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

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)
Optimal quantization

Definition

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

The quantization error of $\rho$ by $N$ points is

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

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

A cornerstone of approximation theory, meshing, clustering, etc. [Foundations of quantization for probability distributions, Graf and Luschgy, 2000]
Optimal quantization

Definition

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

- The quantization error of $\rho$ by $N$ points is

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

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

- Optimal quantization problem:

$$\text{OQ}(\rho, N) := \min_{(\mathbb{R}^d)^N} G_N$$ (1)
Definition

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

The quantization error of $\rho$ by $N$ points is

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

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

Optimal quantization problem:

$$\text{OQ}(\rho, N) := \min_{(\mathbb{R}^d)^N} G_N$$ (1)

A cornerstone of approximation theory, meshing, clustering, etc.

[Foundations of quantization for probability distributions, Graf and Luschgy, 2000]
Optimal quantization

Definition

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

- The quantization error of $\rho$ by $N$ points is

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

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

- Optimal quantization problem:

$$\text{OQ}(\rho, N) := \min_{(\mathbb{R}^d)^N} G_N$$

A cornerstone of approximation theory, meshing, clustering, etc.

[Foundations of quantization for probability distributions, Graf and Luschgy, 2000]

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

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

**Proposition**

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

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

where \( \text{bary}_\rho(X) = \int_X x d\rho(x)/\rho(X) \).
Towards Lloyd’s algorithm

**Proposition**

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

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

where \( \text{bary}_\rho(X) = \int_X x d\rho(x)/\rho(X) \).

- Critical points of the quantization energy = centroidal Voronoi tessellations
  [Du,Faber,Gunzburger '99]
Towards Lloyd’s algorithm

**Proposition**

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

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

where $\text{bary}_\rho(X) = \frac{\int_X x \, d\rho(x)}{\rho(X)}$.

- Critical points of the quantization energy = centroidal Voronoi tessellations [Du,Faber,Gunzburger ’99]
- There exists critical point with (very) high energy.
Lloyd’s algorithm

Optimal quantization: \[ \min_{\mathcal{Y}=(y_1,\ldots,y_N) \in \mathbb{R}^{Nd}} \sum_{i=1}^{N} \int_{\text{Vor}_i(\mathcal{Y})} \|x - y_i\|^2 \, d\rho(x) \]

- Non-convex optimization problem. NP-hard when \( \rho = \frac{1}{N} \sum_j \delta_x \) even in the plane [Mahajan et al. 09] or for \( k = 2 \) in high dimensions [Dasgupta 08].
Lloyd’s algorithm

Optimal quantization: \( \min_{Y=(y_1,...,y_N) \in \mathbb{R}^{Nd}} \sum_{i=1}^{N} \int_{Vor_i(Y)} \|x - y_i\|^2 \ d\rho(x) \)

- 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].
- Lloyd’s algorithm = first-order algorithm to minimize the quantization energy
Lloyd’s algorithm

Optimal quantization: \( \min_{Y=(y_1,\ldots,y_N)\in\mathbb{R}^{Nd}} \sum_{i=1}^{N} \int_{\text{Vor}_i(Y)} \|x - y_i\|^2 \, d\rho(x) \)

- 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].
- Lloyd’s algorithm = first-order algorithm to minimize the quantization energy
- Used intensively in statistics (e.g. clustering) when \( N \) is small.
Lloyd’s algorithm

Optimal quantization: \( \min_{Y=(y_1, \ldots, y_N) \in \mathbb{R}^N} \sum_{i=1}^N \int_{Vor_i(Y)} \|x - y_i\|^2 \, d\rho(x) \)

- 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].
- Lloyd’s algorithm = first-order algorithm to minimize the quantization energy
- Used intensively in statistics (e.g. clustering) when \( N \) is small.

Lloyd’s algorithm: given \( Y = (y_1, \ldots, y_N) \in \Omega^N \)
Lloyd’s algorithm

Optimal quantization: \[ \min_{Y = (y_1, \ldots, y_N) \in \mathbb{R}^{Nd}} \sum_{i=1}^{N} \int_{Vor_i(Y)} \|x - y_i\|^2 \, d\rho(x) \]

- 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].
- Lloyd’s algorithm = first-order algorithm to minimize the quantization energy
- Used intensively in statistics (e.g. clustering) when \( N \) is small.

Lloyd’s algorithm: given \( Y = (y_1, \ldots, y_N) \in \Omega^N \)
1. Compute the Voronoi cells of \( Y \)
Lloyd’s algorithm

Optimal quantization: \( \min_{Y=(y_1, \ldots, y_N) \in \mathbb{R}^{Nd}} \sum_{i=1}^{N} \int_{\text{Vor}_i(Y)} \|x - y_i\|^2 \, d\rho(x) \)

- 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].
- Lloyd’s algorithm = first-order algorithm to minimize the quantization energy
- Used intensively in statistics (e.g. clustering) when \( N \) is small.

Lloyd’s algorithm: given \( Y = (y_1, \ldots, y_N) \in \Omega^N \)

1. Compute the Voronoi cells of \( Y \) and their barycenters \( b_i \) w.r.t. to \( \rho \).
2. Set \( y_i := b_i \) and repeat.
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.
Outline

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)
Optimal uniform quantization

Let $\Omega \subseteq \mathbb{R}^d$ compact convex, and $\mathcal{P}(\Omega) =$ probability measures on $\Omega$. 

Applications:
- Stippling of grayscale images [de Goes et al. 2012],
- Optimal location problems [Bourne, Schmitzer, Wirth, 2018],
- Generation of polycrystalline microstructures [Bourne et al. 2020], etc.
Optimal uniform quantization

Let $\Omega \subseteq \mathbb{R}^d$ compact convex, and $\mathcal{P}(\Omega) =$ probability measures on $\Omega$. The Wasserstein distance $W_p$ on $\mathcal{P}(\Omega)$ is defined through optimal transport:

$$W_p^p(\mu, \rho) = \min \left\{ \int_{\Omega \times \Omega} \|x - y\|^p \, d\gamma(x, y) \mid \Pi_1 \# \gamma = \mu, \Pi_2 \# \gamma = \rho \right\}.$$

Applications:
- Stippling of grayscale images [de Goes et al. 2012],
- Optimal location problems [Bourne, Schmitzer, Wirth, 2018],
- Generation of polycrystalline microstructures [Bourne et al. 2020], etc.
Optimal uniform quantization

- Let $\Omega \subseteq \mathbb{R}^d$ compact convex, and $\mathcal{P}(\Omega) =$ probability measures on $\Omega$. The Wasserstein distance $W_p$ on $\mathcal{P}(\Omega)$ is defined through optimal transport:

$$W_p^p(\mu, \rho) = \min \left\{ \int_{\Omega \times \Omega} \|x - y\|^p \, d\gamma(x, y) \mid \Pi_1\#\gamma = \mu, \Pi_2\#\gamma = \rho \right\}.$$

- Optimal quantization: $\min_{Y=(y_1, \ldots, y_N) \in \Omega^N} W_2^2(\rho, \mu) : \text{spt}(\mu) \subset \{y_1, \ldots, y_N\}$

- Optimal uniform quantization: $\min_{Y=(y_1, \ldots, y_N) \in \Omega^N} W_2^2 \left( \rho, \frac{1}{N} \sum_i \delta_{y_i} \right)$
Optimal uniform quantization

Let $\Omega \subseteq \mathbb{R}^d$ compact convex, and $\mathcal{P}(\Omega) =$ probability measures on $\Omega$. The Wasserstein distance $W_p$ on $\mathcal{P}(\Omega)$ is defined through optimal transport:

$$W_p^p(\mu, \rho) = \min \left\{ \int_{\Omega \times \Omega} \| x - y \|^p d\gamma(x, y) \mid \Pi_1#\gamma = \mu, \Pi_2#\gamma = \rho \right\}.$$

Optimal quantization: $\min_{Y=(y_1, \ldots, y_N) \in \Omega^N} W_2^2(\rho, \mu) : \text{spt}(\mu) \subset \{y_1, \ldots, y_N\}$

Optimal uniform quantization: $\min_{Y=(y_1, \ldots, y_N) \in \Omega^N} W_2^2 \left( \rho, \frac{1}{N} \sum_i \delta_{y_i} \right)$

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

Optimal location problems [Bourne, Schmitzer, Wirth, 2018], Generation of polycrystalline microstructures [Bourne et al. 2020], etc.
Semi-discrete optimal transport

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

\[ F_N: Y = (y_1, \ldots, y_N) \in \Omega^N \mapsto W_2^2 \left( \frac{1}{N} \sum_{i} \delta_{y_i}, \rho \right) \]

By Kantorovich duality, we have 

\[ W_2^2 \left( \frac{1}{N} \sum_{i} \delta_{y_i}, \rho \right) = \max \Phi = (\phi_1, \ldots, \phi_N) \int \min_j \left( \|x - y_j\|_2 - \phi_j \right) \, d\rho(x) + \sum_{1 \leq i \leq N} \frac{1}{N} \phi_i, \]

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

\[ F_N(Y) = \sum_{1 \leq i \leq N} \int \text{Lag}_i(Y, \Phi_Y) \|x - y_i\|_2 \, d\rho(x) \]

where Laguerre cells are defined for \( Y \in \Omega^N \) and \( \Phi \in \mathbb{R}^N 

\[ \text{Lag}_i(Y,\Phi) \text{def} = \{ x \in \mathbb{R}^d | \forall j, \|x - y_i\|_2 - \phi_i \leq \|x - y_j\|_2 - \phi_j \} \]

Indeed, given pairwise distinct points \( Y \in \Omega^N \), the maximizer \( \Phi_Y \in \mathbb{R}^N \) is unique and characterized by \( \rho(\text{Lag}_i(Y, \Phi_Y)) = \frac{1}{N} \): all cells have mass \( \frac{1}{N} \).
Semi-discrete optimal transport

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

\[ F_N : Y = (y_1, \ldots, y_N) \in \Omega^N \mapsto W_2^2 \left( \frac{1}{N} \sum_i \delta_{y_i}, \rho \right) \]
Semi-discrete optimal transport

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

  \[ F_N : Y = (y_1, \ldots, y_N) \in \Omega^N \mapsto W_2^2 \left( \frac{1}{N} \sum_i \delta_{y_i}, \rho \right) \]

- By Kantorovich duality, we have

  \[ W_2^2 \left( \frac{1}{N} \sum_i \delta_{y_i}, \rho \right) = \max_{\Phi=(\phi_1, \ldots, \phi_N)} \int \min_j (\|x - y_j\|^2 - \phi_j) d\rho(x) + \sum_{1 \leq i \leq N} \frac{1}{N} \phi_i, \]

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

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

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

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

Indeed, given pairwise distinct points \( Y \in \Omega^N \), the maximizer \( \Phi_Y \in \mathbb{R}^N \) is unique and characterized by \( \rho(\text{Lag}_i(Y, \Phi_Y)) = \frac{1}{N} : \) all cells have mass \( \frac{1}{N} \).
Optimal quantization energy

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

**Proposition**

$F_N$ is semi-concave on $\Omega^N$, it is $C^1$ on a dense open set and $F_N(Y) = \sum_i \int \text{Lag}_i(Y, \Phi_Y) \|x - y_i\|_2 d\rho(x)$, where $b_i(Y) = \frac{1}{N} \int \text{Lag}_i(Y, \Phi_Y) xd\rho(x)$ is the barycenter of the $i$th cell.
Optimal quantization energy

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

**Proposition**

$F_N$ is semi-concave on $\Omega^N$, it is $C^1$ on a dense open set and

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

where $\text{Lag}_i(Y, \Phi_Y)$ is the barycenter of the $i$th cell.
Optimal quantization energy

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

**Proposition**

$F_N$ is semi-concave on $\Omega^N$, it is $C^1$ on a dense open set and

$$F_N(Y) = \sum_i \int_{\text{Lag}_i(Y, \Phi_Y)} \|x - y_i\|^2 \, d\rho(x), \quad \nabla_{y_i} F_N(Y) = \frac{2}{N} (y_i - b_i(Y))$$

where $b_i(Y) = N \int_{\text{Lag}_i(Y, \Phi_Y)} x \, d\rho(x)$ is the barycenter of the $i$th cell.
Lloyd’s (uniform) algorithm

Lloyd’s algorithm

Optimal quant. of a density $\rho \in \mathcal{P}(\Omega)$,

$$\min_Y \min_{\alpha \in \Delta_N} W_2^2 \left( \sum_i \alpha_i \delta_{y_i}, \rho \right)$$

Algorithm: given $Y \in \Omega^N$
1. Compute the Voronoi cells of $Y$
2. Set $y_i := b_i$ w.r.t. to $\rho$. and their barycenters $b_i$ w.r.t. to $\rho$. 
2. Set $y_i := b_i$ and repeat.
Lloyd’s (uniform) algorithm

Lloyd’s algorithm

Optimal quant. of a density $\rho \in \mathcal{P}(\Omega)$,

$$\min_Y \min_{\alpha \in \Delta_N} W_2^2 \left( \sum_i \alpha_i \delta_{y_i}, \rho \right)$$

$$G_N(Y)$$

Algorithm: given $Y \in \Omega^N$
1. Compute the Voronoi cells of $Y$ and their barycenters $b_i$ w.r.t. to $\rho$.
2. Set $y_i := b_i$ and repeat.

Lloyd’s “uniform” algorithm

Optimal uniform quantization of $\rho$,

$$\min_Y W_2^2 \left( \frac{1}{N} \sum_i \delta_{y_i}, \rho \right)$$

$$F_N(Y)$$

Algorithm: given $Y \in \Omega^N$
1. Compute the Laguerre cells $\text{Lag}_i(Y, \Phi_Y)$ solving the OT problem between $\rho$ and $\mu = \frac{1}{N} \sum_i \delta_{y_i}$ and their barycenters $b_i(Y)$.
2. Set $y_i := b_i(Y)$ and repeat.
Lloyd’s (uniform) algorithm

Lloyd’s algorithm

Optimal quant. of a density $\rho \in \mathcal{P}(\Omega)$,

$$\min_Y \min_{\alpha \in \Delta_N} W_2^2 \left( \sum_i \alpha_i \delta_{y_i}, \rho \right)_{G_N(Y)}$$

**Algorithm**: given $Y \in \Omega^N$
1. Compute the **Voronoi cells** of $Y$ and their **barycenters** $b_i$ w.r.t. to $\rho$.
2. Set $y_i := b_i$ and repeat.

Lloyd’s “uniform” algorithm

Optimal uniform quantization of $\rho$,

$$\min_Y W_2^2 \left( \frac{1}{N} \sum_i \delta_{y_i}, \rho \right)_{F_N(Y)}$$

**Algorithm**: given $Y \in \Omega^N$
1. Compute the **Laguerre cells** $\text{Lag}_i(Y, \Phi_Y)$ solving the OT problem between $\rho$ and $\mu = \frac{1}{N} \sum_i \delta_{y_i}$ and their **barycenters** $b_i(Y)$.
2. Set $y_i := b_i(Y)$ and repeat.

- Lloyd’s algorithms = fixed point algorithms for cancelling $\nabla G_N$ or $\nabla F_N$. 
**Lloyd’s (uniform) algorithm**

**Lloyd’s algorithm**

Optimal quant. of a density $\rho \in \mathcal{P}(\Omega)$,

$$
\min_{\mathbf{Y}} \min_{\alpha \in \Delta_N} W_2^2 \left( \sum_i \alpha_i \delta_{y_i}, \rho \right)
$$

**Algorithm**: given $\mathbf{Y} \in \Omega^N$
1. Compute the **Voronoi cells** of $\mathbf{Y}$ and their **barycenters** $b_i$ w.r.t. to $\rho$.
2. Set $y_i := b_i$ and repeat.

---

**Lloyd’s “uniform” algorithm**

Optimal uniform quantization of $\rho$,

$$
\min_{\mathbf{Y}} W_2^2 \left( \frac{1}{N} \sum_i \delta_{y_i}, \rho \right)
$$

**Algorithm**: given $\mathbf{Y} \in \Omega^N$
1. Compute the **Laguerre cells** $\text{Lag}_i(\mathbf{Y}, \Phi_Y)$ solving the OT problem between $\rho$ and $\mu = \frac{1}{N} \sum_i \delta_{y_i}$ and their **barycenters** $b_i(\mathbf{Y})$.
2. Set $y_i := b_i(\mathbf{Y})$ and repeat.

- Lloyd’s algorithms = fixed point algorithms for cancelling $\nabla G_N$ or $\nabla F_N$.
- The iterates converge (up to subseq.) to a critical point of $F_N$ or $G_N$. 

---

12 / 27
Lloyd’s (uniform) algorithm

Lloyd’s algorithm

Optimal quant. of a density \( \rho \in \mathcal{P}(\Omega) \),

\[
\min_{Y} \min_{\alpha \in \Delta_N} W_2^2 \left( \sum_i \alpha_i \delta_{y_i}, \rho \right)
\]

Algorithm: given \( Y \in \Omega^N \)
1. Compute the **Voronoi cells** of \( Y \) and their **barycenters** \( b_i \) w.r.t. to \( \rho \).
2. Set \( y_i := b_i \) and repeat.

Lloyd’s “uniform” algorithm

Optimal uniform quantization of \( \rho \),

\[
\min_{Y} W_2^2 \left( \frac{1}{N} \sum_i \delta_{y_i}, \rho \right)
\]

Algorithm: given \( Y \in \Omega^N \)
1. Compute the **Laguerre cells** \( \text{Lag}_i(Y, \Phi_Y) \) solving the OT problem between \( \rho \) and \( \mu = \frac{1}{N} \sum_i \delta_{y_i} \) and their **barycenters** \( b_i(Y) \).
2. Set \( y_i := b_i(Y) \) and repeat.

- Lloyd’s algorithms = fixed point algorithms for cancelling \( \nabla G_N \) or \( \nabla F_N \).
- 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 $\rho$, but, if $\rho$ is bounded from above and below on a bounded convex set $\Omega \in \mathbb{R}^d$, then we have the same bound

$$\min_{\Omega^N} F_N \approx \left( \frac{1}{N} \right)^{2/d}.$$
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 $\rho$, but, if $\rho$ is bounded from above and below on a bounded convex set $\Omega \in \mathbb{R}^d$, then we have the same bound

$$\min_{\Omega^N} F_N \approx \left(\frac{1}{N}\right)^{2/d}.$$

- Minimizers for $F_N$ are **critical**, i.e. they satisfy $y_i = b_i(Y)$ for every $i$. 

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

$\rho_N = 20$ $\rho_N = 40$

Figure: Two high-energy critical point for $\rho \equiv 1$ uniform on $\Omega = [0,1]^2$: $F_N(Y) = \Theta(1)$.
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 $\rho$, but, if $\rho$ is bounded from above and below on a bounded convex set $\Omega \subset \mathbb{R}^d$, then we have the same bound

$$\min_{\Omega^N} F_N \approx \left(\frac{1}{N}\right)^{2/d}.$$  

- Minimizers for $F_N$ are **critical**, i.e. they satisfy $y_i = b_i(Y)$ for every $i$.

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

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)
Convergence for well-chosen initial data

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

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

\[ B_N = (b_1(Y^N), \ldots, b_N(Y^N)) \]

\( B_N, N = 7280 \)
Convergence for well-chosen initial data

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

\[ W_2^2 \left( \frac{1}{N} \sum_i \delta_{b_i(Y)}, \rho \right) \ll 1. \]

\[ B_N = (b_1(Y^N), \ldots, b_N(Y^N)) \]

\[ B_N, N = 7280 \]

I.e., a single step Lloyd algorithm yields a good approximation of $\rho$. 

\[ \rho \] 

\[ Y^N \]
Convergence for well-chosen initial data

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

$$W_2^2 \left( \frac{1}{N} \sum_i \delta_{b_i(Y), \rho} \right) \ll 1.$$

I.e., a single step Lloyd algorithm yields a good approximation of $\rho$.

- 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 $\Omega^N$ s.t.

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

Then,

$$W_2^2 \left( \frac{1}{N} \sum_{i=1}^N \delta_{b_i(Y)}, \rho \right) \leq \text{cst}(d, \Omega) \cdot \frac{\varepsilon^{1-d}}{N}.$$
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 $\Omega^N$ s.t. $\forall i \neq j, \|y_i - y_j\| \geq \varepsilon$

Then,

$$W_2^2 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \leq \text{cst}(d, \Omega) \cdot \frac{\varepsilon^{1-d}}{N}.$$ 

- In particular, if $\varepsilon \approx N^{-1/\beta}$, then $W_2^2 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \leq C N^{\frac{d-1}{\beta} - 1}$. This upper bound goes to zero as $N \to +\infty$ provided that $\beta > d - 1$. 

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 $\Omega^N$ s.t.

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

Then,

$$W_2^2 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \leq \text{cst}(d, \Omega) \cdot \frac{\varepsilon^{1-d}}{N}.$$

In particular, if $\varepsilon \approx N^{-1/\beta}$, then $W_2^2 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \leq CN^\frac{d-1}{\beta} - 1$. This 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 $[0, 1]^{d-1} \times \{ \frac{1}{2} \}$ and if $\rho \equiv 1$ on $\Omega = [0, 1]^d$:

$$W_2^2 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \geq \frac{1}{12}$$
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 $\Omega^N$ s.t.

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

Then, 

$$W_2^2 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \leq \text{cst}(d, \Omega) \cdot \frac{\varepsilon^{1-d}}{N}.$$ 

- In particular, if $\varepsilon \approx N^{-1/\beta}$, then $W_2^2 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \leq CN^{\frac{d-1}{\beta} - 1}$. This upper bound goes to zero as $N \to +\infty$ provided that $\beta > d - 1$.
- When $\beta = d$, the upper bound of the theorem is

$$F_N(B_N) = W_2^2 \left( \frac{1}{N} \sum_{i} \delta_{y_i}, \rho \right) \lesssim \left( \frac{1}{N} \right)^{1/d}.$$
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 $\Omega^N$ s.t.

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

Then,

$$W_2^2 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \leq \text{cst}(d, \Omega) \cdot \frac{\varepsilon^{1-d}}{N}.$$  

- In particular, if $\varepsilon \approx N^{-1/\beta}$, then $W_2^2 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \leq C N^{\frac{d-1}{\beta} - 1}$. This upper bound goes to zero as $N \rightarrow +\infty$ provided that $\beta > d - 1$.

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

$$F_N(B_N) = W_2^2 \left( \frac{1}{N} \sum_i \delta_{y_i}, \rho \right) \lesssim \left( \frac{1}{N} \right)^{1/d}.$$  

This does not match the upper bound on $\min_{\Omega^N} F_N$: $\min_{\Omega^N} F_N \lesssim \left( \frac{1}{N} \right)^{2/d}$.
Let \( \Omega \subseteq \mathbb{R}^d \) be convex and let \( \rho \in \mathcal{P}(\Omega) \). Consider a point cloud \( Y \) in \( \Omega^N \) s.t.

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

Then,

\[
W_2^2 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \leq \text{cst}(d, \Omega) \cdot \frac{\varepsilon^{1-d}}{N}.
\]

- In particular, if \( \varepsilon \approx N^{-1/\beta} \), then \( W_2^2 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \leq CN^{\frac{d-1}{\beta}} \). This upper bound goes to zero as \( N \to +\infty \) provided that \( \beta > d - 1 \).
- When \( \beta = d \), the upper bound of the theorem is

\[
F_N(B_N) = W_2^2 \left( \frac{1}{N} \sum_{i} \delta_{y_i}, \rho \right) \lesssim \left( \frac{1}{N} \right)^{1/d}.
\]

This does not match the upper bound on \( \min_{\Omega^N} F_N \): \( \min_{\Omega^N} F_N \lesssim \left( \frac{1}{N} \right)^{2/d} \).

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 $d - 1 < \beta < d$

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

\[ N = 257 \]

- Numerically, it seems that $W_2^2(\mu_N, \rho) \approx N^{-1.01}$, while our upper bound would give an exponent of $\frac{d-1}{\beta} - 1 \approx -0.207$. 
Numerical example with $d - 1 < \beta < d$

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

\[ N = 1025 \]

- Numerically, it seems that $W_2^2(\mu_N, \rho) \approx N^{-1.01}$, while our upper bound would give an exponent of $\frac{d-1}{\beta} - 1 \approx -0.207$.  

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

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

$$N = 4097$$

- Numerically, it seems that $W_2^2(\mu_N, \rho) \approx N^{-1.01}$, while our upper bound would give an exponent of $\frac{d-1}{\beta} - 1 \approx -0.207$. 
Numerical example with $d - 1 < \beta < d$

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

\[ N = 16385 \]

- Numerically, it seems that $W_2^2(\mu_N, \rho) \approx N^{-1.01}$, while our upper bound would give an exponent of $\frac{d - 1}{\beta} - 1 \approx -0.207$. 
Main theorem: sketch of proof

We assume: \( \forall i \neq j, \|y_i - y_j\| \geq \varepsilon \)

**Main idea:** There cannot be “too many” Laguerre cells that are “elongated”
Main theorem: sketch of proof

We assume: \( \forall i \neq j, \|y_i - y_j\| \geq \varepsilon \)

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

- We use the concavity of the Laguerre cells w.r.t the weights \( \Phi \):
  \[
  \frac{1}{2} \text{Lag}_i(Y, 0) \oplus \frac{1}{2} \text{Lag}_i(Y, \Phi) \subset \text{Lag}_i(Y, \Phi/2)
  \]
Main theorem: sketch of proof

We assume: \( \forall i \neq j, \quad \|y_i - y_j\| \geq \varepsilon \)

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

- We use the concavity of the Laguerre cells w.r.t the weights \( \Phi \):

\[
\frac{1}{2} \text{Lag}_i(Y, 0) \oplus \frac{1}{2} \text{Lag}_i(Y, \Phi) \subset \text{Lag}_i(Y, \Phi/2)
\]

\( \implies \) if \( \text{Lag}_i(Y, \Phi) \) is "elongated", then \( |\text{Lag}_i(Y, \frac{1}{2}\Phi)| \) is "large":

![Diagram showing Laguerre cells and their concavity properties.](image-url)
Main theorem: sketch of proof

We assume: ∀i ≠ j, \|y_i - y_j\| ≥ \varepsilon

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

- We use the concavity of the Laguerre cells w.r.t the weights \( \Phi \):

\[
\frac{1}{2} \text{Lag}_i(Y, 0) \oplus \frac{1}{2} \text{Lag}_i(Y, \Phi) \subset \text{Lag}_i(Y, \Phi/2)
\]

\[\implies\] if \( \text{Lag}_i(Y, \Phi) \) is “elongated”, then \( |\text{Lag}_i(Y, \frac{1}{2} \Phi)| \) is “large”:

- The \((\text{Lag}_i(Y, \frac{1}{2} \Phi))_i\) do not overlap: \[
\sum_{i=1}^{N} |\text{Lag}_i(Y, \frac{1}{2} \Phi)| \leq |\Omega|.
\]

Yet, \[
|\text{Lag}_i(Y, \frac{1}{2} \Phi)| \geq c\varepsilon^{d-1} \text{diam}(\text{Lag}_i(Y, \Phi)).
\]
Main theorem: sketch of proof

We assume: \( \forall i \neq j, \|y_i - y_j\| \geq \varepsilon \)

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

- We use the concavity of the Laguerre cells w.r.t the weights \( \Phi \):

\[
\frac{1}{2} \text{Lag}_i(Y, 0) \oplus \frac{1}{2} \text{Lag}_i(Y, \Phi) \subset \text{Lag}_i(Y, \Phi/2)
\]

\[\implies \text{if } \text{Lag}_i(Y, \Phi) \text{ is “elongated”, then } |\text{Lag}_i(Y, \frac{1}{2} \Phi)| \text{ is “large”:}\]

- The \((\text{Lag}_i(Y, \frac{1}{2} \Phi)))_i\) do not overlap: \( \sum_{i=1}^{N} |\text{Lag}_i(Y, \frac{1}{2} \Phi)| \leq |\Omega| \). Yet, \( |\text{Lag}_i(Y, \frac{1}{2} \Phi)| \geq c\varepsilon^{d-1} \text{diam}(\text{Lag}_i(Y, \Phi)) \).

- \( W_1 \left( \frac{1}{N} \sum_{i=1}^{N} \delta_{b_i(Y)}, \rho \right) \lesssim \frac{1}{N} \sum_{i=1}^{N} \text{diam}(\text{Lag}_i(Y, \Phi)) \lesssim \frac{\varepsilon^{1-d}}{N} \), and \( W_2^2 \leq CW_1 \)
Outline

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)
Lagrangian critical measures

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

**Definition (Lagrangian critical measures)**

A measure $\mu$ is said to be Lagrangian critical if in the unique optimal transport plan $\gamma$ (induced by a map $T$ such that $T#\rho = \mu$) for the quadratic cost from $\rho$ to $\mu$ 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 $\gamma_y$ on $T^{-1}(y)$.

The empirical measures $\mu_N$ are Lagrangian critical, and so is any weak limit $\mu$. 
Dimensional decomposition of Lagrangian critical measures

Let $\mu$ be a Lagrangian critical measure and define the sets

$$S_k = \{ y \in \text{spt}(\mu) : \dim(T^{-1}(y)) = d - k \}.$$  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 $\mu$ is absolutely continuous, then $\mu = \rho$.
- For $k = 0, 1, d$ the measure $\mu^k$ is absolutely continuous w.r.t. the $\mathcal{H}^k$–Hausdorff measure. This is conjectured for all $k$, but not proven.
- In particular, if $d = 2$, $\mu$ fully decomposes into three layers, one per dimension.
- If moreover $\mu$ 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 $\rho$ (constant on this support), a critical point cloud for $F_N$ which is not a minimizer and its limit measure. The limit measure $\mu$ is not uniform on the vertical segment (but it is uniform on the lower rectangle).
Outline

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)
Stable critical points

A critical point is *stable* if it is a local minimizer of $F_N$. In general, iterative algorithms converge to stable critical points.

Typical example of an *unstable* critical point:
Proposition

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

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

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

$$\text{diam}(\text{Lag}_i(Y, \Phi_Y)) \leq cN^{-1/d}$$. In particular

$$W_2 \left( \frac{1}{N} \sum_i \delta_{y_i}, \rho \right) \leq c \left( \frac{1}{N} \right)^{1/d}.$$
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: \( Y^{k+1} = (b_1(Y^k), \ldots, b_N(Y^k)) \).
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: $Y^{k+1} = (b_1(Y^k), \ldots, b_N(Y^k))$.

$k=101$
Another unstable critical point

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

$k=121$
Another unstable critical point

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

$k=141$
Another unstable critical point

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

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.

$$\min_{Y \in \Omega^N} W_2^2 \left( \frac{1}{N} \sum_i \delta_{y_i}, \rho \right)$$
	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 $\rho$
- iterations generically converge to stable critical points, which have good values for the energy

(Some) open questions:

- Can estimates be improved if $\rho$ is bounded from above and below?
- Can estimates be improved when $\rho$ 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!
Summary and Perspectives

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

$$\min_{Y \in \Omega^N} W_2^2 \left( \frac{1}{N} \sum_i \delta_{y_i}, \rho \right)$$

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 $\rho$
- iterations generically converge to stable critical points, which have good values for the energy

**(Some) open questions:**

- Can estimates be improved if $\rho$ is bounded from above and below?
- Can estimates be improved when $\rho$ 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!