Convergence of the iterates of Lloyd's algorithm

Léo Portales joint work with my supervisors Elsa Cazelles and Edouard Pauwels

IRIT, TSE, CNRS and Université de Toulouse

24/07/24

Discrete approximation of a continuous measure

μ ν

(Target Measure) $\frac{1}{N}\sum_{k=1}^{N}\delta_{y_k}$ $\sum_{k=1}^{N}\pi_k\delta_{y_k}$

Simulations made using the library PyMongeAmpere by Quentin Mérigot.

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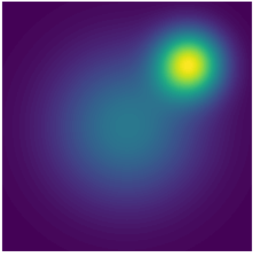

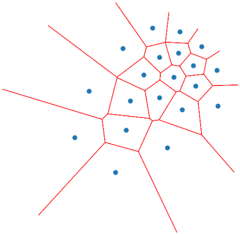

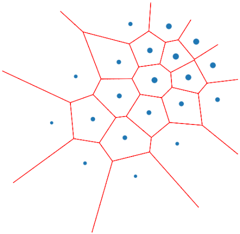

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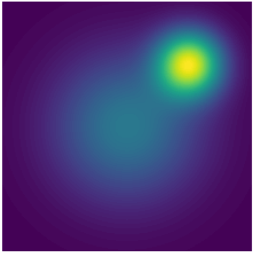

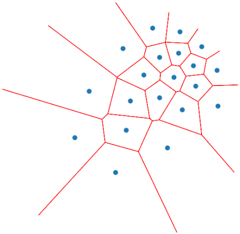

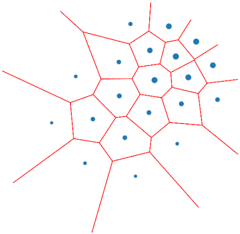

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Discrete approximation of a continuous measure

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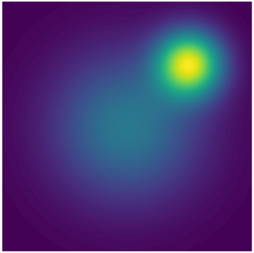
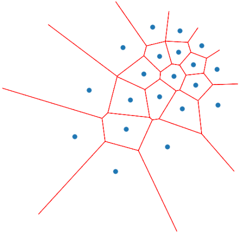


ν

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



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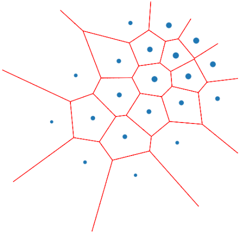

- μ is a compactly supported continuous probability measure on $\mathbb{R}^d$ with density f.
- $\nu(Y) := \sum_{k=1}^{N}\pi_k\delta_{y_k}$ where $Y = (y_1, \ldots, y_N) \in (\mathbb{R}^d)^N$ and $\pi \in \Delta_N$. N is fixed.

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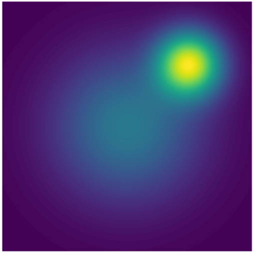

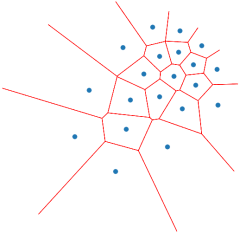

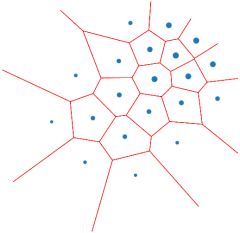

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$$W_2(\mu, \nu(Y)) = \left(\inf_{\gamma\in\Pi(\mu,\nu(Y))}\int_{\mathbb{R}^d\times\mathbb{R}^d}\|x-y\|^2 d\gamma(x,y)\right)^{\frac{1}{2}}$$

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Uniform and optimal quantization

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

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(Optimal Quantization)

Voronoï and Laguerre tesselation

- i'th Voronoï cell:
  $V_i(Y) = \{x \in \mathbb{R}^d \mid \|x - y_i\|^2 < \|x - y_j\|^2 \, \forall j = 1, ..., N\}$

Optimal Quantization

Uniform Quantization

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Optimal Quantization

$$\begin{aligned} G_N(Y) &= \frac{1}{2} \int_{\mathbb{R}^d} \min_{i=1,\dots,N} \|x - y_i\|^2 f(x) dx \\ &= \frac{1}{2} \sum_{i=1}^{N} \int_{V_i(Y)} \|x - y_i\|^2 f(x) dx \end{aligned}$$

Discrete

Uniform Quantization

Voronoï and Laguerre tesselation

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Optimal Quantization

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&= \frac{1}{2} \sum_{i=1}^{N} \int_{V_i(Y)} \left\|x - y_i\right\|^2 f(x) dx
\end{aligned}
$$

Discrete

Uniform Quantization

$$
\begin{aligned}
F_N(Y) &= \max_{w \in \mathbb{R}^N} \frac{1}{2} \left\{ \int_{\mathbb{R}^d} \left(\min_{i=1,\dots,N} \left\|x - y_i\right\|^2 - w_i \right) f(x) dx + \frac{1}{N} \sum_{i=1}^{N} w_i \right\} \\
&= \max_{w \in \mathbb{R}^N} \frac{1}{2} \left\{ \sum_{i=1}^{N} \int_{L_i(Y,w)} \left(\left\|x - y_i\right\|^2 - w_i \right) f(x) dx + \frac{1}{N} \sum_{i=1}^{N} w_i \right\}
\end{aligned}
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Lloyd's algorithm[1]: two equivalent formulations

Can be described in two ways

1. Choose an initial points cloud Y.

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

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1. Choose an initial points cloud Y.
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Which translates to

- UQ:

$$\begin{cases} Y_0 \in (\mathbb{R}^d)^N \setminus D_N \\ Y_{n+1} = Y_n - N.\nabla F_N(Y_n) \end{cases}$$

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- OQ:

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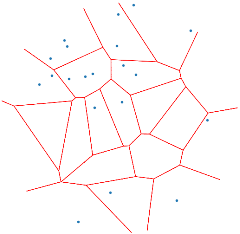
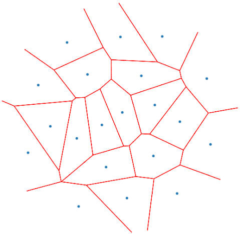
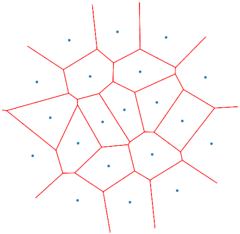
Lloyd's algorithm for (Uniform Quantization): an example with $\mu \sim \mathcal{N}_{\mathbb{S}^1}(0_2, \sigma^2 I_2)$



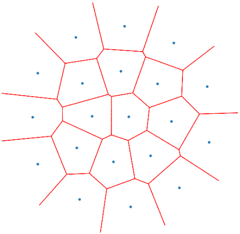
$[n = 0]$



$[n = 1]$



$[n = 2]$



$[n = 20]$

Simulations made using the library PyMongeAmpere by Quentin Mérigot.

Convergence of gradient schemes in non-convex setting

- F_N and G_N both non convex.

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- F_N and G_N do so under an analyticity assumption on the target density.

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Convergence of Lloyd's algorithm for OQ and UQ

Uniform Quantization

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

Optimal Quantization

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Let $(Y_n)_n$ be Lloyd iterates.

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- Convergence to a set of critical points[3]: $\|\nabla F_N(Y_n)\| \underset{n \longrightarrow \infty}{\longrightarrow} 0$

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Let (Z_n) be Lloyd iterates.

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Question:

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

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Main result

Theorem

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

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Remark

Convexity of Supp(μ) is not necessary for uniform quantization.

KL inequality

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 $\Psi : [0, \eta[\longrightarrow \mathbb{R}$ such that:

$$\|\nabla(\Psi \circ f)(x)\| \geq c,\ \forall x \in U \text{ such that } 0 < f(x) < \eta. \tag{1}$$

KL inequality

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 $\Psi : [0, \eta[\longrightarrow \mathbb{R}$ such that:

$$\|\nabla(\Psi \circ f)(x)\| \geq c, \ \forall x \in U \text{ such that } 0 < f(x) < \eta. \tag{1}$$

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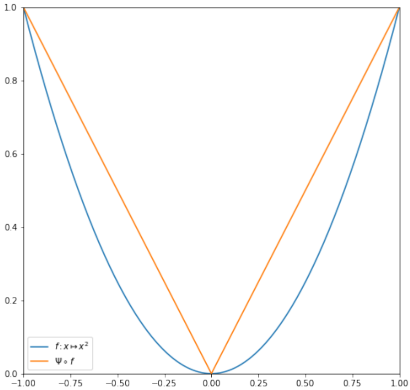
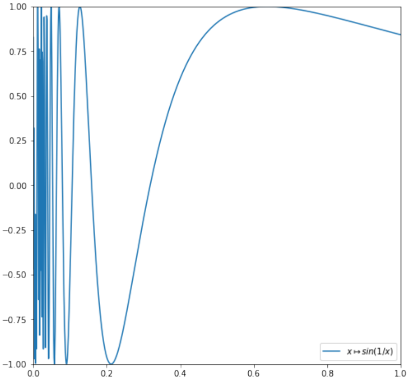
A function whose differential go to zero can have infinitely many oscillations as it goes to 0. The KL property prevents that from happening.

KL inequality

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





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

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

Strong descent conditions

Strong descent conditions: Let $(Y_k)_{k\geq 1}$ be some sequence and F be some differentiable cost function.

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- F_N SDC (can be deduced from Merigot, Santambrogio, Sarrazin [6]).

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Idea of proof

Theorem

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

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Question:

Why are F_N and G_N KL? Because they are definable in an o minimal structure.

A (very quick) overview on o-minimality

$$\mathcal{SA} \subset \mathbb{R}_{\mathsf{an}} \subset \mathbb{R}_{\mathsf{an,exp}} \subset \mathcal{P}(\mathbb{R})$$

[7] H. Hironaka. Introduction to Real-analytic Sets and Real-analytic Maps. 1973

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- Functions definable in an o minimal structure are KL.

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

Proving the definability of G_N and F_N

$$G_N(Y) = \frac{1}{2} \int_{\mathbb{R}^d} \min_{i=1,\dots,N} \|x - y_i\|^2 \underbrace{f(x)}_{\text{GSA}} dx$$

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- $D = W_\epsilon$ (Entropic regularization of the semi-discrete OT problem)

What to remember

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Thank you for listening!

Let $Y \notin D_N$, then

$$\min_{\pi \in \Delta_N} W_2^2\left(\mu, \sum_{i=1}^N \pi_i \delta_{y_i}\right) = \int_{\mathbb{R}^d} \min_{i=1,\dots,N} \|x - y_i\|^2 d\mu(x).$$

Proof.

We denote $\mathcal{H}(Z, Y) = \sum_{i=1}^N \int_{V_i(Z)} \|x - y_i\|^2 d\mu(x)$.
We observe that $\mathcal{H}(Z, Y) = \int_{\mathbb{R}^d} \|x - T(x)\|^2 d\mu(x)$ with $T(x) = \sum_{i=1}^N y_i 1_{V_i(Z)}(x)$. This is the optimal transport map from μ to $\sum_{i=1}^N \mu(V_i(Z))\delta_{y_i}$, so:

$$\mathcal{H}(Z, Y) = W_2^2(\mu, \sum_{i=1}^N \mu(V_i(Z))\delta_{y_i}).$$

Since $\min_Z \mathcal{H}(Z, Y) = \mathcal{H}(Y, Y)$ we finally get

$$\min_Z \mathcal{H}(Z, Y) = \min_\pi W_2^2(\mu, \sum_{i=1}^N \pi_i \delta_{y_i}).$$