SEMI-DISCRETE CONVEX ORDER AND LAGUERRE TESSELLATION FITTING

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ABSTRACT. Laguerre tessellations provide a computationally tractable way to describe a large number of convex partitions of the Euclidean space. For this reason, they have become popular in computational geometry, imaging and numerical analysis, both as a modeling and a discretization tool. In this paper we study the problem of reconstructing a Laguerre tessellation with prescribed cell volumes from its cell barycenters. We show that this problem can be reformulated as a Wasserstein projection onto the convex set of discrete measures dominated in the convex order by an absolutely continuous one. We provide a complete characterization of this set, and exploit this to construct a robust algorithm to solve the reconstruction problem, which can also be applied to fit a Laguerre tessellation to an arbitrary set of barycenters. Interestingly this reconstruction problem is linked to the Semi-Discrete Wasserstein metric extrapolation.

1. Introduction

A partition of \mathbb{R}^d is a list (P_1, \dots, P_N) of non-empty sets P_i , called cells, with pairwise disjoint interiors, and such that

$$\bigcup_{i} P_i = \mathbb{R}^d.$$

Laguerre tessellations, also known as weighted Voronoi tessellations, affine partitions [1], or regular partitions [17], are partitions of \mathbb{R}^d into convex cells that generalize Voronoi tessellations. Specifically, given a vector of distinct generators (or cell centers) $Y = (y_1, \ldots, y_N) \in (\mathbb{R}^d)^N \setminus \Delta_N$, where

$$\Delta_N := \{ Y = (y_1, \dots, y_N) \in (\mathbb{R}^d)^N ; \exists 1 \le i < j \le N \text{ such that } y_i = y_i \},$$

and a vector of weights $\phi = (\phi_1, \dots, \phi_N) \in \mathbb{R}^N$, the associated Laguerre tessellation is the partition of \mathbb{R}^d defined by the cells

$$L_i(Y,\phi) := \{x \in \mathbb{R}^d : \langle x, y_i \rangle - \phi_i \le \langle x, y_j \rangle - \phi_j \ \forall i \ne j \}.$$

Equivalently, a Laguerre tessellation of \mathbb{R}^d is a tessellation which can be obtained by projecting the facets of a convex polyhedron in \mathbb{R}^{d+1} [4, 17]. Setting $\phi_i = |y_i|^2/2$, the definition above yields the classical Voronoi tessellation associated with Y. In general, Laguerre tessellations form a strict subset of the space of all possible convex partitions of \mathbb{R}^d . However, if $d \geq 3$ many convex partition are Laguerre tessellations [15], and if d=2 this is also the case, although with more restrictive geometric conditions (see Figure 1 below). Because of this, Laguerre tessellations have become a common tool for imaging problems in various fields, including biology, material science, or optics, to name a few.

In this work we will be concerned with an inverse problem originally introduced in [5] and arising from applications in imaging for material science: can we recover a Laguerre tessellation provided the cell volumes and their barycenters? We will answer this question by reformulating it as a particular instance of weak optimal transport [12, 11]: the Wasserstein projection problem onto the set of empirical measures in convex order with a given absolutely continuous one. We will provide a precise description of the set of such measures, establishing a clear connection between semi-discrete optimal transport theory and convex order relations involving empirical measures. Using this link we will provide a robust numerical algorithm to solve the reconstruction problem.

1.1. Semi-discrete optimal transport. Laguerre tessellations with prescribed cell volumes arise naturally in the theory of optimal transport. Let $\mathcal{P}_1(\mathbb{R}^d)$ denote the set of probability measures with finite first moments. Given a measure $\rho \in \mathcal{P}_1(\mathbb{R}^d)$ and a vector $v = (v_1, \dots, v_N) \in \mathbb{R}^N_{>0}$ of volumes satisfying $\sum_i v_i = 1$, for any $Y \in (\mathbb{R}^d)^N \setminus \Delta_N$, there always exists a vector of weights $\phi^* \in \mathbb{R}^N$ such that

(1)
$$\rho(L_i(Y, \phi^*)) = v_i, \quad \forall i \in \{1, \dots, N\}.$$

Moreover, there is a unique Laguerre tessellation that satisfies this condition. This result follows from classical theory in semi-discrete optimal transport.

Specifically, consider the optimal transport problem:

(2)
$$\max \left\{ \int \langle x, y \rangle \, d\gamma(x, y) \; ; \; \gamma \in \Gamma(\rho, \nu(Y, v)) \right\},$$

where $\Gamma(\mu, \nu)$ denotes the set of probability measures on $\mathbb{R}^d \times \mathbb{R}^d$ with marginals μ and ν , respectively, and $\nu(Y, v)$ is the empirical measure supported on Y with masses v, i.e.

(3)
$$\nu(Y,v) := \sum_{i=1}^{N} v_i \delta_{y_i} \in \mathcal{P}(\mathbb{R}^d).$$

Since ρ is absolutely continuous, Brenier's theorem guarantees that problem (2) admits a unique solution γ , which is characterized as the only transport plan $\gamma \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ satisfying $\gamma = (\mathrm{Id}, \nabla u)_{\#}\rho$ and

$$(4) \qquad (\nabla u)_{\#} \rho = \nu(Y, v),$$

where $u: \mathbb{R}^d \to \mathbb{R}$ is a convex function known as Brenier potential, and # denotes the push-forward of measures. It can be shown that u necessarily takes the form

(5)
$$u(x) = \max_{i \in \{1,\dots,N\}} \left\{ \langle x, y_i \rangle - \phi_i \right\},\,$$

for an appropriate vector of weights ϕ . Consequently,

$$\nabla u(x) = y_i$$
 for a.e. $x \in L_i(Y, \phi)$.

Expressing condition (4) with this ansatz, one deduces the existence of a vector of weights ϕ^* satisfying (1). Choosing $\phi = \phi^*$ in (5) yields a Brenier potential for the transport problem (2).

1.2. Convex order. Two probability measures $\nu, \rho \in \mathcal{P}_1(\mathbb{R}^d)$ are said to be in convex order, denoted $\nu \leq_C \rho$, if and only if

(6)
$$\int \varphi \, \mathrm{d}\nu \le \int \varphi \, \mathrm{d}\rho$$

for all convex functions $\varphi : \mathbb{R}^d \to \mathbb{R}$. By Strassen's theorem, a convex order relationship between two measures is equivalent to the existence of a martingale coupling between them. This fact has made convex order relations a central tool in economics and finance applications, for example. In particular, common problems in this context are the design of sampling algorithms preserving convex order relations or, conversely, statistical tests to infer convex order relationships from samples. Recently, these problems have been approached using Wasserstein projections: sampling strategies were proposed in [2, 3], while statistical tests for convex order were developed in [13, 14].

The Wasserstein projection of a given probability measure ν onto the set of measures dominated by ρ in the convex order, consists in finding the measure μ solving

(7)
$$\inf\{W_2^2(\mu,\nu); \mu \leq_C \rho\}$$

where W_2 denotes the 2-Wasserstein distance (see equation (12) for the definition). Remarkably, this problem can be reformulated as a weak optimal transport problem [11], i.e. as a minimization problem over couplings $\gamma \in \Gamma(\rho, \nu)$ as in (2), but where the cost of transport takes as argument the probability kernel $x \mapsto \gamma_x$, where $d\gamma(x, y) = d\rho(x)d\gamma_x(y)$ is the disintegration of γ with respect to the projection on its first marginal. This interpretation has been crucial for the recent development of numerical algorithms to solve the projection problem in the fully discrete setting, where all measures are empirical [3, 10, 13].

1.3. Contributions and structure of the paper. Let $C(\rho, v)$ be the set of particle positions $B = (b_1, \ldots, b_N) \in (\mathbb{R}^d)^N$ associated with empirical measures $\nu(B, v)$ that satisfy (6), i.e.

$$\mathcal{C}(\rho, v) := \{ B = (b_1, \dots, b_N) \in (\mathbb{R}^d)^N ; \ \nu(B, v) \leq_C \rho \},$$

where $\rho \in \mathcal{P}_1(\mathbb{R}^d)$ is a given probability measure with bounded density with respect to Lebesgue, and as before $v = (v_1, \dots, v_N) \in \mathbb{R}^N_{>0}$ with $\sum_i v_i = 1$.

Using (6) and the definition of convexity one can verify that $\mathcal{C}(\rho, v)$ is a convex set. Our main contributions concern the structure of this set and its relation to the Laguerre tessellation reconstruction problem. Specifically, we will show that the exposed points of the set $\mathcal{C}(\rho, v)$ are the vectors $B = (b_i)_i$ where

$$b_i = \frac{1}{v_i} \int_{L_i(Y,\phi^*)} x \mathrm{d}\rho(x) \,,$$

where $Y = (\mathbb{R}^d)^N \setminus \Delta_N$ is any vector of generators and ϕ^* is such that condition (1) holds. Moreover we show that the extreme points of $\mathcal{C}(\rho, v)$ can be constructed in a similar way but replacing Laguerre tessellations by an inductive type of tessellation introduced in [1] and which we name hierarchical Laguerre tessellations. Note that in the fully-discrete case, i.e. when also ρ is a fixed empirical measure, the set $\mathcal{C}(\rho, v)$ coincides with the so-called gravity body introduced by Brieden and Gritzmann [6] to

study balanced clusterings of points in \mathbb{R}^d [7]. In that case, $\mathcal{C}(\rho, v)$ is a polytope and its vertices correspond to the barycenters of a certain class of Laguerre tessellations. Our results represent the natural extension of such a characterization to the case of an absolutely continuous reference measure ρ .

Exploiting our characterization of the set $C(\rho, v)$, we show that given a collection of barycenters B of a Laguerre tessellation, one can always recover a hierarchical tessellation whose cell barycenters are arbitrary close to B by solving a Wasserstein projection (7). Finally, we provide a numerical algorithm to solve the reconstruction problem, which can also be used to solve problem (7) in the semi-discrete setting, i.e. whenever ρ is absolutely continuous and ν is empirical.

The rest of the paper is structured as follows. In Section 2 we introduce the concept of hierarchical Laguerre tessellation and describe its relation with classical Laguerre tessellations. In Section 3 we characterize the exposed and extreme points of the set \mathcal{C} . In Section 4 we study the projection problem to recover a Laguerre tessellation with prescribed cell volumes from the cell barycenters. Finally, we propose a subgradient descent method to solve the projection problem, with sublinear rate of convergence, and show numerical results in Section 5.

2. Hierarchical Laguerre tessellations

In this section we describe the concept of hierarchical Laguerre tessellation, which was introduced in [1] to extend Kadets type theorems on specific inductive partitions of convex bodies. Here we focus on the case where the cell volumes of the tessellations are assigned, and descibe the precise relation between hierarchical Laguerre tessellation and classical ones. This will be useful in the next section to characterize the set of empirical measures dominated in the convex order by a given measure.

Let $\rho \in \mathcal{P}_1(\mathbb{R}^d)$ be a reference probability measure. We will also denote by ρ its density with respect to the Lebesgue measure, which we assume to be bounded. We consider partitions with a fixed number of regions and with prescribed volumes. More precisely, given a vector $v = (v_1, \ldots, v_N) \in \mathbb{R}^N_{>0}$ with $\sum_i v_i = 1$, we define the space of convex partitions with volumes v as follows

$$\mathcal{T}_{\text{conv}}(\rho, v) := \{ (P_i)_i \text{ partition of } \mathbb{R}^d : P_i \text{ is convex and } \rho(P_i) = v_i \ \forall i \}.$$

Similarly the space of Laguerre tessellations

$$\mathcal{T}_{\text{Lag}}(\rho, v) := \{ (P_i)_i \text{ Laguerre tessellation of } \mathbb{R}^d : \rho(P_i) = v_i \ \forall i \}.$$

Clearly $\mathcal{T}_{Lag}(\rho, v) \subset \mathcal{T}_{conv}(\rho, v)$. However there are convex partitions that are not Laguerre tessellations. Typical examples in any dimension are binary partitions by hyperplanes (see Figure 2, left). In \mathbb{R}^2 , however, we have further counterexamples due to stronger geometric constraints implied by the definition of Laguerre tessellations, illustrated in Figure 1.

We equip the spaces \mathcal{T}_{conv} and \mathcal{T}_{Lag} with the (pseudo-)metric defined as follows

$$\sum_{i} \rho(P_i \triangle Q_i),$$

for any couple of partitions $(P_i)_i$ and $(Q_i)_i$, where \triangle denotes the symmetric difference.

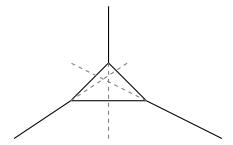


FIGURE 1. An example of convex partition of \mathbb{R}^2 which is not a (hierarchical) Laguerre tessellation. The two-dimensional cells of the partition have as boundaries the solid lines. In order for this tessellation to be Laguerre, it should be possible to recover it as the projection of a polyhedron in \mathbb{R}^3 , but this is impossible if the dashed lines do not meet at a single point.

In the following, it will be important to characterize the closure of $\mathcal{T}_{\text{Lag}}(\rho, v)$. This can be done using the concept of hierarchical Laguerre tessellation:

Definition 2.1 (Hierarchical Laguerre tessellation). By induction, given a hierarchical Laguerre tessellation $(P_i)_i$, the tessellation obtained by partitioning a given cell P_i with a Laguerre tessellation is still a hierarchical Laguerre tessellation.

As for Laguerre tessellations, we define

 $\mathcal{T}_{\text{hLag}}(\rho, v) \coloneqq \{(P_i)_i \text{ hierarchical Laguerre tessellation of } \mathbb{R}^d : \rho(P_i) = v_i \ \forall i \}.$

Proposition 2.2. $\overline{\mathcal{T}_{\text{Lag}}(\rho, v)} = \mathcal{T}_{\text{hLag}}(\rho, v)$.

Proof. Let us show that $\overline{\mathcal{T}_{Lag}(\rho, v)} \subseteq \mathcal{T}_{hLag}(\rho, v)$. Given any sequence of partitions $((L_i^n)_i)_n \subset \mathcal{T}_{Lag}$, let $(Y^n)_n \subset (\mathbb{R}^d)^N/\Delta_N$ be the associated sequence of generators, shifted and normalized so that $y_1^n = 0$ and $\max_{i \neq k} |y_i^n - y_k^n| = 1$. Up to extracting a subsequence (not relabelled), for some $2 \leq M \leq N$ and $Y^{\infty} \in (\mathbb{R}^d)^M \setminus \Delta_M$, and a surjective map $\sigma : \{1, \ldots, N\} \to \{1, \ldots, M\}$,

$$y_i^n \to y_{\sigma(i)}^\infty$$
, $\forall i = 1, \dots, N$.

Moreover,

$$\nu(Y^n, v) = \sum_{i=1}^N v_i \delta_{y_i^n} \rightharpoonup \nu(Y^\infty, w) = \sum_{j=1}^M w_j \delta_{y_i^\infty}, \quad w_j = \sum_{i \in \sigma^{-1}(j)} v_i.$$

Let $(\gamma^n)_n$ be the sequence of optimal transport plans from ρ to $\nu(Y^n, v)$, obtained by solving problem (2). By stability of optimal plans (see, e.g., Theorem 5.20 in [18]), this converges weakly to the optimal transport plan from ρ to $\nu(Y^{\infty}, w)$,

$$\gamma = \sum_{j=1}^{M} \delta_{y_j^{\infty}} \otimes \rho|_{L_j^{\infty}},$$

where $(L_j^{\infty})_j$ is the Laguerre tessellation with generators Y^{∞} and volumes w. In particular,

$$\bigcup_{i \in \sigma^{-1}(j)} L_i^n \to L_j^\infty$$

for $n \to \infty$. Now suppose that for some fixed $j, \tilde{N} := |\sigma^{-1}(j)| > 1$. Let

$$Q_j^n := \bigcup_{i \in \sigma^{-1}(j)} L_i^n.$$

We shift and normalize the set $\tilde{Y}^n = (y_i^n)_{i \in \sigma^{-1}(j)}$ so that $y_{i_1}^n = 0$ for some $i_1 \in \sigma^{-1}(j)$ and $\max_{i \neq k} |y_i^n - y_k^n| = 1$. Up to extracting a subsequence (not relabelled), for some $2 \leq \tilde{M} \leq \tilde{N}$ and $\tilde{Y}^{\infty} \in (\mathbb{R}^d)^{\tilde{M}} \setminus \Delta_{\tilde{M}}$, and a surjective map $\sigma : \{1, \ldots, \tilde{N}\} \to \{1, \ldots, \tilde{M}\}$,

$$y_i^n \to y_{\sigma(i)}^\infty$$
, $\forall i = 1, \dots, \tilde{N}$.

We can then proceed as before, with ρ replaced by $\rho|_{Q_j^n}$, for which $\rho|_{Q_j^n} \to \rho|_{L_j^\infty}$ as $n \to \infty$. Iterating the argument, this implies that $\overline{\mathcal{T}}_{\text{Lag}} \subseteq \mathcal{T}_{\text{hLag}}$.

Let us prove that $\mathcal{T}_{hLag} \subseteq \overline{\mathcal{T}}_{Lag}$. Given any hierarchical Laguerre tessellation $(L_i)_i \in \mathcal{T}_{hLag}(\rho, v)$, using Lemma 3.5 in [1], we can construct a sequence of Laguerre tessellations $(L_i^n)_i$ with generators $Y^n \in (\mathbb{R}^d)^N \setminus \Delta_N$ (but possibly different volumes) such that $L_i^n \to L_i$. In particular, this means that

$$v_i^n \coloneqq \rho(L_i^n) \to v_i$$

for all i. Let $(\tilde{L}_i^n)_i$ be the Laguerre tessellation with generators Y^n , but with weights chosen so that $\rho(\tilde{L}_i^n) = v_i$ for all i. We now show that, up to the extraction of a subsequence, \tilde{L}_i^n also converges towards L_i for all i, which implies that $\mathcal{T}_{\text{hLag}} \subseteq \overline{\mathcal{T}}_{\text{Lag}}$. Proceeding as before, we can assume that, for some $2 \leq M \leq N$ and $Y^{\infty} \in (\mathbb{R}^d)^M \setminus \Delta_M$, and a surjective map $\sigma : \{1, \ldots, N\} \to \{1, \ldots, M\}$,

$$y_i^n \to y_{\sigma(i)}^\infty$$
, $\forall i = 1, \dots, N$.

Denoting $v^n := (v_i^n)_i$, we have

$$\nu(Y^n, v^n) \rightharpoonup \nu(Y^\infty, w)$$
,

and also

$$\nu(Y^n, v) \rightharpoonup \nu(Y^\infty, w).$$

Using again the stability of optimal transport maps we deduce that, up to the extraction of a subsequence,

$$\bigcup_{i \in \sigma^{-1}(j)} \tilde{L}_i^n \to L_j^{\infty}, \quad \text{and} \quad L_j^{\infty} = \bigcup_{i \in \sigma^{-1}(j)} L_i,$$

where $(L_j^{\infty})_j$ is also the Laguerre tessellation with volumes w and generators Y^{∞} . Iterating the argument as before we obtain the result.

3. Semi-discrete convex order

In this section we study the set of empirical measures of prescribed masses in convex order with respect to ρ . We will give a characterization of this set as a convex body of \mathbb{R}^{dN} , and in terms of measures supported on the cell barycenters of Laguerre and hierarchical Laguerre tessellations.

As before, we fix a vector $v = (v_1, \ldots, v_N) \in \mathbb{R}^N_{>0}$ such that $\sum_i v_i = 1$, and a reference measure $\rho \in \mathcal{P}_1(\mathbb{R}^d)$ with bounded density, and we study the following set:

$$\mathcal{C}(\rho, v) := \{ B \in (\mathbb{R}^d)^N ; \ \nu(B, v) \preceq_C \rho \} \subset \mathbb{R}^{dN}$$

where we recall that

$$\nu(B, v) := \sum_{i=1}^{N} v_i \delta_{b_i} \in \mathcal{P}(\mathbb{R}^d),$$

for any $B = (b_1, \ldots, b_N) \in (\mathbb{R}^d)^N$. We will omit to indicate the dependency of \mathcal{C} on ρ and v when clear from the context. It will be convenient to use the weighted l^2 metric on $(\mathbb{R}^d)^N$ defined by

$$\langle Y, Z \rangle_v := \sum_i \langle y_i, z_i \rangle v_i,$$

for any $Y = (y_i)_i$ and $Z = (z_i)_i$ in $(\mathbb{R}^d)^N$. Moreover, we will denote $||Y||_v^2 := \langle Y, Y \rangle_v$. By definition, a point $B \in \mathcal{C}$ if and only if

$$\sum_{i} \varphi(b_i) v_i \le \int \varphi \rho$$

for any convex function $\varphi : \mathbb{R}^d \to \mathbb{R}$. Then by Jensen's inequality, \mathcal{C} is convex. It is also closed, since the functions φ defining the set are continuous. Moreover \mathcal{C} is bounded, since we can use $\varphi : x \to |x|$. Now, if $B \in \mathcal{C}$ using $\varphi : x \to \pm x$, we obtain that

$$\sum_{i} b_{i} v_{i} = \operatorname{bary}(\rho) := \int x d\rho(x).$$

Due to this constraint C cannot have full dimension, and in particular one can check that one has precisely:

Lemma 3.1. $\dim(C) = (N-1)d$.

Proof. We prove this by induction on N. The statement is trivially true for N=1 for any ρ . Suppose it is also true for a given N, and fix a vector of admissible volumes $v=(v_1,\ldots,v_{N+1})$. Let $\tilde{\rho}\in L^\infty(\mathbb{R}^d)$ be any density such that $0\leq \tilde{\rho}\leq \rho$ and $\tilde{\rho}(\mathbb{R}^d)=v_{N+1}$. By Jensen's inequality, we can construct $B=(b_1,\ldots,b_{N+1})\in \mathcal{C}_{N+1}(\rho,v)$ by setting

$$b_{N+1} = \operatorname{bary}(\tilde{\rho}) := \frac{1}{\tilde{\rho}(\mathbb{R}^d)} \int x d\tilde{\rho}(x),$$

and $\tilde{B} = (b_1, \ldots, b_N)$ so that

$$\nu(\tilde{B}, \tilde{v}) \preceq_C \rho - \tilde{\rho}$$
.

Hence we just need to show that b_{N+1} can be chosen arbitrarily in a set of dimension d, since this implies that $\dim(\mathcal{C}_{N+1}) \geq dN$. By convexity, it suffices to find d+1

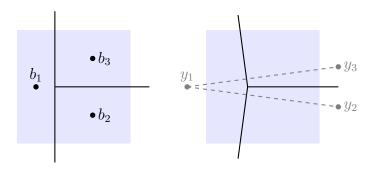


FIGURE 2. An example of configuration $B = (b_1, b_2, b_3) \in \mathcal{B}_{hLag}$, where ρ is uniform on a square (shaded area) and $v_1 = v_2 = v_3$, which is not in \mathcal{B}_{Lag} (left). The vector B can be approximated with arbitrary precision by the barycenters of a Laguerre tessellations with equal volumes and well-chosen cell centers $Y = (y_1, y_2, y_3)$ (right).

densities $\{\tilde{\rho}_i\}_{i=1}^{d+1}$ as above such that the convex hull of b_1, \ldots, b_{d+1} , with $b_i = \text{bary}(\tilde{\rho}_i)$ has dimension d. We can construct them as follows

$$\tilde{\rho}_i = \frac{v_{N+1}}{1 - \varepsilon_i} \left(\rho - \varepsilon_i \frac{\rho|_{A_i}}{\rho(A_i)} \right)$$

where $0 < \varepsilon_i < \min(\rho(A_i), 1 - v_{N+1})$ is a given coefficient and the sets A_i are defined inductively as follows

$$A_1 = \mathbb{R}^d$$
, $A_{i+1} = A_i \cap \{x : \langle h_i, x - p_i \rangle > 0\}$, $p_i = \text{bary}(\rho|_{A_i})$,

where $h_1 = \mathbb{R}^d \setminus \{0\}$ is arbitrary, and for all $i \geq 2$, $h_i \in \text{span}(p_2 - p_1, \dots, p_i - p_1)^{\perp} \setminus \{0\}$ and it is also chosen arbitrarily. It is easy to check that $\rho(A_i) > 0$: in fact, if $\rho(A_i) > 0$, then $\rho(A_{i+1}) > 0$ independently of the choice of h_i , since $p_i = \text{bary}(\rho|_{A_i})$. Moreover, by the bounds on ε_i , we have indeed $0 \leq \tilde{\rho}_i \leq \rho$. Now, since $A_1 = \mathbb{R}^d$, $b_1 = p_1$ and

$$b_i = \text{bary}(\tilde{\rho}_i) = \frac{1}{1 - \varepsilon_i} (p_1 - p_i).$$

Since ρ is absolutely continuous, $p_{i+1} = \text{bary}(\rho|_{A_{i+1}}) \in A_{i+1}$. By definition of A_{i+1} , this means that for all $i \geq 2$,

$$p_{i+1} - p_i \notin \text{span}(p_2 - p_1, \dots, p_i - p_1).$$

Hence, by induction, the vectors $\{b_2 - b_1, \dots, b_{d+1} - b_1\}$ are linearly independent, and we are done.

Given a partition of $(P_i)_{i=1}^N$ of \mathbb{R}^d such that $v_i = \rho(P_i)$ for all i, we can construct an element of $B \in \mathcal{C}$ simply by setting

$$b_i = \operatorname{bary}_{\rho}(P_i) := \frac{1}{v_i} \int_{P_i} x d\rho(x).$$

In particular, denoting by

$$\mathcal{B}_{\text{Lag}}(\rho, v) := \{ B \in (\mathbb{R}^d)^N \; ; \; \exists \, (L_i)_i \in \mathcal{T}_{\text{Lag}}(\rho, v) \text{ such that } b_i = \text{bary}_{\rho}(L_i), \; \forall i \}.$$

and

$$\mathcal{B}_{\mathrm{hLag}}(\rho, v) := \{ B \in (\mathbb{R}^d)^N \; ; \; \exists \, (L_i)_i \in \mathcal{T}_{\mathrm{hLag}}(\rho, v) \text{ such that } b_i = \mathrm{bary}_{\rho}(L_i), \; \forall i \}.$$

the set of barycenters of Laguerre and hierarchical Laguerre tesellations with prescribed volumes, we have $\mathcal{B}_{Lag} \subset \mathcal{B}_{hLag} \subset \mathcal{C}$ by construction. Furthermore, \mathcal{B}_{Lag} is neither convex nor closed. An example showing that the limit of vectors in \mathcal{B}_{Lag} may not belong to the same set is shown in Figure 2. More precisely, as a corollary of Proposition 2.2 we have that:

Lemma 3.2. $\overline{\mathcal{B}}_{\text{Lag}} = \mathcal{B}_{\text{hLag}}$.

Define the function $F:(\mathbb{R}^d)^N\to\mathbb{R}$ as follows

(8)
$$F(Y) := \max \left\{ \int \langle x, y \rangle d\gamma(x, y) \; ; \; \gamma \in \Gamma(\nu(Y, v), \rho) \right\}.$$

We will also use $F_v(Y)$ to denote the same function, when we will need emphasize the dependence on v. The following proposition states that F is the support function of the convex set C.

Proposition 3.3. The function F is convex, it is C^1 on $(\mathbb{R}^d)^N \setminus \Delta_N$, and for all Y in this set

$$\nabla F(Y) = (\text{bary}_{\rho} L_i^*(Y, v))_i$$

where ∇ denotes the gradient with respect to the l^2 inner product weighted by v, $\langle \cdot, \cdot \rangle_v$, and $(L_i^*(Y, v))_i$ is the unique Laguerre tessellation with generators Y and volumes v. Moreover, for all $B \in (\mathbb{R}^d)^N$

$$F^*(B) = \iota_{\mathcal{C}}(B) := \begin{cases} 0 & \text{if } \nu(B, v) \leq_C \rho \\ +\infty & \text{otherwise} \end{cases},$$

where F^* is the Fenchel-Legendre transform of F, again with respect to $\langle \cdot, \cdot \rangle_v$.

Proof. The first part follows from Proposition 5.1 in [16], for example. We give a sketch of the proof for completeness. Given any two vectors $Z, Y \in (\mathbb{R}^d)^N \setminus \Delta_N$ the coupling $\gamma \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ defined by

$$\int \varphi(x,y) d\gamma(x,y) = \sum_{i} \int_{L_{i}^{*}(Z,v)} \varphi(x,y_{i}) d\rho(x)$$

for any bounded continuous function $\varphi : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, belongs to $\Gamma(\rho, \nu(Z, v))$ and is admissible for the problem defining F(Z). In particular, this implies that

$$F(Z) \ge F(Y) + \sum_{i} \int_{L_{i}^{*}(Z,v)} \langle x, z_{i} - y_{i} \rangle d\rho(x)$$

This means that $B(Y) := (\text{bary}_{\rho}L_i^*(Y, v))_i \in \partial F(Y)$, the subgradient of F with respect to the metric $\langle \cdot, \cdot \rangle_v$, and therefore F is convex. By stability of optimal transport, $\text{bary}_{\rho}(L_i^*(Y, v))$ is a continuous function of Y (see Proposition 5.1 in [16]), which implies at once that $B(Y) = \nabla F(Y)$ and that F is C^1 .

For the second part of the statement, by Kantorovich duality

$$F(Y) = \inf \left\{ \int u^* \nu(Y, v) + \int u \rho; u \text{ convex} \right\}$$

Therefore,

$$F^*(B) = \sup_{Y} \sup_{u \text{ convex}} \langle B, Y \rangle_v - \sum_i u^*(y_i) v_i - \int u \rho$$
$$= \sup_{u \text{ convex}} \sum_i u(b_i) v_i - \int u \rho = \iota_{\mathcal{C}}(B).$$

The function F allows us to provide a characterization of the exposed and extreme points of C. We remark that a similar result but in the continuous setting was established in [9], but considering the linear structure on probability measures, which is different from the type of convexity considered in this work. One of our main tools will be Strassen's theorem, which we recall below:

Lemma 3.4 (Strassen's theorem). Let $\mu, \nu \in \mathcal{P}_1(\mathbb{R}^d)$ then $\mu \leq_C \nu$ if and only if there exists a coupling $\theta \in \Gamma(\mu, \nu)$ such that $d\theta(x, y) = d\theta_x(y)d\mu(x)$ and

(9)
$$\int y d\theta_x(y) = x \quad \text{for } \mu\text{-a.e. } x \in \mathbb{R}^d.$$

Theorem 3.5. The following holds:

(10)
$$\mathcal{C} = \operatorname{conv}(\overline{\mathcal{B}}_{Lag}) = \partial F(0)$$

where ∂F denotes the subgradient of F with respect to the metric $\langle \cdot, \cdot \rangle_v$. Moreover,

- 1. \mathcal{B}_{Lag} coincides with the set of exposed points of C;
- 2. the exposed faces of C have dimension d(N-M) for $M=2,\ldots,N$. For a given M, the exposed faces of dimension d(N-M) are given by $\{\mathcal{B}_{Lag}(Y,\sigma)\}_{Y,\sigma}$ where $Y \in (\mathbb{R}^d)^M \setminus \Delta_M$, $\sigma : \{1,\ldots,M\} \to \{1,\ldots,N\}$ is any surjective map and

$$\mathcal{B}_{\text{Lag}}(Y,\sigma) = \Big\{ B \in (\mathbb{R}^d)^N \; ; \; \sum_{j \in \sigma^{-1}(i)} v_j \delta_{b_j} \preceq_C \rho|_{L_i^*(Y,w)} \, , \; \forall i \Big\},$$

where $(L_i^*(Y, w))_i$ is the unique Laguerre tessellation with generators Y and volumes $w = (w_1, \ldots, w_M)$, where

$$w_i = \sum_{j \in \sigma^{-1}(i)} v_j \,, \quad \forall i \,;$$

3. the relative boundary of C can be characterized as follows:

$$\operatorname{rel} \partial \mathcal{C} = \bigcup_{Y,\sigma} \mathcal{B}_{\operatorname{Lag}}(Y,\sigma)$$

where the sum is over any $Y \in (\mathbb{R}^d)^M \setminus \Delta_M$, M = 2, ..., N and $\sigma : \{1, ..., N\} \rightarrow \{1, ..., M\}$ surjective.

Proof. Since, for any $X \in \mathcal{C}$, $0 \in \partial \iota_{\mathcal{C}}(X) = N(X, \mathcal{C})$, the normal cone to \mathcal{C} at X, then $\mathcal{C} = \partial \iota_{\mathcal{C}}^*(0) = \partial F(0)$. Hence, we also have

$$C = \operatorname{conv}\{X \in (\mathbb{R}^d)^N ; \exists Y^n \to 0 \text{ as } n \to \infty : \nabla F(Y^n) \to X \text{ as } n \to \infty\}.$$

If F is differentiable at Y, then $\nabla F(Y) \in \mathcal{B}_{\text{Lag}}$ by Proposition 3.3, and viceversa if $X \in \mathcal{B}_{\text{Lag}}$ then there exists Y such that $\nabla F(Y) = X$. Moreover, by invariance of Laguerre tessellations with respect to the dilation of the generators, if $\nabla F(Y^n) \to X$ then $\nabla F(\lambda_n Y^n) \to X$ for any $(\lambda_n)_n \in \mathbb{R}^n_{>0}$. In particular, we can pick λ_n so that $\lambda_n Y^n \to 0$, which yields the equality in (10). Alternatively, note that we have

$$F(Y) = \sup \{ \langle B, Y \rangle_v ; B \in \mathcal{B}_{\text{Lag}} \}.$$

which implies that $F^* = \iota_{\mathcal{B}_{\text{Lag}}}^{**}$, and therefore $\mathcal{C} = \text{conv}(\overline{\mathcal{B}}_{\text{Lag}})$.

To prove the first point, observer that, since $F = \iota_{\mathcal{C}}^*$,

$$X \in \mathcal{B}_{\text{Lag}} \iff \exists Y : \{B\} = \partial F(Y)$$

 $\iff \exists Y : B = \arg\max\{\langle B, Y \rangle_v ; B \in \mathcal{C}\},$

which is equivalent to X being an exposed point of \mathcal{C} .

To prove the second point, given $Y \in (\mathbb{R}^d)^M \setminus \Delta_M$, for some $M \in \{2, \dots, N\}$, and $\sigma : \{1, \dots, N\} \to \{1, \dots, M\}$ surjective, define $\tilde{Y} = (\tilde{y}_i)_i \in \mathbb{R}^{dN}$ by $\tilde{y}_i = y_{\sigma(i)}$ for all i. Note that all vectors $\tilde{Y} \in \mathbb{R}^{dN}$ different from the constant vector (defined by $y_i = c$ for all i and $c \neq 0$, and which characherizes the affine hull of \mathcal{C}) can be written in this way. The intersection of \mathcal{C} with the separating hyperplane of outward normal \tilde{Y} is $\partial F(\tilde{Y})$ since we have by Fenchel duality

$$B \in \partial F(\tilde{Y}) \iff F(\tilde{Y}) + \iota_{\mathcal{C}}(B) = \langle B, \tilde{Y} \rangle_{v}.$$

Let γ be any maximizer of problem (8) such that

$$F(\tilde{Y}) = \int \langle x, y \rangle d\gamma(x, y).$$

This can be desintegrated with respect to the projection on the second marginal as follows:

$$d\gamma(x,y) = \sum_{i} v_{i} d\theta_{i}(x) \otimes \delta_{Y_{i}}(y)$$

where $\theta_i \in \mathcal{P}(\mathbb{R}^d)$ and verify $\sum_i v_i \theta_i = \rho$. Now, since $F_v(\tilde{Y}) = F_w(Y)$, we can deduce that γ is a maximizer if and only if we have for all i

$$\sum_{j \in \sigma^{-1}(i)} v_j \theta_j = \rho|_{L_i}$$

and in particular we have

$$F(\tilde{Y}) = \sum_{i} v_i \langle \int x d\theta_i(x), \tilde{Y}_i \rangle.$$

We conclude using Strassen's theorem.

Finally, the third point follows from the fact that the relative boundary of a convex body is the union of all its exposed faces whose supporting hyperplane is different from the affine hull of the convex body itself. \Box

4. Projection onto the set of measures in convex order

By Theorem 3.5, the exposed points $B \in \mathcal{C}$ are barycenters of Laguerre tessellations with prescribed volumes. In this section, we consider the problem of recovering from B the generators Y of a Laguerre tessellation with barycenters given by B.

Let us define the following weighted orthogonal projection

(11)
$$P_{\mathcal{C}}(X) := \operatorname{argmin}\{\|B - X\|_{v}^{2} ; B \in \mathcal{C}\}.$$

Fixing an arbitrary point $X \notin \mathcal{C}$ but belonging to the supporting hyperplane of \mathcal{C} , define $Y := X - P_{\mathcal{C}}(X)$. By Theorem 3.5, if $Y \in (\mathbb{R}^d)^N \setminus \Delta_N$, then $P_{\mathcal{C}}(X)$ is an exposed point and Y is the vector of cell-centers of the Laguerre decomposition with volumes v whose barycenters are precisely $P_{\mathcal{C}}(X)$. If $Y \in \Delta_N$, $P_{\mathcal{C}}(X)$ belongs to an exposed face of \mathcal{C} . In particular, by identifying the points in Y occupying the same location, we can construct a vector $Z \in (\mathbb{R}^d)^M \setminus \Delta_M$ such that $z_{\sigma(i)} = y_i$ for some surjective map $\sigma: \{1, \ldots, N\} \to \{1, \ldots, M\}$ and we have

$$\sum_{i \in \sigma^{-1}(j)} v_i \delta_{b_i} \preceq_C \rho|_{L_j^*(Z,w)}, \quad \text{where} \quad w_j = \sum_{i \in \sigma^{-1}(j)} v_i, \quad \forall j,$$

where we used the same notation as in Theorem 3.5.

If X is an exposed point however, $X \in \mathcal{C}$ and Y = 0, so we do not recover any information from Y on the Laguerre tessellation associated with X. The following proposition says that by perturbing X appropriately we can recover an approximation of such tessellation via the orthogonal projection $P_{\mathcal{C}}$.

Proposition 4.1. Suppose that $B \in \mathcal{B}_{Lag}$, the set of exposed points of C. Then for any $\lambda > 1$ sufficiently small $P_{C}(\lambda B) \in \mathcal{B}_{hLag}$ is also an extreme point of C.

Proof. First of all, note that since B is exposed, there exists a $Y \in (\mathbb{R}^d)^N \setminus \Delta_N$ such that B is the unique maximizer of

$$\max \left\{ \langle Y, \tilde{B} \rangle_v ; \tilde{B} \in \mathcal{C} \right\}.$$

Furthermore, we can pick Y in the supporting hyperplane, i.e. $\langle Y, \mathbf{1} \rangle_v = \sum_i v_i y_i = 0$. Then,

$$\langle B, Y \rangle_v > \sum_i v_i \langle \text{bary}(\rho), y_i \rangle = 0.$$

This means that $\lambda B \notin \mathcal{C}$ and furthermore that $P_{\mathcal{C}}(\lambda B)$ must belong to the relative boundary of \mathcal{C} . Hence, if B does not belong to the boundary of any face of dimension larger than 0, the result is evident.

To treat the general case where B may belong to the boundary of a face, we proceed by induction on the number of points. If N=2, by Theorem 3.5 all boundary points are exposed points so the statement holds true. On the other hand, fixing N>2, suppose that the statement is true for any $2 \leq M < N$. Suppose that $\tilde{B} = P_{\mathcal{C}}(\lambda B)$ belongs to the face $\mathcal{B}_{\text{Lag}}(Y,\sigma)$ for a given $Y \in \mathbb{R}^{dM} \setminus \Delta_M$ with $2 \leq M < N$ and $\sigma: \{1,\ldots,N\} \to \{1,\ldots,M\}$ surjective. By the characterization of the face $\mathcal{B}_{\text{Lag}}(Y,\sigma)$ in Theorem 3.5, for any fixed $1 \leq i \leq M$, the vectors $(\tilde{b}_j)_{j \in \sigma^{-1}(i)}$ can be recovered as the projection of $(\lambda b_j)_{j \in \sigma^{-1}(i)}$ on the set of points $(b_j)_{j \in \sigma^{-1}(i)}$ such that

$$\sum_{j \in \sigma^{-1}(i)} v_j \delta_{b_j} \preceq_C \rho|_{L_i^*(Y, w)} \quad \text{where} \quad w_j = \sum_{i \in \sigma^{-1}(j)} v_i.$$

By hypothesis $(\tilde{b}_j)_{j\in\sigma^{-1}(i)}$ must be the set of barycenters of a hierarchical tessellation of $L_i(Y, w)$ with volumes $\{v_j\}_{j\in\sigma^{-1}(i)}$. Hence we find that $P_{\mathcal{C}}(\lambda B) \in \mathcal{B}_{hLag}$, and it is an extreme point by Lemma 3.2.

In practice, instead of computing $P_{\mathcal{C}}(\lambda B)$ we will solve the dual problem given in the following lemma:

Lemma 4.2. let $X \in (\mathbb{R}^d)^N$. The following holds:

$$\inf_{B} \left\{ \frac{\|B - X\|_{v}^{2}}{2} + \iota_{\mathcal{C}}(B) \right\} = -\inf_{Y} \left\{ \frac{\|Y\|_{v}^{2}}{2} - \langle Y, X \rangle_{v} + F_{v}(Y) \right\}.$$

Moreover the problems on the left and right-hand side admit a unique solution, denoted $P_{\mathcal{C}}(X)$ and Y^* respectively, which verify

$$Y^* = X - P_{\mathcal{C}}(X) .$$

Proof. By Proposition 3.3, the convex indicator function $\iota_{\mathcal{C}} = F_v^*$. Then the result is just an application of standard convex duality.

We conclude the section by proving the equivalence between problem (11) and a 2-Wasserstein projection problem (7). In order to state this, let us first recall the definition of the 2-Wasserstein distance W_2 :

(12)
$$W_2^2(\mu,\nu) := \inf_{\gamma \in \Gamma(\mu,\nu)} \left\{ \int |x-y|^2 d\gamma(x,y) \right\}$$

for any $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ are any probability measures with finite second moments, and where $\Gamma(\mu, \nu) \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ is set of probability measures with first and second marginals equal to μ and ν , respectively.

Proposition 4.3. The measure $\nu(P_{\mathcal{C}}(X), v)$ is the unique solution to the projection problem:

$$\inf\{W_2^2(\nu,\nu(X,v)); \nu \leq_C \rho\}.$$

Proof. Existence and uniqueness of the minimizer ν^* has been proven in [11]. In the same work, the authors showed that the optimal transport map from $\nu(X, v)$ and ν^* is Lipschitz continuous. This implies that $\nu^* = \nu(Y^*, v)$ for some vector $Y^* \in (\mathbb{R}^d)^N$. Using the fact that $W_2(\nu(Y, v), \nu(X, V)) \leq ||Y - X||_v$, we obtain

$$||Y^* - X||_v^2 = \inf\{W_2^2(\nu, \nu(X, v)); \nu \preceq_C \rho\} \le \inf\{||Y - X||_v^2; \nu(Y, v) \preceq_C \rho\}.$$
 which implies that $Y^* = P_{\mathcal{C}}(X)$.

Note that this correspondence can be applied directly to the setting considered in Proposition 4.1, where we project onto \mathcal{C} a dilated version of a given vector $B \in (\mathbb{R}^d)^N$. However, in this case, we have a further equivalence with the so-called metric extrapolation problem, which was introduced in [10], as described in the Remark below:

Remark 4.4 (Relation with the metric Wasserstein extrapolation). Let us consider the problem of projecting λX onto \mathcal{C} with $\lambda > 1$, as in Proposition 4.1, but with $X \in (\mathbb{R}^d)^N$ arbitrary. By the change of variable $Y = (\lambda - 1)Z$ the dual problem in Lemma 4.2 becomes up to constant terms

(13)
$$\inf_{Z} \left\{ \lambda(\lambda - 1) \frac{\|Z - X\|_{v}^{2}}{2} - (\lambda - 1) \frac{W_{2}^{2}(\nu(Z, v), \rho)}{2} \right\}$$

Setting $t = \lambda/(\lambda - 1)$ this is larger than

(14)
$$\lambda \inf_{\mu} \left\{ \frac{W_2^2(\mu, \nu(X, v))^2}{2(t-1)} - \frac{W_2^2(\mu, \rho)}{2t} \right\}.$$

In fact, $||Z - X||_v \ge W_2(\nu(Z, v), \nu(X, v))$, and we get problem (14) by replacing the minimization over Z with a minimization over any probability measure μ with finite second moments. This is precisely the metric extrapolation problem, which was introduced in [10] to extend up to time t > 1 the W_2 -geodesic connecting ρ at time 0 to $\nu(X, v)$ at time 1. It was proven in [10] that the solution to this problem is unique and in the form $\mu^* = T_{\#}\nu(X, v)$ where T is a Lipschitz map. This implies that problem (14) actually coincides with (13) and $\mu^* = \nu(Z^*, v)$ with Z^* solving (13).

5. Subgradient descent and numerical tests

Let us go back to the dual problem in Lemma 4.2, i.e.

(15)
$$\inf_{Y} G_v(Y), \quad \text{where} \quad G_v(Y) := \frac{\|Y\|_v^2}{2} - \langle Y, X \rangle_v + F_v(Y).$$

Given any $Y \in (\mathbb{R}^d)^N$ let $M \in \{1, ..., N\}$ and $\tilde{Y} \in (\mathbb{R}^d)^M / \Delta_M$ be such that $y_i = \tilde{y}_{\sigma}(i)$ for all i, for some surjective map $\sigma : \{1, ..., N\} \to \{1, ..., M\}$. Define $w = (w_1, ..., w_M)$ by

$$w_j = \sum_{i \in \sigma^{-1}(j)} v_i.$$

Then, as a consequence of Theorem 3.5 and Fenchel duality:

$$B(Y) := (\text{bary}_o(L^*_{\sigma(i)}(\tilde{Y}, w)))_i \in \partial F(Y),$$

where ∂F^* denotes the subgradient of F^* with respect to the metric $\langle \cdot, \cdot \rangle_v$.

Lemma 5.1. Suppose $\rho \in \mathcal{P}_2(\mathbb{R}^d)$, i.e.

$$m_2^2(\rho) := \int |x|^2 \mathrm{d}\rho(x) < +\infty.$$

Then, F is $m_2(\rho)$ -Lipschitz. Moreover denoting by Y^* the unique solution to (15), $||Y^*-X||_v \leq m_2(\rho)$ and $G_v(Y)$ is $2m_2(\rho)$ -Lipschitz on the set $\{Y : ||Y-X||_v \leq m_2(\rho)\}$.

Proof. For any $Y, Z \in (\mathbb{R}^d)^N$

$$F(Z) - F(Y) \le \langle B(Z), Z - Y \rangle_v$$

$$\le ||B(Z)||_v ||Z - Y||_v$$

$$\le m_2(\rho) ||Z - Y||_v,$$

where the last inequality is due to Jensen's inequality. Exchanging Y and Z we obtain that F is $m_2(\rho)$ -Lipschitz. Moreover, by Lemma 4.2

$$||Y^* - X||_v = ||P_{\mathcal{C}}(X)||_v \le m_2(\rho),$$

where the last inequality follows from the definition of convex order and choosing as test function $\varphi: x \to |x|^2$. We conclude by observing that

$$\partial G(Y) = Y - X + \partial F(Y)$$

and using the triangular inequality.

Given the considerations above, we can formulate a projected subgradient descent method with varying stepsize η_t (see, e.g., Section 3.4.1 in [8]) as follows: given $Y_1 \in (\mathbb{R}^d)^N$, for all k > 1,

(16)
$$Z_k = Y_k - \eta_t(Y_k - X + B(Y_k)),$$

$$Y_{k+1} = X + \max\left(\frac{\|Z_k - X\|_v}{m_2(\rho)}, 1\right)^{-1} (Z_k - X).$$

As a consequence of Lemma 5.1, the strong convexity of G, and Theorem 3.9 in [8] we have that the subgradient method defined by (16) converges with sublinear rate with an appropriate choice of step-size. More precisely:

Corollary 5.2. Choosing $\eta_k = 2/(k+1)$,

$$G(Y_k) - G(Y^*) \le \frac{4m_2^2(\rho)}{k+1}$$
.

Remark 5.3. In [5] a different approach was proposed in order to reconstruct the generators Y from given cell barycenters B. The proposed algorithm consists in solving the following concave maximization problem

$$\sup_{Y} \{ \langle B, Y \rangle_v - F_v(Y) \}.$$

In view of our results, this corresponds to computing the Legendre transform of F_v , which is just the convex indicator function of $C(\rho, v)$. In general, however, this requires enforcing the constraint that $Y \notin \Delta_N$, i.e. that generators are distinct points, to retrieve a solution, in particular when $B \notin \mathcal{B}_{Lag}(\rho, v)$. Our approach bypasses this issue and allows generators to collide, both during the iterations and at convergence. However, exploiting Proposition 4.1, simply replacing B with λB , where $\lambda > 1$ is a regularization parameter, we can ensure that at least when $B \in \mathcal{B}_{Lag}$ we can find a hierarchical Laguerre tessellation whose barycenters are $P_C(\lambda B)$. When this exists, it can always be computed explicitly using algorithm (16), possibly iteratively whenever particles collide (as in the proof of Proposition 4.1).

5.1. Numerical tests. We now present some numerical results that illustrate the behavior of our method for reconstruction and fitting problems. More precisely, given a set of volumes v and barycenters B, we reconstruct the generators of the associated tessellation by setting

$$Y = \lambda B - P_{\mathcal{C}}(\lambda B)$$
,

where $\lambda = t/(t-1)$ with t > 1 is a regularization parameter. In practice, Y is computed via algorithm (16), where for numerical stability, we identify two given particles y_i and y_j if $|y_i - y_j| < \delta$, where $\delta > 0$ is a given tolerance ($\delta = 10^{-6}$ for all the tests below).

We stress that the regularization parameter $\lambda > 1$ is necessary here since if $B \in \mathcal{B}_{\text{Lag}}$ and we just set $\lambda = 1$, the dual problem (15) would yield the trivial solution Y = 0. In contrast, by Proposition 4.1, if λ is sufficiently close to 1 (or equivalently, t is sufficiently large), $P_{\mathcal{C}}(\lambda B) \in \mathcal{B}_{\text{hLag}}$, and up to identifying particles occupying the same position, the dual problem yields the generators Y for a Laguerre tessellation containing the hierarchical tessellation whose barycenters are given by $P_{\mathcal{C}}(\lambda B)$. In principle, one can iterate the procedure (just as in the proof of Proposition 4.1) to compute such hierarchical tessellation, but we find numerically that this is generally not necessary since the numerical solution verifies $Y \notin \Delta_N$ (up to the specified tolerance δ) and this generates a classical Laguerre tessellation.

5.1.1. Reconstruction of Laguerre tessellations. We consider the problem of reconstructing a Laguerre tessellation given its cell volumes and barycenters. For all tests in this section, we use as reference measure $\rho = \mathbf{1}_{[0,1]^2} \mathrm{d}x$.

Figure 3 shows the result obtained using algorithm 16 with t = 1250 and N = 20. The convergence of the scheme is illustrated in Figure 4, both in terms of number of iterations and increasing the regularization parameter t. One can observe that the scheme appears to converge faster than what predicted from Corollary 5.2.

The results corresponding to a larger test (N = 924) are shown in Figures 5, 6, and 7. Note that while the reconstructed barycenters match the data (as in the previous test), the reconstructed generators are very different (see Figure 6) and the shape of specific Laguerre cells may differ considerably with respect to the true ones (see Figure 5).

5.1.2. Fitting a Laguerre tessellation to data. As in [5], we apply our method to fit a Laguerre tessellation to an electron backscatter diffraction (EBSD) image of a single-phase steel (provided by Tata Steel Research & Development), shown in Figure 8. The pixels are colored according to their crystallographic orientation, and the regions where this is constant are called grains. The image we consider has N=243 grains.

We used the areas v and the barycenters B of the grains as data in our method to generate a vector of generators Y. Note that since by construction $B \in \mathcal{C}$, we do need to include a regularization also in this case. For the tests presented here we set t = 10. We used as reference measure $\rho = \mathbf{1}_{\Omega} dx$ where $\Omega = [0, 252.25]^2$ is the image domain (measured in microns). The results are shown in Figures 8 and 9. Note that as in the previous examples, the convergence is faster than expected from Corollary 5.2, at least up to $k \approx 100$.

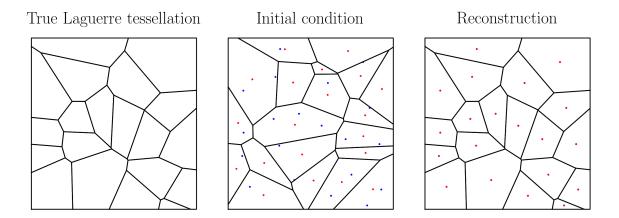


FIGURE 3. Reconstruction of a Laguerre tessellation, for t=1250. The barycenters of the true solutions are in blue and those of the reconstruction are in red.

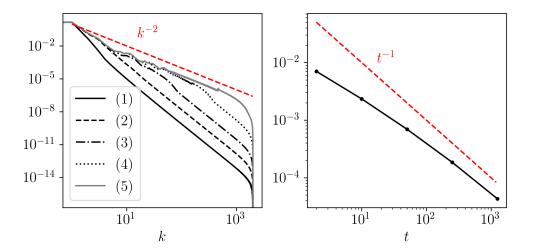


FIGURE 4. On the left: $G(Y^k) - G(Y^K)$, for $1 \le k \le K$, for different values of t (the curve (i) corresponds to $t = 2 \cdot 5^{i-1}$), and the data in Figure 3. On the right: $||B^K - B||_v$, error on barycenter reconstruction at the last iteration K, for different t.

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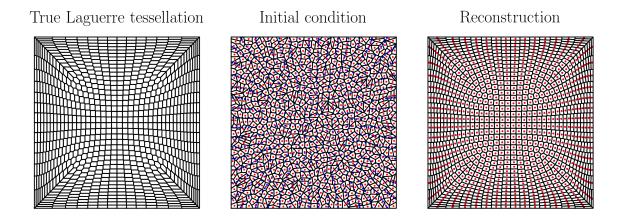


FIGURE 5. Reconstruction of a Laguerre tessellation, for t=100. The barycenters of the true solutions are in blue and those of the reconstruction are in red.

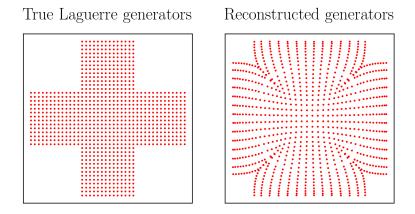


FIGURE 6. Generators of true Laguerre tessellation in Figure 5 (left) and generators for reconstruction for t = 100 (right).

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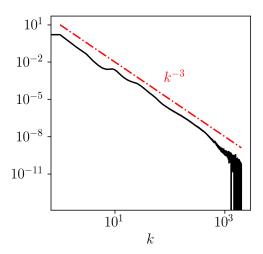


FIGURE 7. Convergence of the scheme for the data represented in Figure 5 and t = 100, shown in terms of $G(Y^k) - G(Y^K)$, for $1 \le k \le K$.

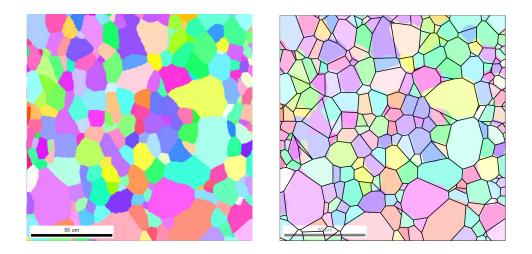


FIGURE 8. EBSD image (left) and fitted Laguerre tessellation from centroids and barycenters (right) computed with t = 10.

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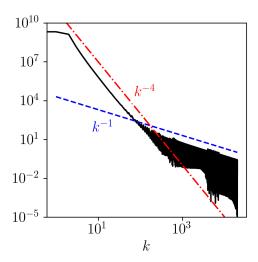


FIGURE 9. Convergence of the scheme for the data extracted from the EBSD image in Figure 8 and t = 10, shown in terms of $G(Y^k) - G(Y^K)$, for $1 \le k \le K$.

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