Bridging the gap between Optimal Transport and MMD with Sinkhorn Divergences

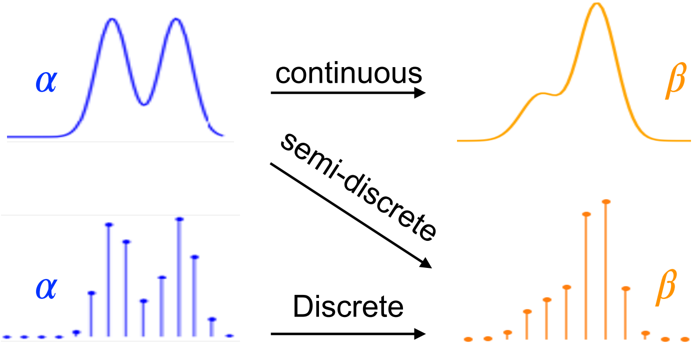
Aude Genevay

MIT CSAIL

CIRM Workshop - March 2020

Joint work with Gabriel Peyré, Marco Cuturi, Francis Bach, Lénaïc Chizat

Comparing Probability Measures



Discrete Setting (Quantization)

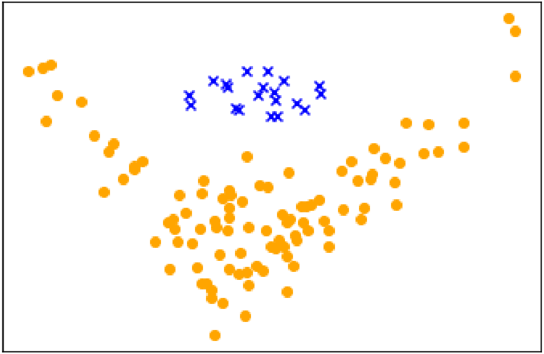


Figure 1 – $\min_{(x_1,\ldots,x_k)} \mathcal{D}(\frac{1}{k}\sum_{i=1}^{k}\delta x_i, \frac{1}{n}\sum_{i=1}^{n}\delta y_j)$

Discrete Setting (Quantization)

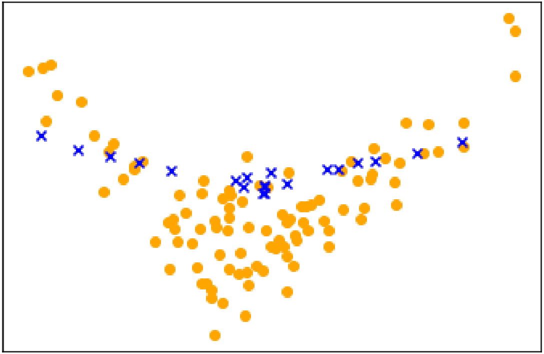


Figure 1 – $\min_{(x_1,\ldots,x_k)} \mathcal{D}\left(\frac{1}{k}\sum_{i=1}^{k} \delta x_i, \frac{1}{n}\sum_{i=1}^{n} \delta y_j\right)$

Discrete Setting (Quantization)

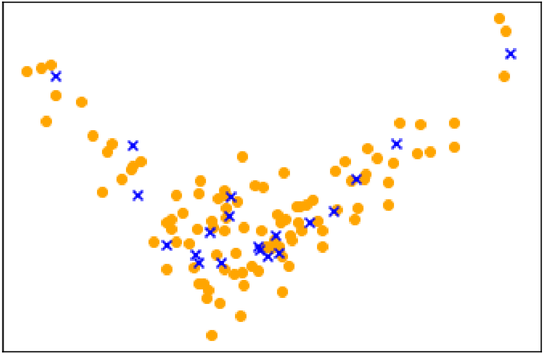


Figure 1 – $\min_{(x_1,\ldots,x_k)} \mathcal{D}\left(\frac{1}{k}\sum_{i=1}^{k} \delta x_i, \frac{1}{n}\sum_{i=1}^{n} \delta y_j\right)$

Discrete Setting (Quantization)

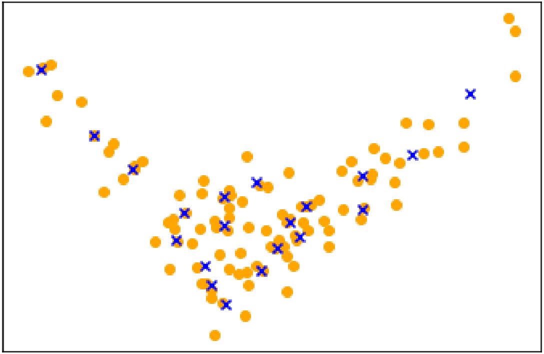


Figure 1 – $\min_{(x_1,\ldots,x_k)} \mathcal{D}\left(\frac{1}{k}\sum_{i=1}^{k}\delta x_i, \frac{1}{n}\sum_{i=1}^{n}\delta y_j\right)$

Semi-discrete Setting (Density Fitting)

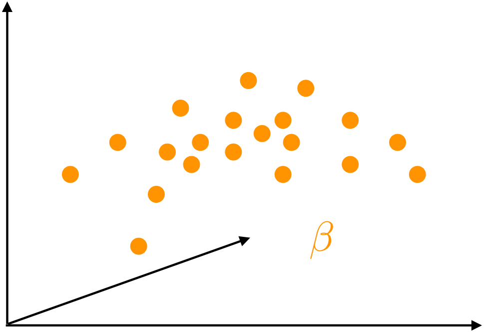


Figure 2 – $\min_\theta \mathcal{D}(\alpha_\theta, \beta)$

Semi-discrete Setting (Density Fitting)

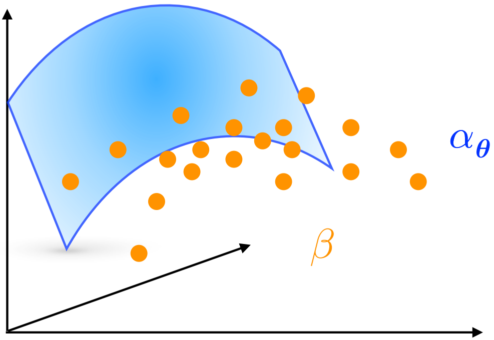


Figure 2 – $\min_{\theta} \mathcal{D}(\alpha_{\theta}, \beta)$

Semi-discrete Setting (Density Fitting)

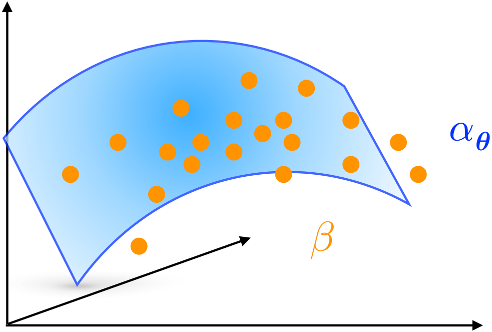


Figure 2 – $\min_\theta \mathcal{D}(\alpha_\theta, \beta)$

Semi-discrete Setting (Density Fitting)

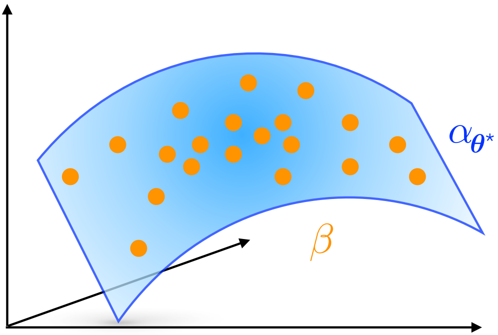


Figure 2 – $\min_\theta \mathcal{D}(\alpha_\theta, \beta)$

φ-divergences (Czisar '63)

Definition (φ-divergence)

Let φ convex l.s.c. function such that $\varphi(1) = 0$, the φ-divergence D_φ between two measures α and β is defined by :

$$D_\varphi(\alpha|\beta) \stackrel{\text{def.}}{=} \int_{\mathcal{X}} \varphi\left(\frac{\mathrm{d}\alpha(x)}{\mathrm{d}\beta(x)}\right)\mathrm{d}\beta(x).$$

Example (Kullback Leibler Divergence)

$$D_{KL}(\alpha|\beta) = \int_{\mathcal{X}} \log\left(\frac{\mathrm{d}\alpha}{\mathrm{d}\beta}(x)\right)\mathrm{d}\alpha(x) \quad \leftrightarrow \quad \varphi(x) = x\log(x)$$

Weak Convergence of measures

Example

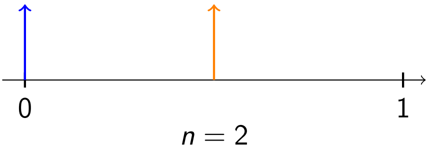
On $\mathbb{R}$, $\alpha = \delta_0$ and $\alpha_n = \delta_{1/n}$: $D_{KL}(\alpha_n|\alpha) = +\infty$.

$n = 1$

Weak Convergence of measures

Example

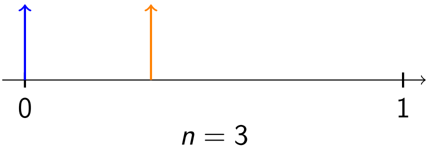
On $\mathbb{R}$, $\alpha = \delta_0$ and $\alpha_n = \delta_{1/n}$: $D_{KL}(\alpha_n|\alpha) = +\infty$.



Weak Convergence of measures

Example

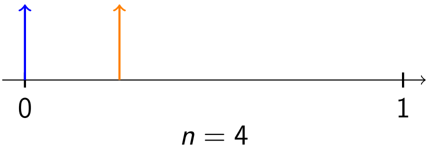
On $\mathbb{R}$, $\alpha = \delta_0$ and $\alpha_n = \delta_{1/n}$: $D_{KL}(\alpha_n|\alpha) = +\infty$.



Weak Convergence of measures

Example

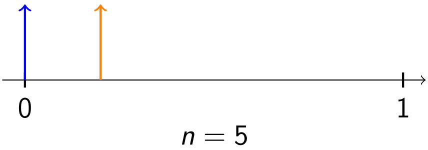
On $\mathbb{R}$, $\alpha = \delta_0$ and $\alpha_n = \delta_{1/n}$: $D_{KL}(\alpha_n|\alpha) = +\infty$.



Weak Convergence of measures

Example

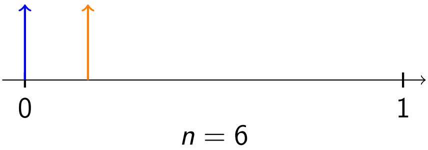
On $\mathbb{R}$, $\alpha = \delta_0$ and $\alpha_n = \delta_{1/n}$: $D_{KL}(\alpha_n|\alpha) = +\infty$.



Weak Convergence of measures

Example

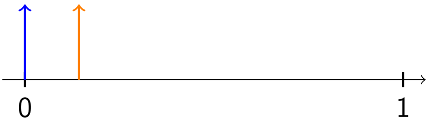
On $\mathbb{R}$, $\alpha = \delta_0$ and $\alpha_n = \delta_{1/n}$: $D_{KL}(\alpha_n|\alpha) = +\infty$.



Weak Convergence of measures

Example

On $\mathbb{R}$, $\alpha = \delta_0$ and $\alpha_n = \delta_{1/n}$: $D_{KL}(\alpha_n|\alpha) = +\infty$.

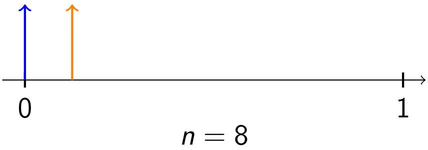


$n = 7$

Weak Convergence of measures

Example

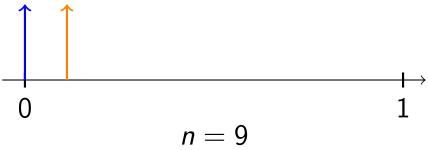
On $\mathbb{R}$, $\alpha = \delta_0$ and $\alpha_n = \delta_{1/n}$: $D_{KL}(\alpha_n|\alpha) = +\infty$.



Weak Convergence of measures

Example

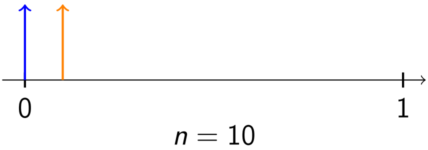
On $\mathbb{R}$, $\alpha = \delta_0$ and $\alpha_n = \delta_{1/n}$: $D_{KL}(\alpha_n|\alpha) = +\infty$.



Weak Convergence of measures

Example

On $\mathbb{R}$, $\alpha = \delta_0$ and $\alpha_n = \delta_{1/n}$: $D_{KL}(\alpha_n|\alpha) = +\infty$.



Definition (Weak Convergence)

α_n **weakly converges** to α, (denoted $\alpha_n \rightharpoonup \alpha$)
$\Leftrightarrow \int f(x)\mathrm{d}\alpha_n(x) \to \int f(x)\mathrm{d}\alpha(x)\ \forall f \in \mathcal{C}_b(\mathcal{X})$.
Let $\mathcal{D}$ distance between measures , $\mathcal{D}$ **metrises weak convergence** IFF$\left(\mathcal{D}(\alpha_n, \alpha) \to 0 \Leftrightarrow \alpha_n \rightharpoonup \alpha\right)$.

Maximum Mean Discrepancies (Gretton '06)

Definition (RKHS)

Let $\mathcal{H}$ a Hilbert space with kernel k, then $\mathcal{H}$ is a Reproducing Kernel Hilbert Space (RKHS) IFF :

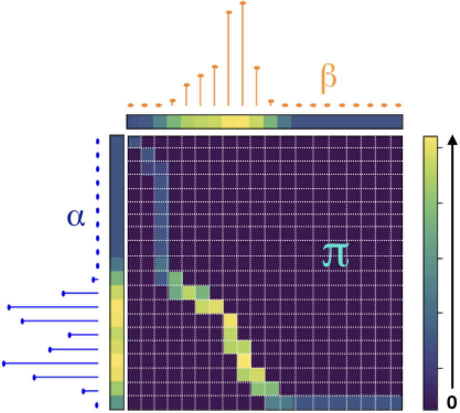
1. $\forall x \in \mathcal{X}, \quad k(x, \cdot) \in \mathcal{H}$,
2. $\forall f \in \mathcal{H}, \quad f(x) = \langle f, k(x, \cdot) \rangle_{\mathcal{H}}$.

Let $\mathcal{H}$ a RKHS avec kernel k, the distance **MMD** between two probability measures α and β is defined by :

$$
\begin{aligned}
MMD_k^2(\alpha, \beta) &\overset{\text{def.}}{=} \left(\sup_{\{f \mid \|f\|_{\mathcal{H}} \leqslant 1\}} |\mathbb{E}_\alpha(f(X)) - \mathbb{E}_\beta(f(Y))| \right)^2 \\
&= \mathbb{E}_{\alpha \otimes \alpha}[k(X, X')] + \mathbb{E}_{\beta \otimes \beta}[k(Y, Y')] \\
&\quad -2\mathbb{E}_{\alpha \otimes \beta}[k(X, Y)].
\end{aligned}
$$

Optimal Transport (Monge 1781, Kantorovitch '42)

- $c(x, y)$: cost of moving a unit of mass from x to y
- $\pi(x, y)$ (coupling) : how much mass moves from x to y



The Wasserstein Distance

Minimal cost of moving all the mass from α to β ?

Let $\alpha \in \mathcal{M}_+^1(\mathcal{X})$ and $\beta \in \mathcal{M}_+^1(\mathcal{Y})$,

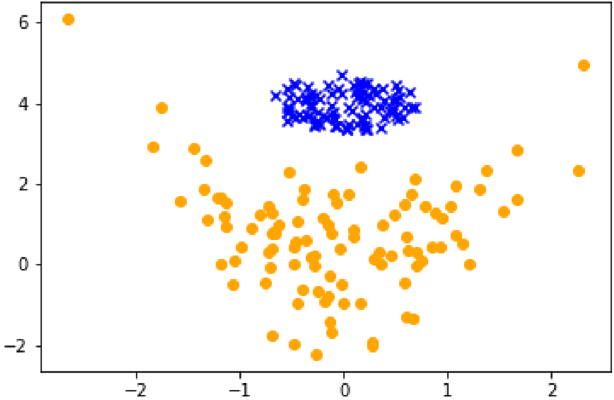
$$W_c(\alpha, \beta) = \min_{\pi \in \Pi(\alpha,\beta)} \int_{\mathcal{X}\times\mathcal{Y}} c(x,y)\mathrm{d}\pi(x,y) \qquad (\mathcal{P})$$

For $c(x,y) = \|x-y\|_2^p$, $W_c(\alpha,\beta)^{1/p}$ is the **p-Wasserstein distance**.

Optimal Transport vs. MMD

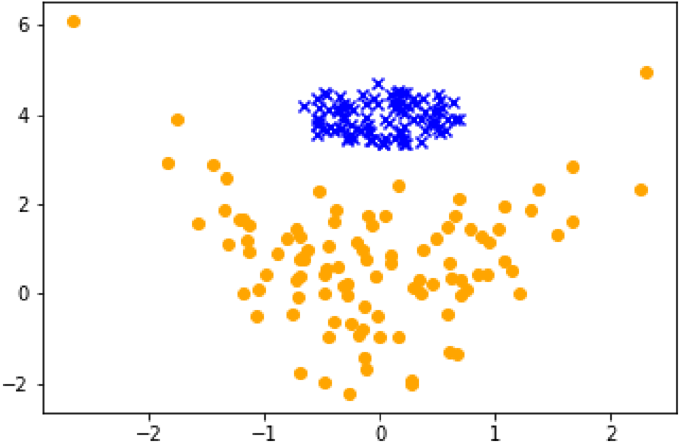
	MMD	**OT**
sample complexity	$(\frac{1}{\sqrt{n}})$	$O(n^{-1/d})$ (curse of dimension)
computation	$O(n^2)$	$O(n^3\log(n))$

Simple example

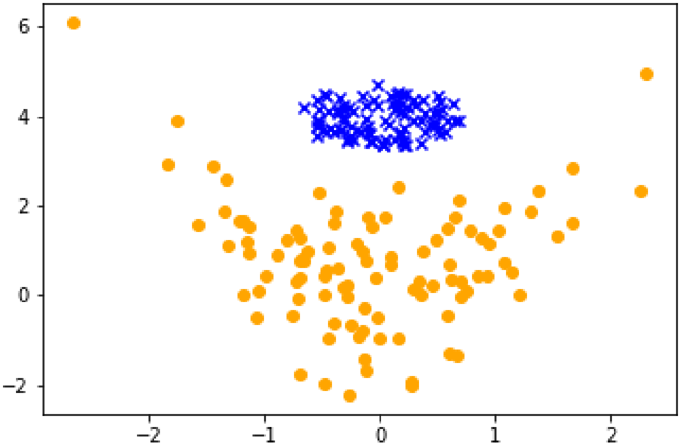


$$\underset{(x_1,\ldots,x_n)}{min} \mathcal{D}\left(\frac{1}{n}\sum_{i=1}^{n}\delta x_i, \frac{1}{n}\sum_{i=1}^{n}\delta y_j\right)$$

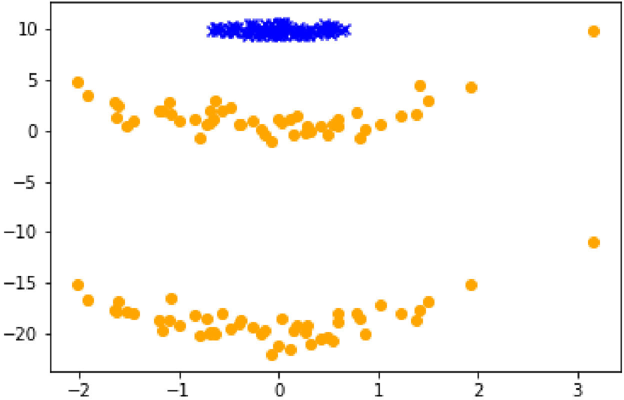
Discrete gradient flow of *MMD*



Discrete gradient flow of OT

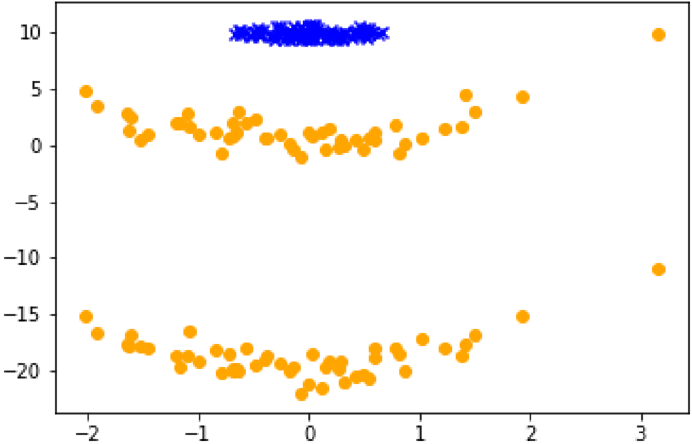


Another example

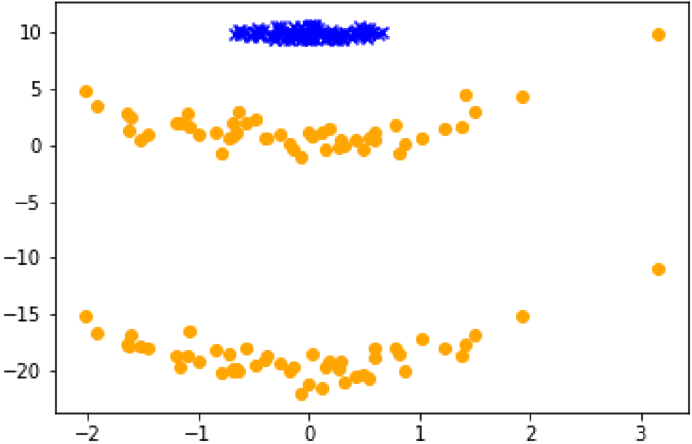


$$\underset{(x_1,\dots,x_n)}{min} \mathcal{D}\left(\frac{1}{n}\sum_{i=1}^{n}\delta x_i, \frac{1}{n}\sum_{i=1}^{n}\delta y_j\right)$$

Discrete gradient flow of *MMD*

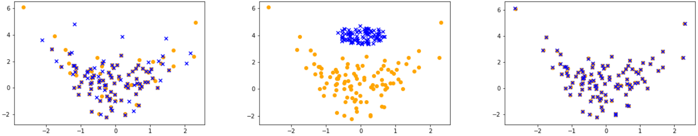


Discrete gradient flow of OT



Optimal Transport vs. MMD

	MMD	**OT**
sample complexity	$\left(\frac{1}{\sqrt{n}}\right)$	$O(n^{-1/d})$ (curse of dimension)
computation	$O(n^2)$	$O(n^3 \log(n))$
		better gradients !



$\underset{(x_1,\ldots,x_k)}{min} \mathcal{D}\left(\frac{1}{k}\sum_{i=1}^{k} \delta x_i, \frac{1}{n}\sum_{i=1}^{n} \delta y_j\right)$ after 200 steps of grad. descent.

1. Notions of Distance between Measures
2. Entropic Regularization of Optimal Transport
   - The basics
   - A magic regularizing tool !
   - Sample Complexity
3. Sinkhorn Divergences : Interpolation between OT and MMD
4. Conclusion

Entropic Regularization (Cuturi '13)

Let $\alpha \in \mathcal{M}_+^1(\mathcal{X})$ and $\beta \in \mathcal{M}_+^1(\mathcal{Y})$,

$$W_c \ (\alpha, \beta) \stackrel{\text{def.}}{=} \min_{\pi \in \Pi(\alpha, \beta)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) \mathrm{d}\pi(x, y) \qquad (\mathcal{P})$$

Entropic Regularization (Cuturi '13)

Let $\alpha \in \mathcal{M}_+^1(\mathcal{X})$ and $\beta \in \mathcal{M}_+^1(\mathcal{Y})$,

$$W_{c,\varepsilon}(\alpha, \beta) \overset{\text{def.}}{=} \min_{\pi \in \Pi(\alpha,\beta)} \int_{\mathcal{X}\times\mathcal{Y}} c(x,y)\mathrm{d}\pi(x,y) + \varepsilon H(\pi|\alpha \otimes \beta), \quad (\mathcal{P}_\varepsilon)$$

where

$$H(\pi|\alpha \otimes \beta) \overset{\text{def.}}{=} \int_{\mathcal{X}\times\mathcal{Y}} \log\left(\frac{\mathrm{d}\pi(x,y)}{\mathrm{d}\alpha(x)\mathrm{d}\beta(y)}\right)\mathrm{d}\pi(x,y).$$

relative entropy of the transport plan π with respect to the product measure $\alpha \otimes \beta$.

Entropic Regularization

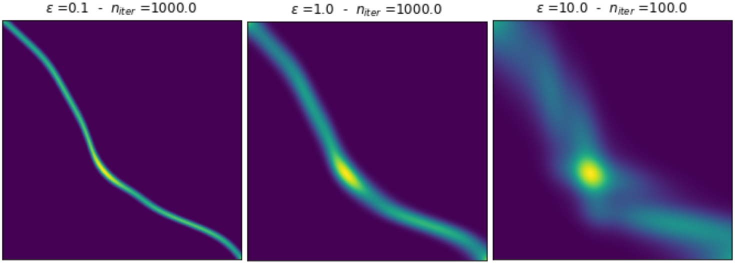


Figure 3 – Influence of the regularization parameter ε on the transport plan π.

Intuition : the entropic penalty 'smoothes' the problem and avoids over fitting (think of ridge regression for least squares)

Dual Formulation

Contrary to standard OT, no constraint on the dual problem :

$$W_c \; (\alpha, \beta) = \max_{\substack{u \in \mathcal{C}(\mathcal{X}) \\ v \in \mathcal{C}(\mathcal{Y})}} \int_{\mathcal{X}} u(x) \mathrm{d}\alpha(x) + \int_{\mathcal{Y}} v(y) \mathrm{d}\beta(y) \qquad (\mathcal{D})$$

such that $\quad \{ u(x) + v(y) \leqslant c(x,y) \, \forall \, (x,y) \in \mathcal{X} \times \mathcal{Y} \}$

Dual Formulation

Contrary to standard OT, no constraint on the dual problem :

$$W_{c,\varepsilon}(\alpha,\beta) = \max_{\substack{u \in \mathcal{C}(\mathcal{X}) \\ v \in \mathcal{C}(\mathcal{Y})}} \int_{\mathcal{X}} u(x)\mathrm{d}\alpha(x) + \int_{\mathcal{Y}} v(y)\mathrm{d}\beta(y)$$

$$- \varepsilon \int_{\mathcal{X}\times\mathcal{Y}} e^{\frac{u(x)+v(y)-c(x,y)}{\varepsilon}} \mathrm{d}\alpha(x)\mathrm{d}\beta(y) + \varepsilon.$$

Sinkhorn's Algorithm

Iterative algorithm : alternate between optimizing over u with fixed v and optimizing over v with fixed u.

Sinkhorn's Algorithm

Iterative algorithm : alternate between optimizing over u with fixed v and optimizing over v with fixed u.

Sinkhorn's Algorithm

Let $\mathbf{K}_{ij} = e^{-\frac{c(x_i, y_j)}{\varepsilon}}, \mathbf{a} = e^{\frac{\mathbf{u}}{\varepsilon}}, \mathbf{b} = e^{\frac{\mathbf{v}}{\varepsilon}}$.

$$\mathbf{a}^{(\ell+1)} = \frac{1}{\mathbf{K}(\mathbf{b}^{(\ell)} \odot \boldsymbol{\beta})} \quad ; \quad \mathbf{b}^{(\ell+1)} = \frac{1}{\mathbf{K}^T(\mathbf{a}^{(\ell+1)} \odot \boldsymbol{\alpha})}$$

Complexity of each iteration : $O(n^2)$,
Linear convergence, constant degrades when $\varepsilon \to 0$.

Differentiable approximation of OT

Bonus : Sinkhorn procedure is fully differentiable with auto-diff tools (e.g TensorFlow) $\Rightarrow$ yields a differentiable approximation of OT !

Some applications :

- Differentiable sorting (Cuturi et al '19)
- Differentiable (or 'soft') assignments
- Differentiable clustering (G. et al '19)
- Learning with a regularized Wasserstein loss ($\rightarrow$ more on that later...)

The 'sample complexity'

Informal Definition

*Given a distance between measures , its **sample complexity** corresponds to the error made when approximating this distance with samples of the measures.*

$\rightarrow$ Bad sample complexity implies bad generalization (over-fitting).

Known cases :

- OT : $\mathbb{E}|W(\alpha, \beta) - W(\hat{\alpha}_n, \hat{\beta}_n)| = O(n^{-1/d})$
  $\Rightarrow$ curse of dimension (Dudley '84, Weed and Bach '18)
- MMD : $\mathbb{E}|MMD(\alpha, \beta) - MMD(\hat{\alpha}_n, \hat{\beta}_n)| = O(\frac{1}{\sqrt{n}})$
  $\Rightarrow$ independent of dimension (Gretton '06)

What about $\mathbb{E}|W_\varepsilon(\alpha, \beta) - W_\varepsilon(\hat{\alpha}_n, \hat{\beta}_n)|$?

'Sample Complexity' of W_ε.

Theorem (G., Chizat, Bach, Cuturi, Peyré '19) (Mena, Weed '19)

Let $\mathcal{X}, \mathcal{Y} \subset \mathbb{R}^d$ bounded , and $c \in \mathcal{C}^\infty$ L-Lipschitz. Then

$$\mathbb{E}|W_\varepsilon(\alpha, \beta) - W_\varepsilon(\hat{\alpha}_n, \hat{\beta}_n)| = O\left(\frac{1}{\sqrt{n}}\left(1 + \frac{1}{\varepsilon^{\lfloor d/2 \rfloor}}\right)\right),$$

where constants depend on $|\mathcal{X}|$, $|\mathcal{Y}|$, d, and $\left\|c^{(k)}\right\|_\infty$ pour $k = 0 \ldots \lfloor d/2 \rfloor + 1$.

'Sample Complexity' of W_ε.

We get the following asymptotic behavior

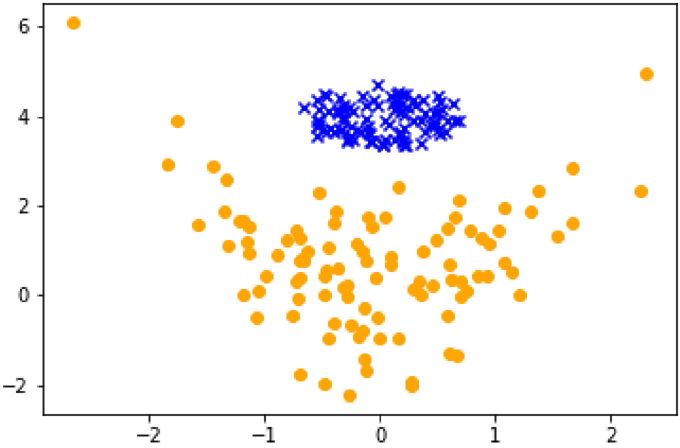
$$\mathbb{E}|W_\varepsilon(\alpha, \beta) - W_\varepsilon(\hat{\alpha}_n, \hat{\beta}_n)| = O\left(\frac{1}{\varepsilon^{\lfloor d/2 \rfloor}\sqrt{n}}\right) \qquad \text{when } \varepsilon \to 0$$

$$\mathbb{E}|W_\varepsilon(\alpha, \beta) - W_\varepsilon(\hat{\alpha}_n, \hat{\beta}_n)| = O\left(\frac{1}{\sqrt{n}}\right) \qquad \text{when } \varepsilon \to +\infty.$$

$\rightarrow$ A large enough regularization breaks the curse of dimension.

1. Notions of Distance between Measures
2. Entropic Regularization of Optimal Transport
3. Sinkhorn Divergences : Interpolation between OT and MMD
   - Definition and properties
   - Learning with Sinkhorn Divergences
4. Conclusion

Discrete gradient flow of W_ε, $\varepsilon = 1$



The effect of entropy

Entropic Transport is Maximum Likelihood under Gaussian noise (Rigollet Weed '18)

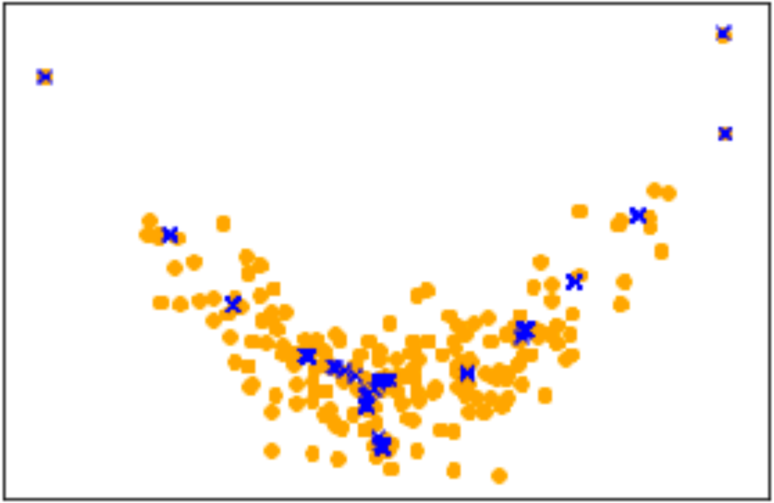
Consider a sample $(x_1, \dots, x_n) \sim X$ from the model

$$X = Y + \zeta \quad \text{where } Y \sim \alpha_\theta,\ \zeta \sim \mathcal{N}(0, \varepsilon).$$

Then,

$$\hat{\theta}^{MLE} = min_\theta W_\varepsilon(\alpha_\theta, \frac{1}{n}\sum_{i=1}^{n} \delta x_i)$$

The effect of entropy



Sinkhorn Divergences

Issue of regularized Wass. Distance : $W_{c,\varepsilon}(\alpha, \alpha) \neq 0$
Proposed Solution : introduce corrective terms to 'debias' regularized Wasserstein distance

Definition (Sinkhorn Divergences)

Let $\alpha \in \mathcal{M}_+^1(\mathcal{X})$ and $\beta \in \mathcal{M}_+^1(\mathcal{Y})$,

$$SD_{c,\varepsilon}(\alpha, \beta) \stackrel{\text{def.}}{=} W_{c,\varepsilon}(\alpha, \beta) - \frac{1}{2} W_{c,\varepsilon}(\alpha, \alpha) - \frac{1}{2} W_{c,\varepsilon}(\beta, \beta),$$

Interpolation Property

Theorem (G., Peyré, Cuturi '18), (Ramdas and al. '17)

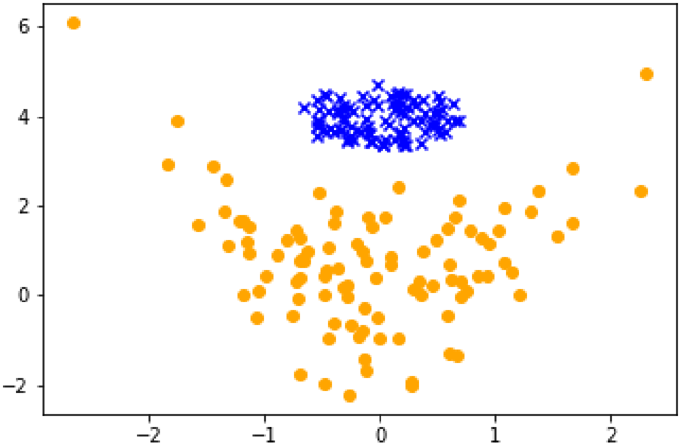
Sinkhorn Divergences have the following asymptotic behavior :

$$\text{when } \varepsilon \to 0, \quad SD_{c,\varepsilon}(\alpha, \beta) \to W_c(\alpha, \beta), \tag{1}$$

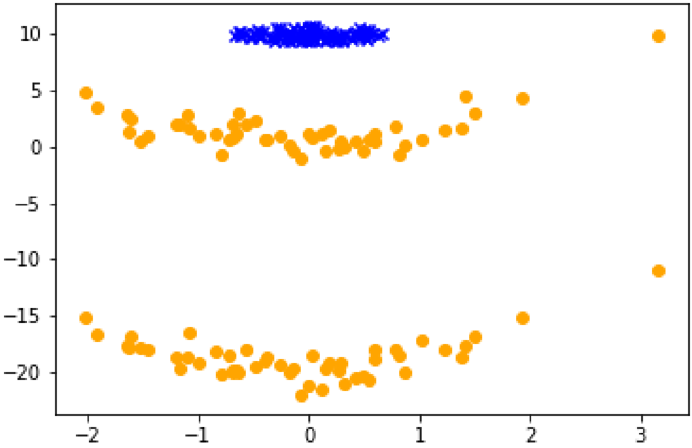
$$\text{when } \varepsilon \to +\infty, \quad SD_{c,\varepsilon}(\alpha, \beta) \to \frac{1}{2} MMD^2_{-c}(\alpha, \beta). \tag{2}$$

Remark : To get an MMD, $-c$ must be positive definite. For $c = \| \cdot \|_2^p$ with $0 < p < 2$, the MMD is called Energy Distance.

Discrete gradient flow of SD_ε, $\varepsilon = 1$



Discrete gradient flow of SD_ε, $\varepsilon = 1$



Summary

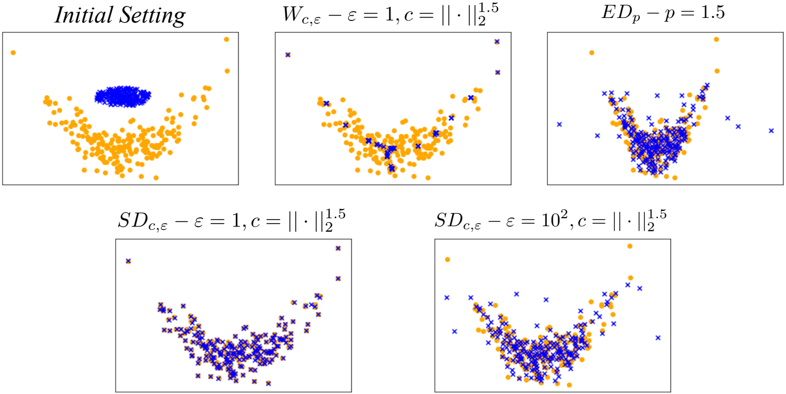
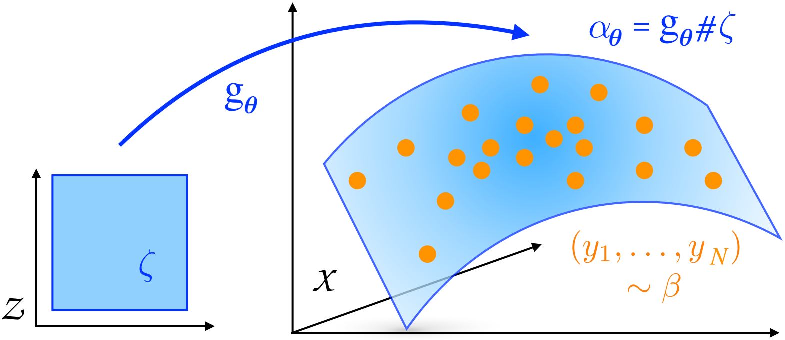


Figure 4 – Goal : Recover the positions of the Diracs with gradient descent. Orange circles : target distribution β, blue crosses : parametric model after convergence α_{θ^*}. Upper right : initial setting α_{θ_0}.

Generative Models



Problem Formulation

- β the **unknown** measure of the data :
  finite number of samples $(y_1, \ldots, y_N) \sim \beta$
- α_θ the parametric model of the form $\alpha_\theta \stackrel{\text{def.}}{=} g_{\theta\#}\zeta$:
  to sample $x \sim \alpha_\theta$, draw $z \sim \zeta$ and take $x = g_\theta(z)$.

We are looking for the optimal parameterθ^* defined by

$$\theta^* \in \underset{\theta}{\operatorname{argmin}}\ SD_{c,\varepsilon}(\alpha_\theta, \beta)$$

NB : α_θ and β are only known via their samples.

The Optimization Procedure

We want to solve by gradient descent

$$\min_{\theta} SD_{c,\varepsilon}(\alpha_\theta, \beta)$$

At each descent step k instead of approximating $\nabla_\theta SD_{c,\varepsilon}(\alpha_\theta, \beta)$:

- we approximate $SD_{c,\varepsilon}(\alpha_{\theta^{(k)}}, \beta)$ by $SD^{(L)}_{c,\varepsilon}(\hat{\alpha}_{\theta^{(k)}}, \hat{\beta})$ via
  - minibatches : draw n samples from $\alpha_{\theta^{(k)}}$ and m in the dataset (distributed according to β),
  - L Sinkhorn iterations : we compute an approximation of the SD between both samples with a fixed number of iterations
- we compute the gradient $\nabla_\theta SD^{(L)}_{c,\varepsilon}(\hat{\alpha}_{\theta^{(k)}}, \hat{\beta})$ by backpropagation (with automatic differentiation library)
- we do an update $\theta^{(k+1)} = \theta^{(k)} - C_k \nabla_\theta SD^{(L)}_{c,\varepsilon}(\hat{\alpha}_{\theta^{(k)}}, \hat{\beta})$

Computing the Gradient in Practice

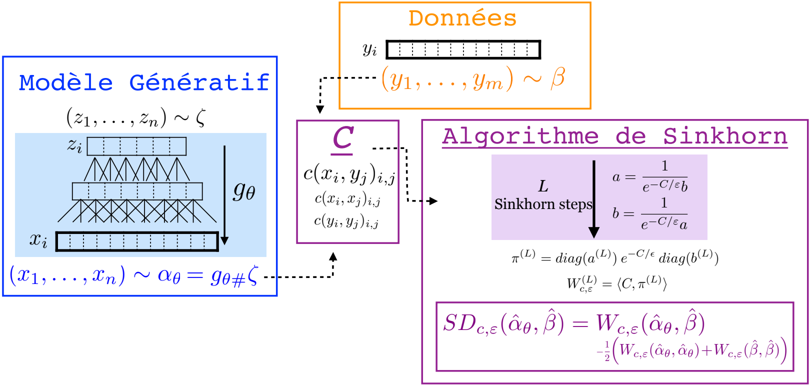


Figure 5 – Scheme of the approximation of the Sinkhorn Divergence from samples (here, $g_\theta : z \mapsto x$ is represented as a 2-layer NN).

Empirical Results

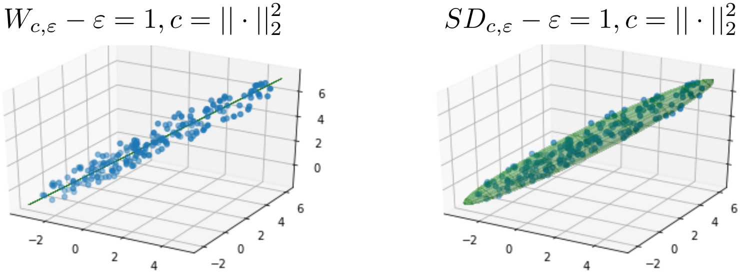
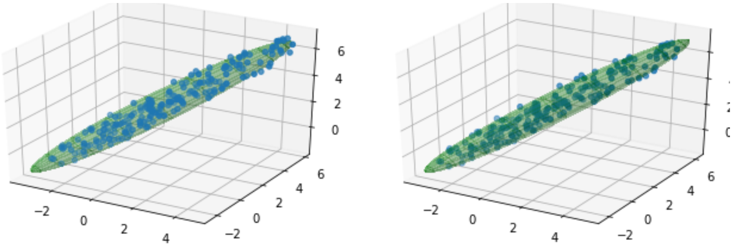


Figure 6 – Influence of the 'debiasing' of the Sinkhorn Divergence (SD_ε) compared to regularized OT (W_ε). Data are generated uniformly inside an ellipse, we want to infer the parameters A, ω (covariance and center).

Empirical Results

$ED_p - \ p = 1.5$ $\qquad$ $SD_{c,\varepsilon} - \varepsilon = 1, c = ||\cdot||_2^2$



ED_p 1.5,-		
3.12	1.74	2.08
2.25	2.83	2.09
2.30	1.74	3.07
(0.63 , 1.75 , 2.75)		

ground truth		
3	2	2
2	3	2
2	2	3
(1,2,3)		

$SD_{c,\varepsilon}$ 2, 1		
2.90	1.96	2.13
2.02	3.03	2.10
2.06	1.95	3.03
(0.94 , 1.96 , 2.90)		

Figure 7 – Comparison of the Sinkhorn Divergence ($SD_{c,\varepsilon}$) and Energy Distance (ED_p) on the ellipse fitting task (we retained best parameters for each)

Learning the cost function

In high dimension (e.g. images), the Euclidean distance is not relevant $\rightarrow$ choosing the cost c is a complex problem.

Idea : the cost should yield high values for the Sinkhorn Divergence when $\alpha_\theta \neq \beta$ to differenciate between synthetic samples (from α_θ) and 'real' data (from β). (Li and al '18)

We learn a parametric cost of the form :

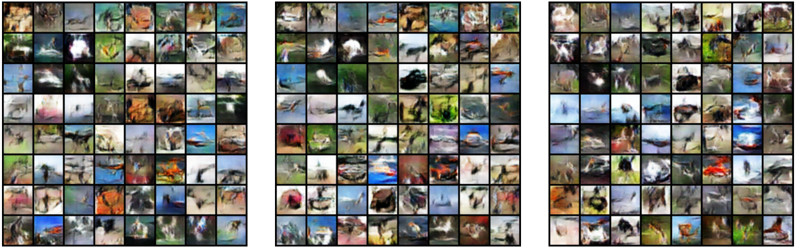
$$c_\varphi(x, y) \stackrel{\text{def.}}{=} \|f_\varphi(x) - f_\varphi(y)\|^p \quad \text{where} \quad f_\varphi : \mathcal{X} \rightarrow \mathbb{R}^{d'},$$

The optimization problem becomes a min-max on (θ, φ)

$$\min_\theta \max_\varphi SD_{c_\varphi, \varepsilon}(\alpha_\theta, \beta)$$

$\rightarrow$ GAN-type problem, cost c acts as a discriminator.

Empirical Results - CIFAR10



(a) MMD (b) $\varepsilon = 100$ (c) $\varepsilon = 1$

MMD (Gaussian)	$\varepsilon = 100$	$\varepsilon = 10$	$\varepsilon = 1$
4.56 ± 0.07	4.81 ± 0.05	4.79 ± 0.13	4.43 ± 0.07

Table 1 – Inception Scores on CIFAR10 (same setting as MMD-GAN paper (Li et al. '18)).

Take Home Message

Sinkhorn Divergences are a great notion of distance between measures !

- ‘debias’ regularized Wasserstein Distance
- interpolate between OT (small ε) and MMD (large ε) and get the best of both worlds :
  - inherit geometric properties from OT
  - break curse of dimension for ε large enough
- fast algorithms for implementation in ML tasks