of u^*, v^* we have also $D_\varepsilon(u^*, (u^*)^{(c,\varepsilon)}) \leq D_\varepsilon(u^*, v^*)$;

So we conclude that $D_\varepsilon(u^*, (u^*)^{(c,\varepsilon)}) = D_\varepsilon(u^*, v^*)$.

Therefore $v^* = (u^*)^{(c,\varepsilon)}$.

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Shannon Entropy-Regularized Optimal Transport
A duality approach

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Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

$$2 \implies 3$$

Shannon Entropy-Regularized Optimal Transport

A duality approach

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4. *(Duality attainement)* $\mathrm{OT}_\varepsilon(\rho_1, \rho_2) = D_\varepsilon(u^*, v^*) + \varepsilon$.

Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

$2 \implies 3$ For every $u \in L_\varepsilon^{\exp}(\rho_1)$ and $v \in L_\varepsilon^{\exp}(\rho_2)$ we have

$$(\pi_1)_\sharp(e^{(u+v-c)/\varepsilon}\rho_1 \otimes \rho_2) = e^{(u-v^{(c,\varepsilon)})/\varepsilon}\rho_1$$

$$(\pi_2)_\sharp(e^{(u+v-c)/\varepsilon}\rho_1 \otimes \rho_2) = e^{(v-u^{(c,\varepsilon)})/\varepsilon}\rho_2$$

So if we assume 2 then we have $\gamma^* = e^{(u^*+v^*-c)/\varepsilon} \in \Pi(\rho_1, \rho_2)$.

Shannon Entropy-Regularized Optimal Transport
A duality approach

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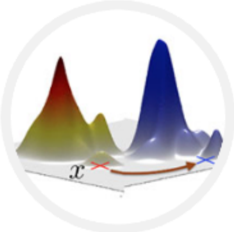
Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

$3 \implies 4$



Shannon Entropy-Regularized Optimal Transport

A duality approach

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4. *(Duality attainement)* $\mathrm{OT}_\varepsilon(\rho_1, \rho_2) = D_\varepsilon(u^*, v^*) + \varepsilon$.

Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

$3 \implies 4$ Since $\gamma^* \in \Pi(\rho_1, \rho_2)$, we have

$$\varepsilon \mathrm{KL}(\gamma^* | e^{-c/\varepsilon}) \geq D_\varepsilon(u, v) + \varepsilon \qquad \forall\, u \in L^{\exp}_\varepsilon(\rho_1), v \in L^{\exp}_\varepsilon(\rho_2)$$

$$\varepsilon \mathrm{KL}(\gamma | e^{-c/\varepsilon}) \geq D_\varepsilon(u^*, v^*) + \varepsilon \qquad \forall\, \gamma \in \Pi(\rho_1, \rho_2).$$

Shannon Entropy-Regularized Optimal Transport

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Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

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$$\varepsilon \mathrm{KL}(\gamma^* | e^{-c/\varepsilon}) \geq D_\varepsilon(u, v) + \varepsilon \qquad \forall\, u \in L^{\exp}_\varepsilon(\rho_1), v \in L^{\exp}_\varepsilon(\rho_2)$$

$$\varepsilon \mathrm{KL}(\gamma | e^{-c/\varepsilon}) \geq D_\varepsilon(u^*, v^*) + \varepsilon \qquad \forall\, \gamma \in \Pi(\rho_1, \rho_2).$$

Since by definition $\gamma^* = e^{u^*/\varepsilon} e^{v^*/\varepsilon} e^{-c/\varepsilon}$, one also has $\varepsilon \mathrm{KL}(\gamma^* | e^{-c/\varepsilon}) \geq D_\varepsilon(u^*, v^*) + \varepsilon$.

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A duality approach

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Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

$3 \implies 4$ Since $\gamma^* \in \Pi(\rho_1, \rho_2)$, we have

$$\varepsilon \mathrm{KL}(\gamma^* | e^{-c/\varepsilon}) \geq D_\varepsilon(u, v) + \varepsilon \qquad \forall\, u \in L^{\exp}_\varepsilon(\rho_1), v \in L^{\exp}_\varepsilon(\rho_2)$$

$$\varepsilon \mathrm{KL}(\gamma | e^{-c/\varepsilon}) \geq D_\varepsilon(u^*, v^*) + \varepsilon \qquad \forall\, \gamma \in \Pi(\rho_1, \rho_2).$$

Since by definition $\gamma^* = e^{u^*/\varepsilon} e^{v^*/\varepsilon} e^{-c/\varepsilon}$, one also has $\varepsilon \mathrm{KL}(\gamma^* | e^{-c/\varepsilon}) \geq D_\varepsilon(u^*, v^*) + \varepsilon$.

Putting everything together we get

$$\varepsilon \mathrm{KL}(\gamma | \mathcal{K}) \geq D_\varepsilon(u^*, v^*) + \varepsilon = \varepsilon \mathrm{KL}(\gamma^* | e^{-c/\varepsilon}) \geq D_\varepsilon(u, v) + \varepsilon;$$

Shannon Entropy-Regularized Optimal Transport

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Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

$4 \implies 1$

Shannon Entropy-Regularized Optimal Transport

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Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

$4 \implies 1$ Since $\varepsilon \mathrm{KL}(\gamma | e^{-c/\varepsilon}) \geq D_\varepsilon(u, v) + \varepsilon$, with equality iff $\gamma = e^{\frac{u+v-c}{\varepsilon}}$.

minimizing in γ we find that $\mathrm{OT}_\epsilon(\rho_1, \rho_2) \geq D_\varepsilon(u, v) + \varepsilon \qquad \forall\, u \in L^{\exp}_\varepsilon(\rho_1),\ v \in L^{\exp}_\varepsilon(\rho_2)$;

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Proof idea: $1 \implies 2 \implies 3 \implies 4 \implies 1$

$4 \implies 1$ Since $\varepsilon \mathrm{KL}(\gamma | e^{-c/\varepsilon}) \geq D_\varepsilon(u, v) + \varepsilon$, with equality iff $\gamma = e^{\frac{u+v-c}{\varepsilon}}$.

minimizing in γ we find that $\mathrm{OT}_\epsilon(\rho_1, \rho_2) \geq D_\varepsilon(u, v) + \varepsilon \qquad \forall\, u \in L^{\exp}_\varepsilon(\rho_1),\ v \in L^{\exp}_\varepsilon(\rho_2)$;

using that by hypotesis $\mathrm{OT}_\varepsilon(\rho_1, \rho_2) = D_\varepsilon(u^*, v^*) + \varepsilon$, we get that

$$D_\varepsilon(u^*, v^*) \geq D_\varepsilon(u, v) \qquad \forall\, u \in L^{\exp}_\varepsilon(\rho_1),\ v \in L^{\exp}_\varepsilon(\rho_2).$$

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4. *(Duality attainement)* $\mathrm{OT}_\varepsilon(\rho_1, \rho_2) = D_\varepsilon(u^*, v^*) + \varepsilon$.

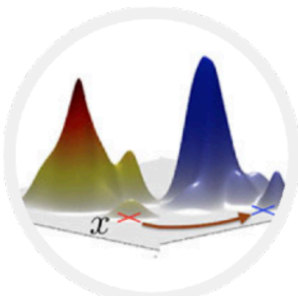
Remark (the role of the reference measure)

Let $(X, d_X, \mathfrak{m}_1)$, $(Y, d_Y, \mathfrak{m}_2)$ be Polish metric measure spaces, $c : X \times Y \to \mathbb{R}$
$\rho_1 \in \mathcal{P}(X)$ and $\rho_2 \in \mathcal{P}(Y)$ be probability measures such that $\mathrm{KL}(\rho_1|\mathfrak{m}_1) + \mathrm{KL}(\rho_2|\mathfrak{m}_2) < \infty$.

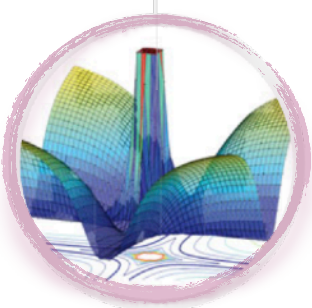
$$
\begin{aligned}
S_\varepsilon(\rho_1, \rho_2; \mathfrak{m}_1, \mathfrak{m}_2) :&= \min_{\gamma \in \Pi(\rho_1, \rho_2)} \left\{ \int_{X \times Y} c \, d\gamma + \varepsilon \, \mathrm{KL}(\gamma | \mathfrak{m}_1 \otimes \mathfrak{m}_2) \right\} \\
&= \mathrm{OT}_\varepsilon(\rho_1, \rho_2) + \varepsilon \, \mathrm{KL}(\rho_1|\mathfrak{m}_1) + \varepsilon \, \mathrm{KL}(\rho_2|\mathfrak{m}_2)
\end{aligned}
$$

Dual potentials: $u_0 - \varepsilon \log \rho_1 \in L^\infty(\mathfrak{m}_1)$ and $v_0 - \varepsilon \log \rho_2 \in L^\infty(\mathfrak{m}_2)$.

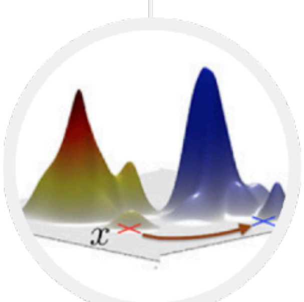
Outline



Duality approach for the Shannon Entropy-Regularized Optimal Transport



Convergence proof of the Sinkhorn algorithm (variational)



Applications

Shannon entropy regularized OT and Sinkhorn algorithm

$$\mathrm{OT}_\varepsilon(\rho_1, \rho_2) = \min_{\gamma \in \Pi(\rho_1,\rho_2)} \varepsilon \int_{X \times Y} \gamma \log\left(\frac{\gamma}{e^{-c/\varepsilon}}\right) d(\rho_1 \otimes \rho_2) \qquad \varepsilon > 0$$

$$= \min_{\gamma \in \Pi(\rho_1,\rho_2)} \int_{X \times Y} c(x,y)\, d\gamma(x,y) + \varepsilon \int_{X \times Y} \gamma(x,y) \log \gamma(x,y)\, d(\rho_1 \otimes \rho_2)\,.$$

There exists a unique minimizer γ^ε *(strictly convex)* $\gamma^\varepsilon(x,y) = a^\varepsilon(x) b^\varepsilon(y) e^{-c(x,y)/\varepsilon}$

If and only if solves the Schrödinger system

[E. Schrödinger, 1932]

$$\begin{cases} a^\varepsilon(x) \displaystyle\int_Y b^\varepsilon(y) e^{-c(x,y)/\varepsilon} d\rho_2(y) = 1 \\ b^\varepsilon(y) \displaystyle\int_X a^\varepsilon(y) e^{-c(x,y)/\varepsilon} d\rho_1(x) = 1 \end{cases}$$

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The algorithm: $a^0(x) = b^0(y) = 1$

Define the sequences (iteratively) $(a^n)_{n\in\mathbb{N}}$ and $(b^n)_{n\in\mathbb{N}}$ by

$$b^n(y) = \frac{1}{\int e^{-c(x,y)/\varepsilon}a^{n-1}(x)d\rho_1(x)},\ a^n(x) = \frac{1}{\int e^{-c(x,y)/\varepsilon}b^n(y)d\rho_2(y)}.$$

Shannon entropy regularized OT and Sinkhorn algorithm

Lemma: Let (X, d_X), (Y, d_Y) be Polish spaces, $c : X \times Y \to \mathbb{R}$ be a Borel bounded cost, $\rho_1 \in \mathcal{P}(X)$, $\rho_2 \in \mathcal{P}(Y)$ be probability measures. Then

$$D_\varepsilon(u, u^{(c,\varepsilon)}) \geq D_\varepsilon(u, v) \qquad \forall v \in L^{\exp}_\varepsilon(\rho_2),$$
$$D_\varepsilon(u, u^{(c,\varepsilon)}) = D_\varepsilon(u, v) \text{ if and only if } v = u^{(c,\varepsilon)}.$$

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Lemma

There exist $u^* \in L^{\exp}_\varepsilon(\rho_1)$ and $v^* \in L^{\exp}_\varepsilon(\rho_2)$ such that $D_\varepsilon(u, v) \leq D_\varepsilon(u^*, v^*)$ with $\|v^*\|_\infty, \|u^*\|_\infty \leq 3\|c\|_\infty/2$.
Moreover, there exist $a \in \mathbb{R}$ such that $u^* = (v + a)^{(c,\varepsilon)}$ and $v^* = (u^*)^{(c,\varepsilon)}$.

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Theorem (S. Di Marino & AG, 2020)

The following are equivalent:

1. *(Maximizers)* u^* and v^* are maximizing potentials for dual problem;
2. *(Maximality condition)* $\mathcal{F}_1^{(c,\varepsilon)}(u^*) = v^*$ and $\mathcal{F}_2^{(c,\varepsilon)}(v^*) = u^*$;
3. *(Schrödinger system)* let $\gamma^* = e^{(u^*(x)+v^*(y)-c(x,y))/\varepsilon} \cdot \rho_1 \otimes \rho_2$, then $\gamma^* \in \Pi(\rho_1, \rho_2)$;
4. *(Duality attainement)* $\mathrm{OT}_\varepsilon(\rho_1, \rho_2) = D_\varepsilon(u^*, v^*) + \varepsilon$.

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Convergence proof

Sinkhorn algorithm aka Iterative Proportional fitting procedure (IPFP)

Define the sequences (iteratively) $(a^n)_{n\in\mathbb{N}}$ and $(b^n)_{n\in\mathbb{N}}$ by

$$b^n(y) = \frac{1}{\int e^{-c(x,y)/\varepsilon} a^{n-1}(x) d\rho_1(x)},$$

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Theorem

If $(a^n)_{n\in\mathbb{N}}$ and $(b^n)_{n\in\mathbb{N}}$ are the IPFP sequences defined above, then there exists $(\lambda^n)_{n\in\mathbb{N}}, \lambda^n \in \mathbb{R}$ such that

$a^n/\lambda^n \to a$ in $L^p(\rho_1)$ and $\lambda^n b^n \to b$ in $L^p(\rho_2)$, $1 \le p < +\infty$, where (a, b) solve the Schrödinger problem.

In particular, the sequence $\gamma^n = a^n b^n e^{-c/\varepsilon}$, converges in $L^p(\rho_1 \otimes \rho_2)$ to γ_ε for any $1 \le p < +\infty$.

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Proof idea: Let us write $a^n = e^{u_n/\varepsilon}$, $b^n = e^{v_n/\varepsilon}$

$$\begin{cases} v_{2n+1} = (u_{2n})^{(c,\varepsilon)} \\ u_{2n+1} = u_{2n} \end{cases}, \quad \begin{cases} v_{2n+2} = v_{2n+1} \\ u_{2n+2} = (v_{2n+1})^{(c,\varepsilon)} \end{cases}.$$

$\exists\ \ell_n \in \mathbb{R}$ such that
$\|u_n - \ell_n\|_\infty, \|v_n + \ell_n\| \le \frac{3}{2}\|c\|_\infty$

$$D_\varepsilon(u_n, v_n) \le D_\varepsilon(u_{n+1}, v_{n+1}) \le \cdots \le \mathrm{OT}_\varepsilon(\rho_1, \rho_2) - \varepsilon.$$

$u_n - \ell_n$ and $v_n + \ell_n$ are precompact in every L^p, for $1 \le p < \infty$

One obtain

$$D_\varepsilon(v^{(c,\varepsilon)}, v) - D_\varepsilon(u, v) = \lim_{n_k\to\infty} D_\varepsilon(u_{n_k+1}, v_{n_k+1}) - D_\varepsilon(u_{n_k}, v_{n_k}) = 0.$$

$$D_\varepsilon(u, u^{(c,\varepsilon)}) - D_\varepsilon(u, v) = \lim_{n_k\to\infty} D_\varepsilon(u_{n_k+2}, v_{n_k+2}) - D_\varepsilon(u_{n_k}, v_{n_k}) = 0.$$

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Robustness of the Sinkhorn algorithm

Proposition (Continuity with respect to the marginals)

The functional $\mathrm{OT}_\varepsilon(\rho_1, \rho_2)$ is continuous: if $(\rho_1^n)_{n\in\mathbb{N}} \subset \mathcal{P}(X)$ and $(\rho_2^n)_{n\in\mathbb{N}} \subset \mathcal{P}(Y)$ are sequences weakly converging respectively to ρ_1 and ρ_2, then the corresponding Kantorovich potentials $(u_n)_{n\in\mathbb{N}}$ and $(v_n)_{n\in\mathbb{N}}$ converges uniformly in L^∞ to (u^*, v^*).

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For each $n \in \mathbb{N}$ consider the couple of optimal potentials (u_n, v_n).

WLOG assume that one is the $u_n = (v_n)^{(c,\varepsilon)}$ and $v_n = (u_n)^{(c,\varepsilon)}$.

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The potentials u_n and v_n are bounded for all $n \in \mathbb{N}$ and then, by Banach-Alaoglu theorem, there exists subsequences $(u_{n_k})_{n_k\in\mathbb{N}}$ and $(v_{n_k})_{n_k\in\mathbb{N}}$ such that $u_{n_k} \to u^*$ and $v_{n_k} \to v^*$ (unif.).

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Similarly, one can show that (u^*, v^*) is a maximizer couple for ρ_1 and ρ_2.

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Wasserstein distance as a loss function

$$\min_{\nu \in \mathcal{P}(X)} \mathrm{OT}_\varepsilon(\nu, \rho_1)$$

Wasserstein distance as a loss function

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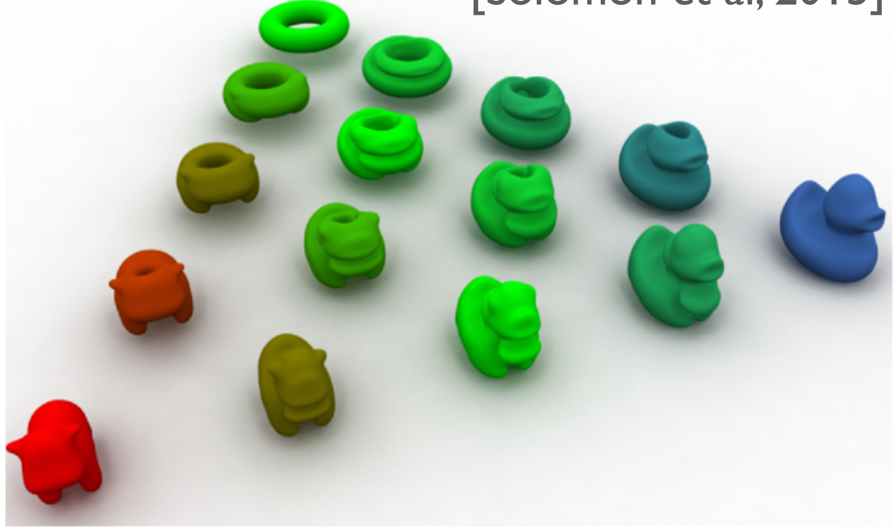
Wasserstein Barycenters $\rho_1, \cdots, \rho_N$ be probability measures in X and $\lambda_1, \ldots, \lambda_N \geq 0$ such that $\sum_{j=1}^N \lambda_j = 1$.

$$\min_{\nu \in \mathcal{P}(X)} \sum_{i=1}^N \lambda_i \mathrm{OT}_\varepsilon(\nu, \rho_i)$$

[Solomon et al, 2015]



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$$\min_{\nu \in \mathcal{P}(X)} \mathrm{OT}_\varepsilon(\nu, \rho_1)$$

How to compute "$\nabla \mathrm{OT}_\varepsilon(\nu, \rho_1)$" ?

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Wasserstein distance as a loss function

$$\min_{\nu \in \mathcal{P}(X)} \mathrm{OT}_\varepsilon(\nu, \rho)$$

How to compute "$\nabla \mathrm{OT}_\varepsilon(\nu, \rho)$" ?

Theorem

Let (X, d_X), (Y, d_Y) be Polish spaces, $c : X \times Y \to \mathbb{R}$ be a Borel bounded cost, $\nu \in \mathcal{P}(X)$, $\rho \in \mathcal{P}(Y)$ be probability measures.The Fréchet differential of $\mathrm{OT}_\varepsilon(\nu, \rho)$ is given by

$$\nabla \mathrm{OT}_\varepsilon(\nu, \rho) := \left(\frac{\delta \mathrm{OT}_\varepsilon(\nu, \rho)}{\delta \nu}, \frac{\delta \mathrm{OT}_\varepsilon(\nu, \rho)}{\delta \rho} \right) = (u^*, v^*)\,,$$

where (u^*, v^*) are Kantorovich potentials such that $u^* = (v^*)^{(c,\varepsilon)}$

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Wasserstein distance as a loss function

Proof idea:

Wasserstein distance as a loss function

Proof idea: Let $\nu^t = \nu + t\chi$, $\rho^t = \rho + t\alpha$ and

(u, v) (resp. (u_t, v_t)) the optimal potentials for $\mathrm{OT}_\varepsilon(\nu, \rho)$ (resp. $\mathrm{OT}_\varepsilon(\nu^t, \rho^t)$).

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$$\frac{\mathrm{OT}_\varepsilon(\nu^t, \rho^t) - \mathrm{OT}_\varepsilon(\nu, \rho)}{t} \leq \int_X u_t d\chi - \varepsilon \int_{X\times Y} \exp\left(\frac{u_t(x) - v_t(y) - c(x,y)}{\varepsilon}\right) d(\chi \otimes \rho) +$$
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Combining both inequalities we have $\dfrac{\delta \mathrm{OT}_\varepsilon}{\delta \nu}(\nu, \rho) = u$ and $\dfrac{\delta \mathrm{OT}_\varepsilon}{\delta \rho}(\nu, \rho) = v.$

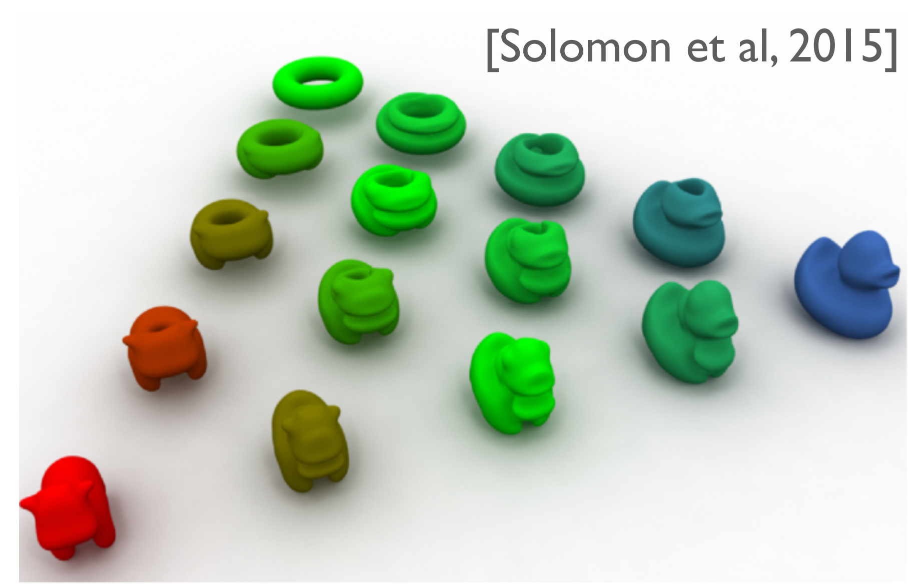
Wasserstein distance as a loss function

$$\min_{\nu \in \mathcal{P}(X)} \mathrm{OT}_{\varepsilon}(\nu, \rho)$$

Wasserstein Barycenters

$\rho_1, \cdots, \rho_N$ be probability measures in X and $\lambda_1, \ldots, \lambda_N \geq 0$ such that $\sum_{j=1}^{N} \lambda_j = 1$.

$$\min_{\nu \in \mathcal{P}(X)} \sum_{i=1}^{N} \lambda_i \mathrm{OT}_{\varepsilon}(\nu, \rho_i)$$



[Solomon et al, 2015]