The (nonconvex) uniform optimal quantization problem.

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Dynamics and Discretization: PDEs, Sampling, and Optimization
Simons Institute, October 2021

Optimal quantization and Lloyd's algorithm

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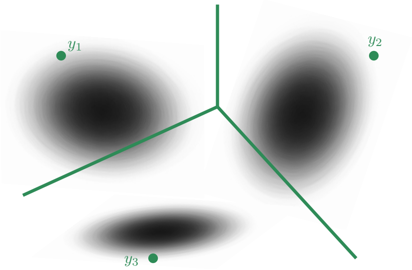

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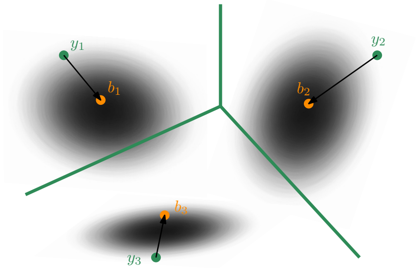

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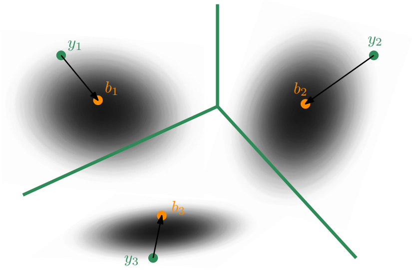

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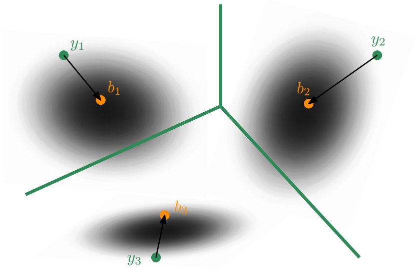

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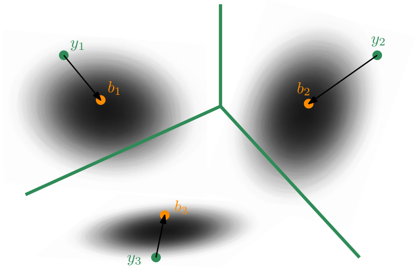

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$$\min_\theta \mathrm{W}_1(\rho, \mu_\theta) \qquad \text{[Arjovsky \textit{et. al}, 2017,][Genevay \textit{et al.} 2018]}$$

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$$\min_{Y=(y_1,\ldots,y_N)\in\Omega^d} \mathrm{W}_2^2\left(\rho, \frac{1}{N}\sum_i \delta_{y_i}\right)$$

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Does gradient descent lead to low-energy configurations?

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- By Kantorovich duality [Kantorovich 1942][Aurenhammer *et al.* 1998],

$$F_N(Y) = \max_{\Phi} \sum_i \alpha_i \phi_i + \int_{\Omega} \min_i \|x - y_i\|^2 - \phi_i \mathrm{d}\rho(x)$$

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where *Laguerre cells* are defined for $Y \in \Omega^N$ and $\Phi \in \mathbb{R}^N$:

$$\mathrm{Lag}_i(Y, \Phi) \stackrel{\text{def}}{=} \left\{x \in \mathbb{R}^d \;\middle|\; \forall j,\; \|x - y_i\|^2 - \phi_i \leq \|x - y_j\|^2 - \phi_j\right\}$$

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- Given pairwise distinct points $Y \in \Omega^N$, the maximizer $\Phi_Y \in \mathbb{R}^N$ is unique and characterized by $\rho(\mathrm{Lag}_i(Y, \Phi_Y)) = \frac{1}{N}$: all cells have mass $\frac{1}{N}$.

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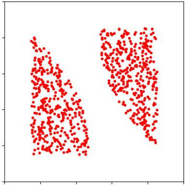
Proposition

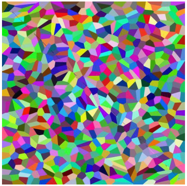
F_N is semi-concave on Ω^N, it is $\mathcal{C}^1$ on a dense open set and

$$F_N(Y) = \sum_i \int_{\mathrm{Lag}_i(Y,\Phi_Y)} \|x - y_i\|^2 \,\mathrm{d}\rho(x),$$

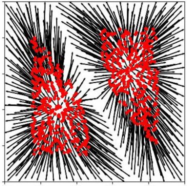
where $b_i(Y) = N \int_{\mathrm{Lag}_i(Y,\Phi_Y)} x d\rho(x)$ is the barycenter of the ith cell.



Point cloud Y



$\mathrm{Lag}_i(Y, \Phi_Y)$



$-\frac{N}{2}\nabla_{y_i} F_N(Y)$

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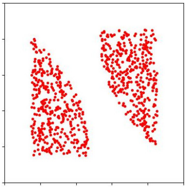

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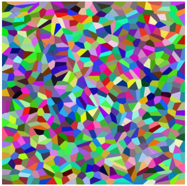

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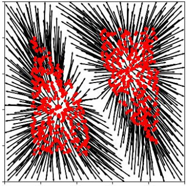

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- The iterates converge (up to subseq.) to a critical point of F_N or G_N.
- In both cases, there may exist critical points with high energy

Low- and high-energy critical points of F_N

- Given ρ bounded from above and below on a bounded convex set $\Omega \in \mathbb{R}^d$,

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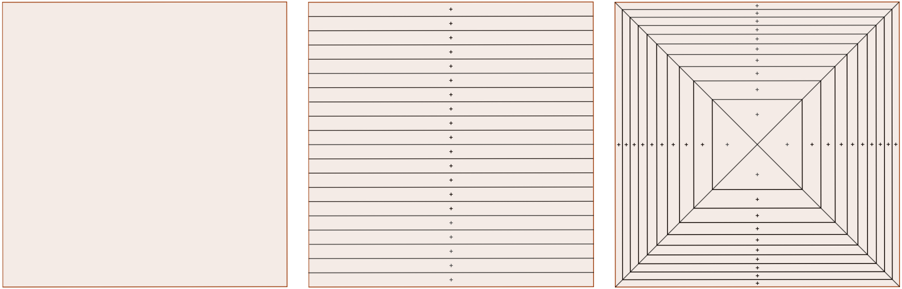
- Due to the non-convexity of F_N, some critical points are NOT minimizers:



ρ $\qquad$ $N = 20$ $\qquad$ $N = 40$

Figure: Two high-energy critical point for $\rho \equiv 1$ uniform on $\Omega = [0,1]^2$: $F_N(Y) = \Theta(1)$.

Convergence under a dimensionality condition

- Experimentally, when the point cloud $Y = (y_1, \ldots, y_N)$ is not chosen adversely, one observes that

$$\mathrm{W}_2^2\left(\frac{1}{N}\sum_i \delta_{b_i(Y)}, \rho\right) \ll 1.$$

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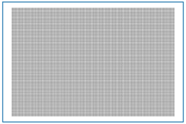

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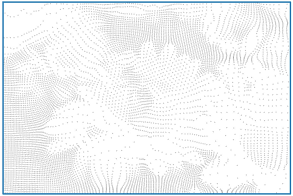

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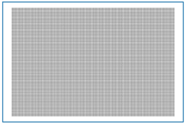

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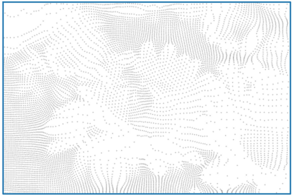

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I.e., a *single step* Lloyd algorithm yields a good approximation of ρ.

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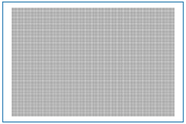
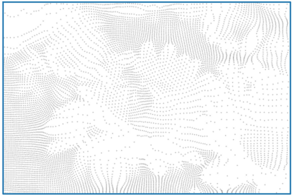


Y^N

$B_N = (b_1(Y^N), \dots, b_N(Y^N))$



$B^N, N = 7280$

I.e., a *single step* Lloyd algorithm yields a good approximation of ρ.

- Our main theorem explains this behaviour.

Convergence under a dimensionality condition

Theorem (Santambrogio, Sarrazin, M. (2021))

Let $\Omega \subseteq \mathbb{R}^d$ be convex and let $\rho \in \mathcal{P}(\Omega)$. Consider a point cloud Y in Ω^N s.t.

$$\forall i \neq j, \quad \|y_i - y_j\| \geq C_0 N^{-\frac{1}{\beta}}, \text{ with } \beta \text{ and } C_0 > 0$$

Then,
$$\boxed{\mathrm{W}_2^2\left(\frac{1}{N}\sum_{i=1}^N \delta_{b_i(Y)}, \rho\right) \leq \mathrm{cst}(d, \Omega, C_0) \cdot N^{\frac{d-1}{\beta}-1}.}$$

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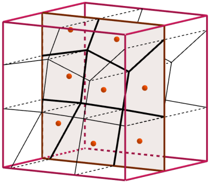
- The upper bound goes to zero as $N \to +\infty$ provided that $\beta > d-1$. This is **tight**: If $(y_i)_{1 \leq i \leq N}$ lie on the $(d-1)$ hypercube $[0,1]^{d-1} \times \left\{\frac{1}{2}\right\}$ and if $\rho \equiv 1$ on $\Omega = [0,1]^d$:

$$\mathrm{W}_2^2\left(\frac{1}{N}\sum_{i=1}^N \delta_{b_i(Y)}, \rho\right) \geq \frac{1}{12}$$



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- The upper bound goes to zero as $N \to +\infty$ provided that $\beta > d-1$.
- When $\beta = d$, the upper bound of the theorem is

$$F_N(B_N) = \mathrm{W}_2^2\left(\frac{1}{N}\sum_i \delta_{y_i}, \rho\right) \lesssim \left(\frac{1}{N}\right)^{1/d}.$$

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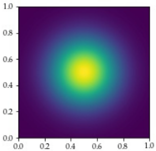
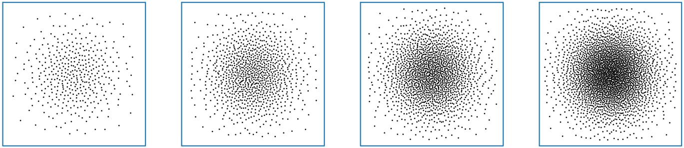
This does not match the upper bound on $\min_{\Omega^N} F_N$: $\min_{\Omega^N} F_N \lesssim \left(\frac{1}{N}\right)^{2/d}$.
However, the exponent in the upper bound **cannot be improved** !

Tightness in the case $\beta = d$

ρ



Random:



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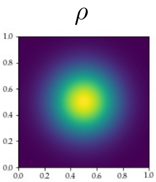

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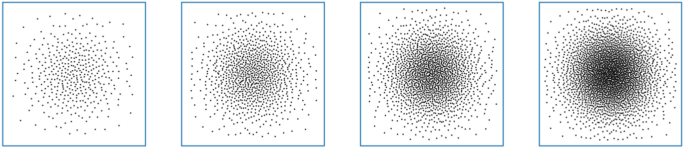
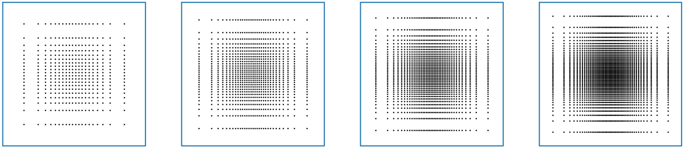


Grid-like:



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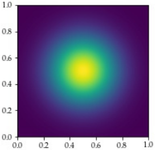

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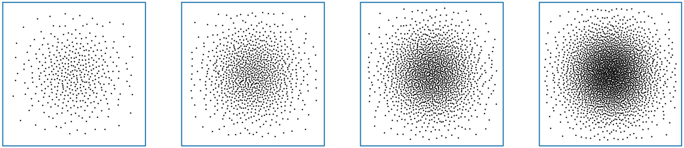

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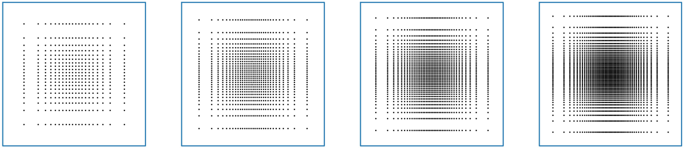
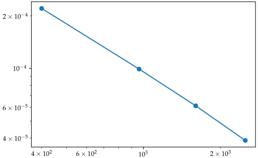
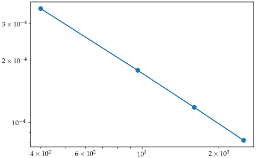


$N = 400$ $N = 961$ $N = 1600$ $N = 2500$



Random $\sim N^{-0.99}$



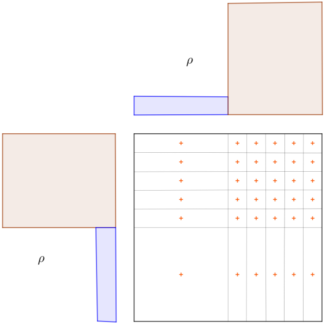
Grid-like $\sim N^{-0.78}$

Tightness in the case $\beta = d$

- On $\Omega = [-1,1]^d$, let $n \in \mathbb{N}^*$, $N = n^d$

$$\rho(x) = \frac{1}{n}\mathbb{1}_{[-1;0]} + \left(1 - \frac{1}{n}\right)\mathbb{1}_{[0;1]}, \qquad \rho_N = \underbrace{\rho \otimes \ldots \otimes \rho}_{d \text{ times}}$$

and Y^N a "grid-like" cloud of N points as on the picture.



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- Then, $\nabla_Y F_N(Y^N) = 0$, so that Y^N is a fixed point of Lloyd's algorithm, and

$$\mathrm{W}_2^2\left(\frac{1}{N}\sum_{i=1}^N \delta_{b_i(Y^N)}, \rho_N\right) \geq CN^{-1/d}$$

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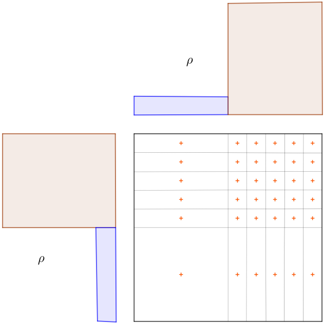

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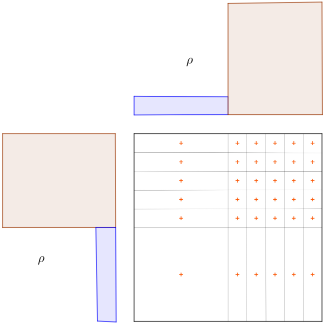
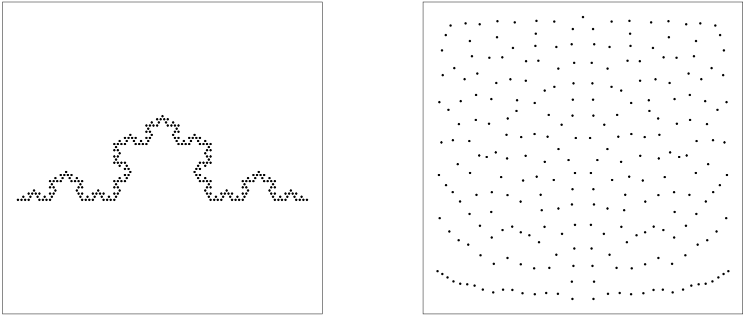


Numerical example with $d - 1 < \beta < d$

- Point are sampled from the Von Koch fractal (dimension $\beta = \frac{\ln 4}{\ln 3} \simeq 1.26$), $\rho \equiv 1$ on $\Omega = [0,1]^2$.



$N = 257$

- Numerically, it seems that $\mathrm{W}_2^2(\mu_N, \rho) \simeq N^{-1.01}$, while our upper bound would give an exponent of $\frac{d-1}{\beta} - 1 \simeq -0.207$.

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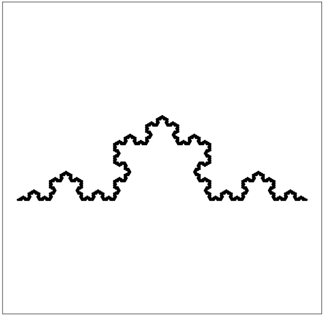

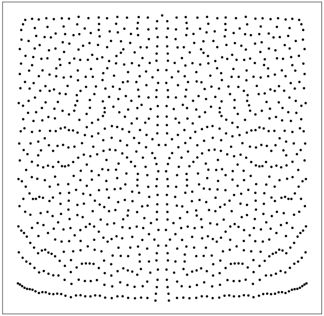

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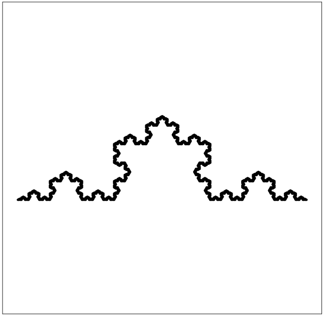

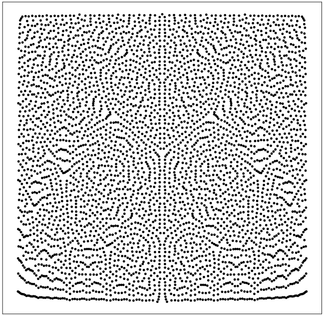

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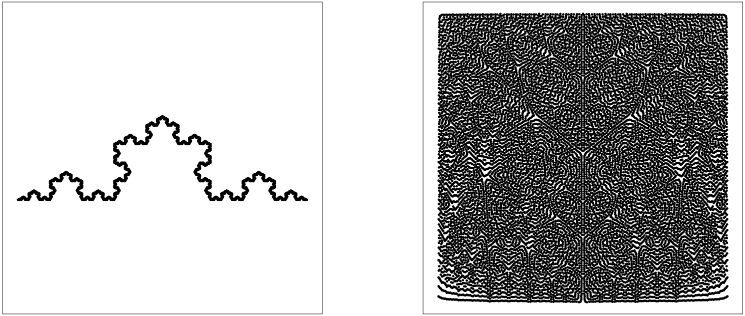

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Main theorem: sketch of proof

We assume: $\forall i \neq j, \quad \|y_i - y_j\| \geq C_0 N^{-\frac{1}{\beta}}$, with β and $C_0 > 0$

Main idea: There cannot be "too many" Laguerre cells that are "elongated"

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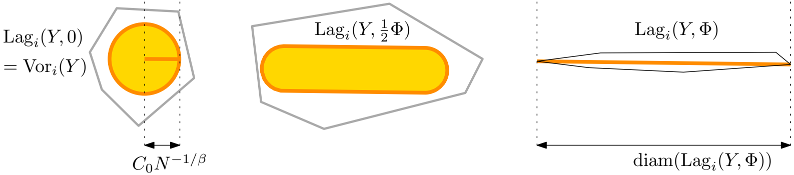

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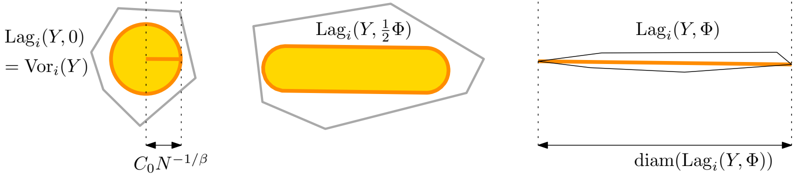

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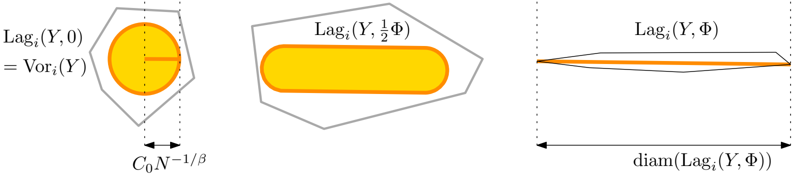

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Limit of critical points as $N \to \infty$:

- If $Y^N \in \Omega^N$ is a critical point of $F_N(Y) = \mathrm{W}_2^2(\rho, \delta_Y)$, what are the possible narrow limit of the "discrete critical measure" $\mu_N = \frac{1}{N} \sum_{i=1}^N \delta_{y_i^N}$?

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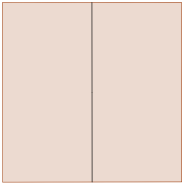
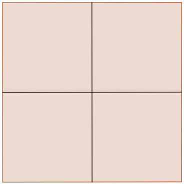
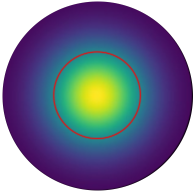




$\rho =$ Lebesgue on $[0;1]^2$



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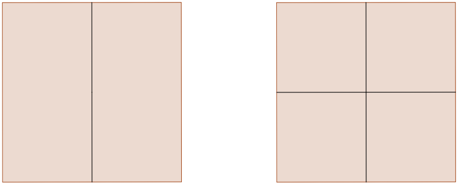

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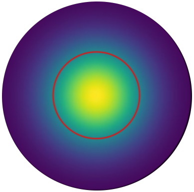

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- Can this behavior be proven ? More generally, what can we say about limits of discrete critical measures?

Lagrangian critical measures

- **Disintegration of OT plan** Let $\rho, \mu \in \mathcal{P}(\Omega)$ and γ be the quadratic optimal transport plan, which we disintegrate into $\gamma = \int_\Omega \rho_y \mathrm{d}\mu(y)$.

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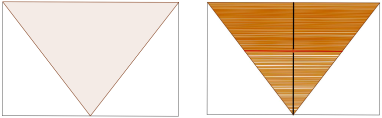

$(\rho_y)_y \simeq$ Laguerre cells.

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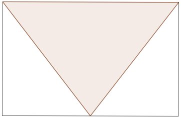
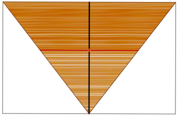

$(\rho_y)_y \simeq$ Laguerre cells.

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$$\iff \boxed{\forall \xi \in \mathcal{C}_c^0(\Omega, \mathbb{R}^d), \quad \frac{\mathrm{d}}{\mathrm{dt}} \mathrm{W}_2^2((\mathrm{id} + t\xi)_{\#}\mu, \rho)\Big|_{t=0} = 0.}$$

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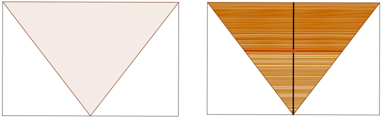

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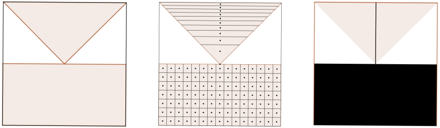
- **Narrow limit of critical points of F_N are Lagrangian critical:**

Assume that $\nabla_Y F_N(Y^N) = 0$ and $\lim_{N \to +\infty} \frac{1}{N} \sum_i \delta_{y_i^N} = \mu$. Then μ is Lagrangian critical.



ρ $\quad$ $\frac{1}{N} \sum_i \delta_{y_i^N}$ $\quad$ μ

Classification of Lagrangian critical measures

- Given $\mu \in \mathcal{P}(\Omega)$, let $\mathcal{E}_k$ the points of $\mathrm{spt}(\mu)$ whose "Laguerre cell" ρ_y has dimension $d - k$:

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- Very preliminary result: most of the questions about Lagrangian critical measures are open.

Summary and Perspectives

Take-home message: Despite the non-convexity, gradient descent strategies for optimal uniform quantization problem, i.e.

$$\min_{Y \in \Omega^N} \mathrm{W}_2^2 \left(\frac{1}{N} \sum_i \delta_{y_i}, \rho \right)$$

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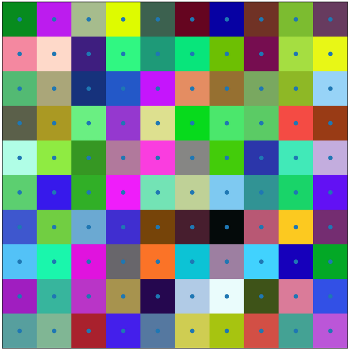
Thank you for your attention!

An unstable critical point

- $\Omega = [-\pi, \pi]^2, \rho \equiv 1/(4\pi^2), N = 10^2, Y^0 =$ uniform grid.
- Iterates follow Lloyd's algorithm: $Y^{k+1} = (b_1(Y^k), \ldots, b_N(Y^k))$.



k=1

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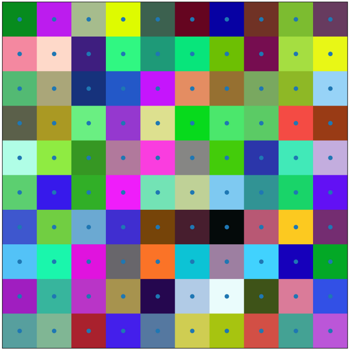

k=101

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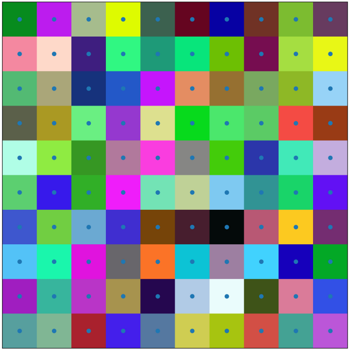

k=121

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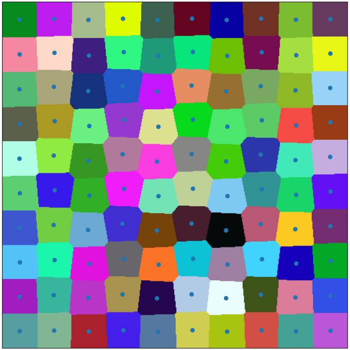

k=141

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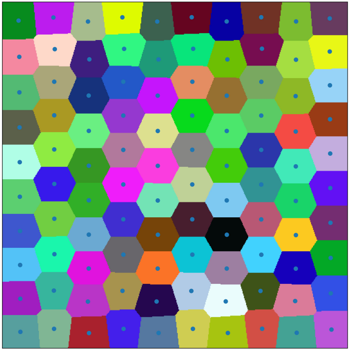

k=161

- Lloyd's iterate escape the critical point due to numerical error + instability.