Points critiques dans la quantification optimale uniforme

Filippo Santambrogio
Université Claude Bernard Lyon 1 et IUF

10 ans du Labez Bézout – Marne la Vallée, 14 juin 2022

Overview

1. Optimal quantization
2. Optimal uniform quantization
3. Non-asymptotic bounds (from a NeurIPS paper with Q. Mérigot and C. Sarrazin)
4. Limit measures of critical points (from C. Sarrazin's PhD thesis)
5. Stable critical points of Lloyd's energy (from an ongoing work with A. Figalli and Q. Mérigot)

Outline

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Optimal quantization

Definition

Let ρ be a probability density on a compact domain Ω of $\mathbb{R}^d$.

- *The quantization error of ρ by N points is*

$$G_N(y_1, \ldots, y_N) = \int_\Omega \min_{1 \le i \le N} \|x - y_i\|^2 \, \mathrm{d}\rho(x),$$

which measures how well ρ is approximated by $Y = (y_1, \ldots, y_N)$.

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- Denote $\mathrm{Vor}_i(Y) = \{x \mid \forall j, \|x - y_i\|^2 \leq \|x - y_j\|^2\}$ the **Voronoi cells**. Then,

$$G_N(y_1, \ldots, y_N) = \sum_{1 \leq i \leq N} \int_{\mathrm{Vor}_i(Y)} \|x - y_i\|^2 \, \mathrm{d}\rho(x).$$

Towards Lloyd's algorithm

Proposition

Assume that all the cells have positive mass (i.e. $\rho(\mathrm{Vor}_i(Y)) > 0$). Then,

$$\nabla_{y_i} G_N(y_1, \ldots, y_N) = 2\rho(\mathrm{Vor}_i(Y)) \cdot (y_i - \mathrm{bary}_\rho(\mathrm{Vor}_i(Y)),$$

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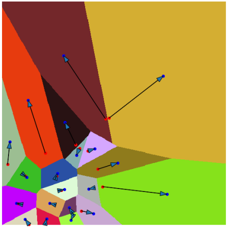

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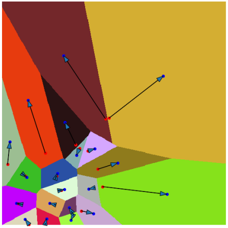

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- There exists critical point with (very) high energy.

Lloyd's algorithm

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- Non-convex optimization problem. NP-hard when $\rho = \frac{1}{N}\sum_j \delta_{x_j}$ even in the plane [Mahajan et al. 09] or for $k=2$ in high dimensions [Dasgupta 08].

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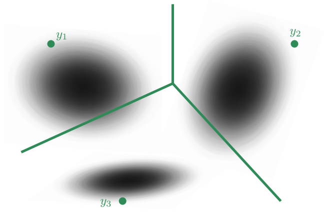

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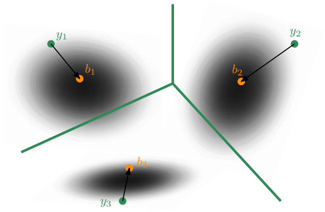

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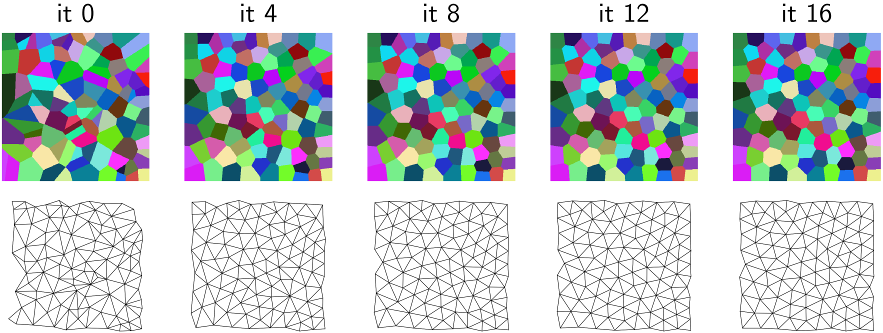
Iterates of Lloyd's algorithm



- Lloyd's algorithm has a rather slow convergence.
- ... and can (in principle) get stuck at configurations with high quant. error.

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- **Applications:** Stippling of grayscale images [de Goes *et al.* 2012],

ρ

$y_1, \ldots, y_N$

Optimal location problems [Bourne, Schmitzer, Wirth, 2018], Generation of polycrystalline microstructures [Bourne *et al.* 2020], etc.

Semi-discrete optimal transport

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- The uniform quantization energy involves a **semi-discrete** OT problem:

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- By Kantorovich duality,we have

$$\mathrm{W}_2^2\left(\frac{1}{N}\sum_i \delta_{y_i}, \rho\right) = \max_{\Phi=(\phi_1,\dots,\phi_N)} \int \min_j(\|x - y_j\|^2 - \phi_j)\mathrm{d}\rho(x) + \sum_{1\leq i\leq N} \frac{1}{N}\phi_i,$$

which can be re-written using the optimal $\Phi = \Phi_Y$ as

$$F_N(Y) = \sum_{1\leq i\leq N} \int_{\mathrm{Lag}_i(Y,\Phi_Y)} \|x - y_i\|^2 \,\mathrm{d}\rho(x)$$

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

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

Indeed, 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 $\frac{1}{N}$.

Optimal quantization energy

- We minimize $F_N : Y \in \Omega^N \mapsto \mathrm{W}_2^2\left(\frac{1}{N}\sum_i \delta_{y_i}, \rho\right)$.
- W_2^2 is convex on $\mathcal{P}(\Omega)$, yet F_N is **not convex** on Ω^N.

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

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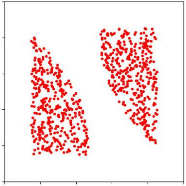
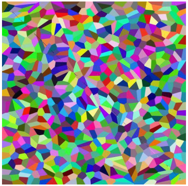


Point cloud Y



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

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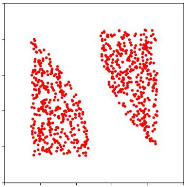
where $b_i(Y) = N \int_{\mathrm{Lag}_i(Y,\Phi_Y)} x d\rho(x)$ is the barycenter of the ith cell.



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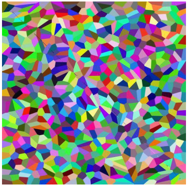

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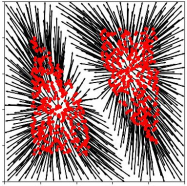

$-\frac{N}{2}\nabla_{y_i} F_N(Y)$

Lloyd's (uniform) algorithm

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Algorithm: given $Y \in \Omega^N$
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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

- The minimal value for the optimal quantization is always at most of order $N^{-2/d}$. For optimal uniform quantization the same estimate can depend on ρ, but, if ρ is bounded from above and below on a bounded convex set $\Omega \in \mathbb{R}^d$, then we have the same bound

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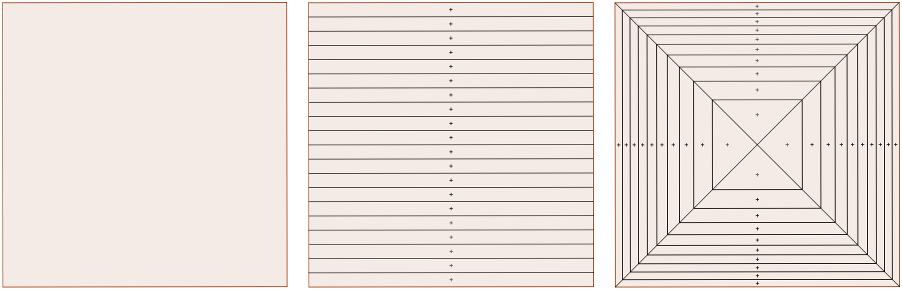
- Due to the non-convexity of F_N, some critical points are NOT minimizers:



ρ $\quad$ $N = 20$ $\quad$ $N = 40$

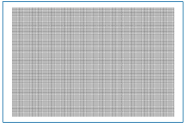
Outline

Convergence for well-chosen initial data

- Experimentally, Lloyd's algorithms converge well. Even better, when the point cloud $Y = (y_1, \dots, y_N)$ is not chosen adversely, one observes

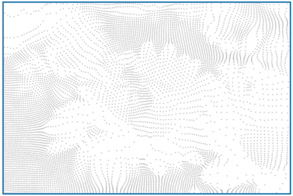
$$\mathrm{W}_2^2\left(\frac{1}{N}\sum_i \delta_{b_i(Y)}, \rho\right) \ll 1.$$

ρ



Y^N

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



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Convergence for well-chosen initial data

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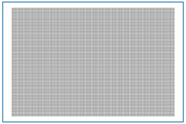

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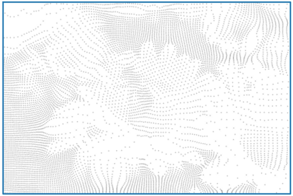

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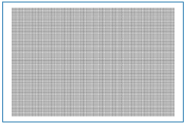

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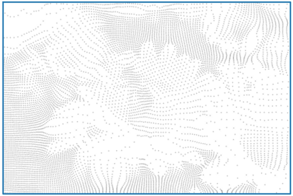

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- Our main theorem explains this behaviour.

Convergence under a dimensionality condition

Theorem

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.*

$$\forall i \neq j, \quad \|y_i - y_j\| \geq \varepsilon$$

Then,

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

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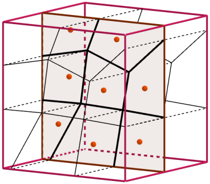
  This is **tight**: If $(y_i)_{1\leq i\leq N}$ lie on the $(d-1)$ hypercube $[0,1]^{d-1}\times\left\{\frac{1}{2}\right\}$ and if $\rho \equiv 1$ on $\Omega = [0,1]^d$:

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



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- When $\beta = d$, the upper bound of the theorem is

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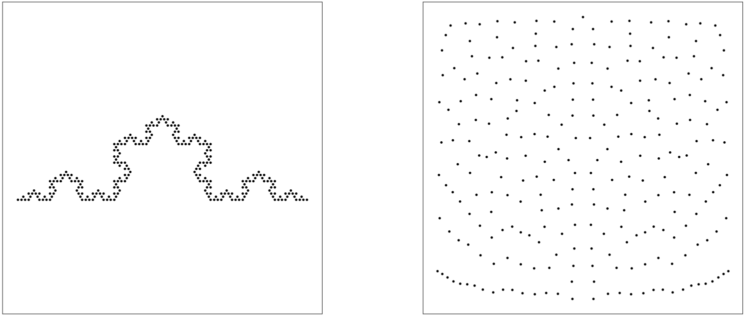
Yet, this is sharp taking $d=1$, $\rho = \frac{1}{N}$ on $[-1,0]$ and $\rho = (1-\frac{1}{N})$ on $(0,1]$ (or, in higher dimension, products of this distribution).

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 $\Omega = [0, 1]^2$.



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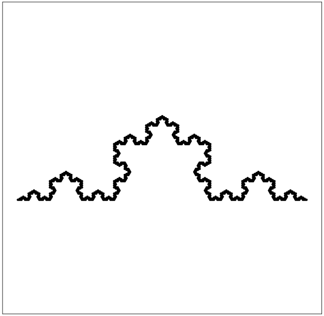

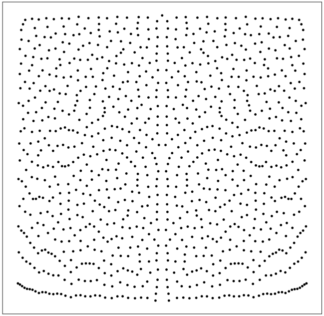

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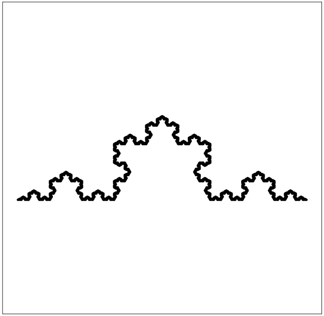

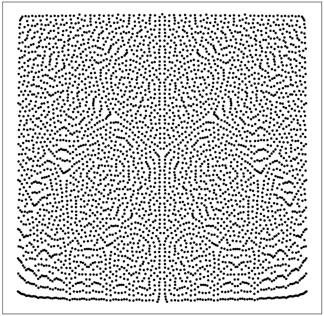

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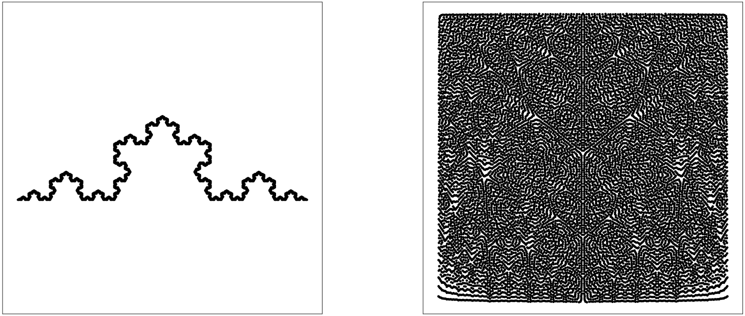

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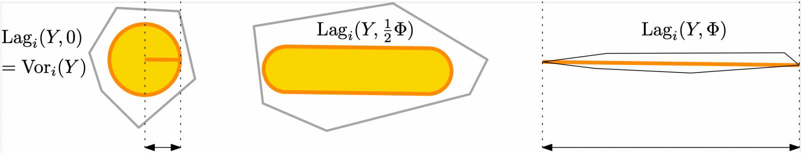

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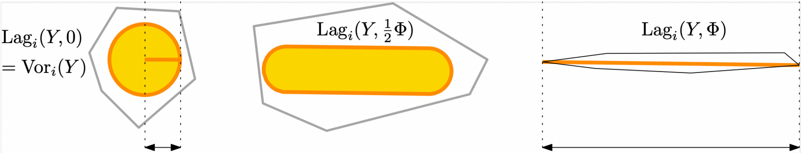

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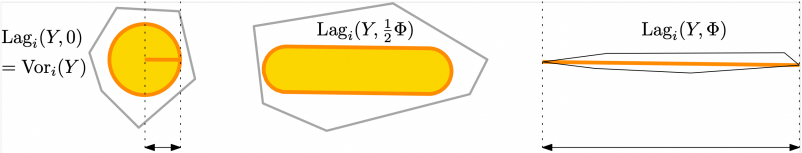

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- $\mathrm{W}_1\left(\frac{1}{N}\sum_{i=1}^N \delta_{b_i(Y)},\rho\right) \lesssim \frac{1}{N}\sum_{i=1}^N \mathrm{diam}(\mathrm{Lag}_i(Y,\Phi)) \lesssim \frac{\varepsilon^{1-d}}{N}$, and $\mathrm{W}_2^2 \leq C\mathrm{W}_1$.

Outline

Lagrangian critical measures

Let $Y = (y_1, \ldots, y_N)$ be a critical point for the optimal uniform quantization of a density ρ. Let $\mu_N := \frac{1}{N}\sum_{i=1}^N \delta_{y_i}$ be the associated empirical measure. What about the weak limits of μ_N, $N \to \infty$?

Definition (Lagrangian critical measures)

A measure μ is said to be Lagrangian critical if in the unique optimal transport plan γ (induced by a map T such that $T_\# \rho = \mu$) for the quadratic cost from ρ to μ we do have

$$\int \xi(y) \cdot (y - x) d\gamma(x, y) = 0$$

for all $\xi \in C(\Omega; \mathbb{R}^d)$.
This corresponds to saying that $\mu-$a.e. y is the barycenter of the conditional distribution γ_y on $T^{-1}(y)$.

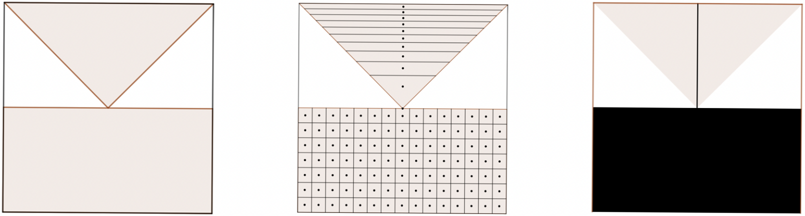
The empirical measures μ_N are Lagrangian critical, and so is any weak limit μ.

Dimensional decomposition of Lagrangian critical measures

Let μ be a Lagrangian critical measure and define the sets $S_k = \{y \in \mathrm{spt}(\mu) : \dim(T^{-1}(y)) = d - k\}$. Then $\mu = \sum_{k=0}^{d} \mu^k$ where $\mu^k = \mu_{|S_k}$. We then have

- Every set S_k is contained in a countable union of $C^{1,1}$ $k-$dimensional hypersurfaces.
- For $k = d$, we have $\mu^k = \rho_{|S_d}$. In particular, if μ is absolutely continuous, then $\mu = \rho$.
- For $k = 0, 1, d$ the measure μ^k is absolutely continuous w.r.t. the $\mathcal{H}^k$-Hausdorff measure. This is conjectured for all k, but not proven.
- In particular, if $d = 2$, μ fully decomposes into three layers, one per dimension.
- If moreover μ is a limit of empirical measures corresponding to discrete critical points Y_N, then $\mu^0 = 0$ (also proven for $d = 1, 2$ only but conjectured in the general case).

A Lagrangian critical measure with 1D and 2D parts

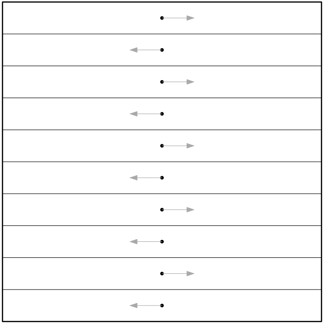


From left to right, the support of the probability density ρ (constant on this support), a critical point cloud for F_N which is not a minimizer and its limit measure. The limit measure μ is not uniform on the vertical segment (but it is uniform on the lower rectangle).

Outline

Stable critical points

A critical point is *stable* if it is a local minimizer of F_N. In general, iteratvie algorithms converge to stable critical points.
Typical example of an *unstable* critical point:



Stable critical points in 2D

Proposition

For every dimension d there exists $c > 0$ such that if

$$\mathcal{H}^{d-1}(\mathrm{Lag}_i(Y, \Phi_Y) \cap \mathrm{Lag}_j(Y, \Phi_Y)) \geq cN^{-\frac{d-1}{d}}$$

for some $i \neq j$, then the configuration is unstable.

Elaborating on this, but only for $d = 2$ one can prove (work in progress)

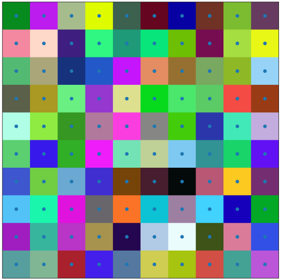
Theorem

In dimension $d = 2$, $\exists c > 0$ s.t. for any a stable critical point $Y \in \mathbb{R}^{dN}$, we have $\mathrm{diam}(\mathrm{Lag}_i(Y, \Phi_Y)) \leq cN^{-1/d}$. *In particular*

$$\mathrm{W}_2\left(\frac{1}{N}\sum_i \delta_{y_i}, \rho\right) \leq c\left(\frac{1}{N}\right)^{1/d}.$$

Another 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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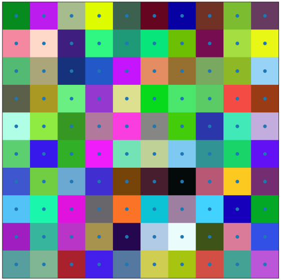

k=101

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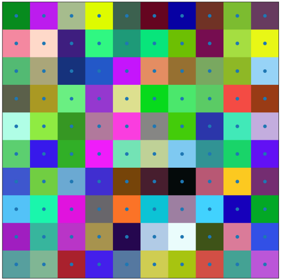

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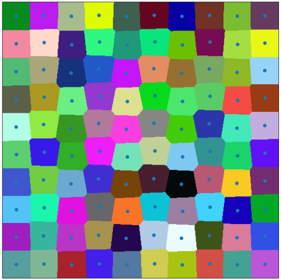

k=141

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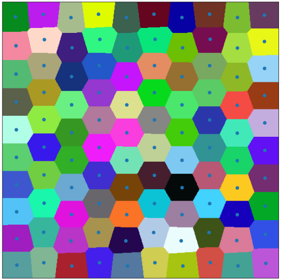

k=161

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

Summary and Perspectives

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

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

often lead to low energy configurations. This is related to several points raised in this presentation

- when the points are far enough from each other the corresponding barycenters provide good values for the quantization energy
- when the limit configuration is not too much concentrated the limit measure coincides with ρ
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(Some) open questions:

- Can estimates be improved if ρ is bounded from above and below?
- Can estimates be improved when ρ is supported on a submanifold of $\mathbb{R}^d$?
- What can we say about the limits of discrete critical points in dim. $d > 2$?
- What about *stable* critical points in dimension $d > 2$?
- Are non-optimal grids with reasonable energy unstable?

Thank you for your attention!