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Optimal quantization of the mean measure and applications to statistical learning

Frédéric Chazal, Clément Levrard, and Martin Royer

Abstract: This paper addresses the case where data come as point sets, or more generally as discrete measures. Our motivation is twofold: first we intend to approximate with a compactly supported measure the mean of the measure generating process, that coincides with the intensity measure in the point process framework, or with the expected persistence diagram in the framework of persistence-based topological data analysis. To this aim we provide two algorithms that we prove almost minimax optimal.

Second we build from the estimator of the mean measure a vectorization map, that sends every measure into a finite-dimensional Euclidean space, and investigate its properties through a clustering-oriented lens. In a nutshell, we show that in a mixture of measure generating process, our technique yields a representation in \mathbb{R}^k , for $k \in \mathbb{N}^*$ that guarantees a good clustering of the data points with high probability. Interestingly, our results apply in the framework of persistence-based shape classification via the ATOL procedure described in [36]. At last, we assess the effectiveness of our approach on simulated and real datasets, encompassing text classification and large-scale graph classification.

1. Introduction

This paper handles the case where we observe n i.i.d measures X_1, \dots, X_n , rather than n i.i.d sample points, the latter case being the standard input of many machine learning algorithms. Such kind of observations naturally arise in many situations, for instance when data are spatial point patterns: in species distribution modeling [35], repartition of clusters of diseases [16], modelisation of crime repartition [38] to name a few. The framework of i.i.d sample measures also encompasses analysis of multi-channel time series, for instance in embankment dam anomaly detection from piezometers [22], as well as topological data analysis via persistence diagrams [18, 8]. The objective of the paper is twofold: first we want to build from data a compact representation of the mean of the measure, in the arithmetic sense. Second, based on the first construction, we intend to provide an embedding of the sample measures that allows for a provably efficient clustering or classification.

Applications for the first objective might be found whenever the sample measures are organized around a central measure of interest, for instance in image analysis [14] or point processes modeling [35, 16, 38]. In [14], the central measure is defined as the Wasserstein barycenter of the distribution of measures. Namely, if we assume that X_1, \dots, X_n are i.i.d measures on \mathbb{R}^d drawn from X , where X is a probability distribution on the space of measures, then the

central measure is defined as $\mu_W = \arg \min_{\nu} \mathbb{E} (W_2(X, \nu))^2$, where ν ranges in the space of measures and W_2 denotes the Wasserstein distance. Note that this definition only makes sense in the case where $X(\mathbb{R}^d)$ is constant a.s., that is when we draw measures with the same total mass. Moreover, computing the Wasserstein barycenter of X_1, \dots, X_n in practice is too costly for large n 's, even with approximating algorithms [14, 33]. To overcome these difficulties, we choose to define the central measure as the arithmetic mean of X , denoted by $\mathbb{E}(X)$, that assigns the weight $\mathbb{E}[X(A)]$ to a borelian set A . In the point process theory, the mean measure is often referred to as the intensity function of the process.

An easily computable estimator of this mean measure is the sample mean measure $\bar{X}_n = (\sum_{i=1}^n X_i) / n$. We intend to build a k -points approximation of $\mathbb{E}(X)$, that is a distribution $P_{\mathbf{c}}$ supported by $\mathbf{c} = (c_1, \dots, c_k)$ that approximates well $\mathbb{E}(X)$, based on X_1, \dots, X_n . To this aim, we introduce two algorithms (batch and mini-batch) that extend classical quantization techniques intended to solve the k -means problem [28]. In fact, these algorithms are build to solve the k -means problem for \bar{X}_n . We prove in Section 2.2 that these algorithms provide minimax optimal estimators of a best possible k -points approximation of $\mathbb{E}(X)$, provided that $\mathbb{E}(X)$ satisfies some structural assumption. Interestingly, our results also proves optimality of the classical quantization techniques [28, 26] in the point sample case.

The second objective, clustering or classification of measures, has a wide range of possible applications: in the case where data come as a collection of finite point sets for instance, including ecology [35], genetics [36, 2], graphs clustering [7, 21] and shapes clustering [8]. Our technique is based on a vectorization of the measures, that is a map v that sends every measure X_i into \mathbb{R}^k . We build this vectorization using the optimal k -points $\mathbf{c} = (c_1, \dots, c_k)$ obtained in the first part (Section 2.2), transforming each X_i into a vector $v_i \in \mathbb{R}^k$ that roughly encodes how much weight X_i spreads around every c_j . Note that a vectorization based on a fixed grid of \mathbb{R}^d is possible, however the dimension of such a vectorization is constrained and can grow quite large. In the particular framework of topological data analysis and persistence diagrams clustering, vectorization via evaluation onto a fixed grid is the technique exposed in [3], whereas our method has clear connections with the procedures described in [46, 36].

For this vectorization scheme, we provide general conditions on the structure of the sample measures that allow an almost exact clustering based on the vectorization space. It is worth mentioning that our theoretical results include vectorization via evaluations of kernel functions around each point c_j , for a general class of kernel functions that encompasses the one used in [36]. Further, we also prove in Section 4 that theses structural conditions are fulfilled in a framework of shape classification via persistence diagrams. As a consequence, we theoretically asses the performance of the procedure exposed in [36]. Up to our knowledge, this provides the only theoretical guarantee on a measure-based clustering algorithm.

At last, we perform numerical experiments in Section 5 to assess the effectiveness of our approach on real and synthetic data, in a classification framework. In a nutshell, our vectorization scheme combined with standard algorithms provides

state-of-the-art performances on various classification and clustering problems, with a lighter computational cost. The classification problems encompass sentiment analysis of IMDB reviews [27] as well as large-scale graph classification [37, 43]. Surprisingly, our somehow coarse approach turns out to outperform more involved methods in several large-scale graph classification problems.

The paper is organized as follows: in Section 2, we introduce notation along with the exposition of the problem of mean measure quantization. Then, two theoretically grounded algorithms are described to solve this problem from the sample X_1, \dots, X_n . Section 3 exposes our general vectorization technique, and conditions that guarantee a correct clustering based on it. Section 4 investigates the special case where the measures are persistence diagrams built from samplings of different shapes, showing that all the previously exposed theoretical results apply in this framework. The numerical experiments are exposed in Section 5. Sections 6, 7 and 8 gather the main proofs of the results. Proofs of intermediate and technical results are deferred to Section 9.

2. Quantization of the mean measure

2.1. Definition and notation

Throughout the paper we will consider finite measures on the d -dimensional ball $\mathcal{B}(0, R)$ of the Euclidean space \mathbb{R}^d . Let $\mathcal{M}(R, M)$ denote the set of such measures of total mass smaller than M . For an element $\mu \in \mathcal{M}(R, M)$ we denote by $M(\mu)$ its total mass. Further, if $\mu \in \mathcal{M}(R, M)$ and f is a borelian function from \mathbb{R}^d to \mathbb{R} , we denote by $\mu(du) \bullet f(u)$ integration of f with respect to μ , whenever $\mu(du) \bullet |f|(u)$ is finite. We let X denote a random variable taking values in $\mathcal{M}(R, M)$, and X_1, \dots, X_n denote an i.i.d. sample with the same distribution as X . Definition 1 below introduces the mean measure.

Definition 1. Let $\mathcal{B}(\mathbb{R}^d)$ denote the borelian sets of \mathbb{R}^d . The mean measure $\mathbb{E}(X)$ is defined as the measure such that

$$\forall A \in \mathcal{B}(\mathbb{R}^d) \quad \mathbb{E}(X)(A) = \mathbb{E}(X(A)).$$

The empirical mean measure \bar{X}_n may be defined via $\bar{X}_n(A) = \frac{1}{n} \sum_{i=1}^n X_i(A)$.

In the case where the measures of interest are persistence diagrams, the mean measure defined above is the expected persistence diagram, defined in [11]. If the sample measures are point processes, $\mathbb{E}(X)$ is the intensity function of the process. It is straightforward that, if $\mathbb{P}(X \in \mathcal{M}(R, M)) = 1$, then both $\mathbb{E}(X)$ and \bar{X}_n are (almost surely) elements of $\mathcal{M}(R, M)$. The goal of this paper is to build a k -points approximation of $\mathbb{E}(X)$ based on X_1, \dots, X_n .

If $\mu_1, \mu_2 \in \mathcal{M}(R, M)$ satisfy $M(\mu_1) = M(\mu_2)$, and $p \in \llbracket 1, +\infty \rrbracket$, we may define $W_p(\mu_1, \mu_2)$ as the p -Wasserstein distance between μ_1 and μ_2 . Let $\mathcal{M}_k(R, M)$ denote the subset of $\mathcal{M}(R, M)$ that consists of distributions supported by k points. Adopting the quantization terminology, each support point of a finite k -points distribution is called a codepoint. A vector made of k codepoints c_1, \dots, c_k

is called a codebook. For a codebook $\mathbf{c} = (c_1, \dots, c_k) \in \mathcal{B}(0, R)^k$, we let

$$\begin{aligned} W_j(\mathbf{c}) &= \{x \in \mathbb{R}^d \mid \forall i < j \quad \|x - c_j\| < \|x - c_i\| \quad \text{and} \quad \forall i > j \quad \|x - c_j\| \leq \|x - c_i\|\}, \\ N(\mathbf{c}) &= \{x \mid \exists i < j \quad x \in W_i(\mathbf{c}) \quad \text{and} \quad \|x - c_j\| = \|x - c_i\|\}, \end{aligned}$$

so that $(W_1(\mathbf{c}), \dots, W_k(\mathbf{c}))$ forms a partition of \mathbb{R}^d and $N(\mathbf{c})$ represents the skeleton of the Voronoi diagram associated with \mathbf{c} . Given a codebook \mathbf{c} , a standard way to approximate $\mathbb{E}(X)$ with a probability distribution supported by \mathbf{c} is to consider $P_{\mathbf{c}} = \sum_{j=1}^k \mathbb{E}(X)(W_j(\mathbf{c}))\delta_{c_j}$. It is then easy to see that, for any other distribution $P'_k = \sum_{j=1}^k \mu_j \delta_{c_j}$ such that $\sum_{j=1}^k \mu_j = M(\mathbb{E}(X))$, supported by \mathbf{c} ,

$$W_2^2(\mathbb{E}(X), P'_k) \geq W_2^2(\mathbb{E}(X), P_{\mathbf{c}}) = \mathbb{E}(X)(du) \bullet \min_{j=1, \dots, k} \|u - c_j\|^2 = R(\mathbf{c}).$$

Thus, finding the best k -points approximation of $\mathbb{E}(X)$ in terms of W_2 boils down to minimize $R(\mathbf{c})$. Note that $R(\mathbf{c})$ is often referred to as the distortion of \mathbf{c} , in the quantization framework. According to [19, Corollary 3.1], since $\mathbb{E}(X) \in \mathcal{M}(R, M)$, there exist minimizers \mathbf{c}^* of $R(\mathbf{c})$, and we let \mathcal{C}_{opt} denote the set of such minimizers. In what follows, R^* will denote the optimal distortion achievable with k points, that is $R^* = R(\mathbf{c}^*)$, where $\mathbf{c}^* \in \mathcal{C}_{opt}$. Basic properties of \mathcal{C}_{opt} are recalled below.

Proposition 2. [25, Proposition 1] *Recall that $\mathbb{E}(X) \in \mathcal{M}(R, M)$, then*

1. $B = \inf_{\mathbf{c}^* \in \mathcal{C}_{opt}, j \neq i} \|c_i^* - c_j^*\| > 0$,
2. $p_{min} = \inf_{\mathbf{c}^* \in \mathcal{C}_{opt}, j=1, \dots, k} \mathbb{E}(X)(W_j(\mathbf{c}^*)) > 0$.

In what follows, we will further assume that $\mathbb{E}(X)$ satisfies a so-called *margin condition*, defined in [23, Definition 2.1] and recalled below. For any subset A of an Euclidean space, and $r > 0$, we denote by $\mathcal{B}(A, r)$ the set $\cup_{u \in A} \mathcal{B}(u, r)$.

Definition 3. $\mathbb{E}(X) \in \mathcal{M}(R, M)$ *satisfies a margin condition with radius $r_0 > 0$ if and only if, for all $0 \leq t \leq r_0$,*

$$\sup_{\mathbf{c}^* \in \mathcal{C}_{opt}} \mathbb{E}(X)(\mathcal{B}(N(\mathbf{c}^*), t)) \leq \frac{B p_{min}}{128 R^2} t.$$

In a nutshell, a margin condition ensures that the mean distribution $\mathbb{E}(X)$ is well-concentrated around k poles. Following [25], a margin condition will ensure that usual k -means type algorithms are almost optimal in terms of distortion. These algorithms are recalled below and adapted to the mean-measure quantization framework.

2.2. Batch and mini-batch algorithms

Let X_1, \dots, X_n be i.i.d random measures in $\mathcal{M}(R, M)$. This section exposes two algorithms that are intended to approximate a best k -points empirical codebook,

that is a codebook $\hat{\mathbf{c}}_n$ which minimizes $W_2(\bar{X}_n, \hat{P}_{\mathbf{c}})$, for $\mathbf{c} \in \mathcal{B}(0, R)^k$, $\hat{P}_{\mathbf{c}}$ being defined by $\sum_{j=1}^k \bar{X}_n(W_j(\mathbf{c}))\delta_{c_j}$. These algorithms are extensions of two well-known clustering algorithms, namely the Lloyd algorithm ([26]) and Mac Queen algorithm ([28]). We first introduce the counterpart of Lloyd algorithm.

Algorithm 1: Batch algorithm (Lloyd)

<p>Input : X_1, \dots, X_n and k ;</p> <p># Initialization</p> <p>Sample $c_1^{(0)}, c_2^{(0)}, \dots, c_k^{(0)}$ from \bar{X}_n ;</p> <p>while $\mathbf{c}^{(t+1)} \neq \mathbf{c}^{(t)}$ do :</p> <p style="padding-left: 20px;"># Centroid update.</p> <p style="padding-left: 40px;">for j in $1..k$:</p> <p style="padding-left: 80px;">$c_j^{(t+1)} = \frac{1}{\bar{X}_n(W_j(\mathbf{c}^{(t)}))} \bar{X}_n(du) \bullet \left[u \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u) \right]$;</p> <p>Output : $\mathbf{c}^{(T)}$ (codebook of the last iteration) .</p>
--

Note that Algorithm 1 is a batch algorithm, in the sense that every iteration need to process the whole data set X_1, \dots, X_n . Fortunately, Theorem 4 below ensures that a limited number of iterations are required for Algorithm 1 to provide an almost optimal solution. In the sample point case, that is when we observe n i.i.d points $X_i^{(1)}$, Algorithm 1 is the usual Lloyd's algorithm. In this case, the mean measure $\mathbb{E}(X)$ is the distribution of $X_1^{(1)}$, that is the usual sampling distribution of the n i.i.d points. As well, the counterpart of Mac-Queen algorithm [28] for standard k -means clustering is the following mini-batch algorithm. We let $\pi_{\mathcal{B}(0,R)^k}$ denote the projection onto $\mathcal{B}(0, R)^k$.

Algorithm 2: Mini-batch algorithm (Mac-Queen)

<p>Input : X_1, \dots, X_n, divided into mini-batches (B_1, \dots, B_T) of sizes (n_1, \dots, n_T), and k. For $j = 1, \dots, T$, B_j is divided in two halves, $B_j^{(1)}$ and $B_j^{(2)}$. Maximal radius R ;</p> <p># Initialization</p> <p>Sample $c_1^{(0)}, c_2^{(0)}, \dots, c_k^{(0)}$ from \bar{X}_n ;</p> <p>for $j = 0, \dots, T - 1$ do :</p> <p style="padding-left: 20px;"># Centroid update.</p> <p style="padding-left: 40px;">for j in $1..k$:</p> <p style="padding-left: 80px;">$c_j^{(t+1)} = \pi_{\mathcal{B}(0,R)^k} \left(c_j^{(t)} - \frac{\bar{X}_{B_{t+1}^{(2)}}(du) \bullet \left[(c_j^{(t)} - u) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u) \right]}{(t+1) \bar{X}_{B_{t+1}^{(1)}}(W_j(\mathbf{c}^{(t)}))} \right)$;</p> <p>Output : $\mathbf{c}^{(T)}$ (codebook of the last iteration) .</p>

Note that the mini-batches split in two halves is motivated by technical considerations only that are exposed in Section 6.2. Whenever $n_i = 1$ for $i = 1, \dots, n$ (and $B_i^{(1)} = B_i^{(2)} = \{X_i\}$), Algorithm 2 is a slight modification of

the original Mac-Queen algorithm [28]. Indeed, the Mac-Queen algorithm takes mini-batches of size 1, and estimates the population of the cell j at the t -th iteration via $\sum_{\ell=1}^t \hat{p}_j^{(\ell)}$ instead of $t\hat{p}_j^{(t)}$, where $\hat{p}_j^{(t)} = \bar{X}_{B_t^{(1)}}(W_j(\mathbf{c}^{(t)}))$. These modifications are motivated by Theorem 5, that guarantees near-optimality of the output of Algorithm 2, provided that the mini-batches are large enough.

2.3. Theoretical guarantees

This section exposes theoretical guarantees for the two algorithms introduced in Section 2.2. Note that these guarantees are stated on the excess distortion $R(\mathbf{c}_T) - R^*$, where \mathbf{c}_T is the output of the considered algorithm. In fact, the same bounds hold also for $\|\mathbf{c}_T - \mathbf{c}^*\|^2$, up to the $M(\mathbb{E}(X))$ factor. A special interest will be paid to the sample-size dependency of the excess distortion. From this standpoint, a first negative result may be derived from the quantization framework. Indeed, from [25, Proposition 7], we may deduce that, for any empirically designed codebook $\hat{\mathbf{c}}$,

$$\inf_{\{X|\mathbb{E}(X) \text{ has a } r_0\text{-margin}\}} \mathbb{E}(R(\hat{\mathbf{c}}) - R^*) \geq c_0 M(\mathbb{E}(X)) R^2 \frac{k^{1-\frac{2}{d}}}{n}. \quad (1)$$

In fact, this bound holds in the special case where X satisfies the additional assumption $X = \delta_{X^{(1)}}$ a.s., pertaining to the vector quantization case. Thus it holds in the general case. This small result ensures that the sample-size dependency of the minimax excess distortion over the class of distribution of measures whose mean measure satisfies a margin condition with radius r_0 is of order $1/n$ or greater.

A first upper bound on this minimax excess distortion may be derived from the following Theorem 4, that investigates the performance of the output of Algorithm 1.

Theorem 4. *Let $X \in \mathcal{M}_{N_{max}}(R, M)$, for some $N_{max} \in \mathbb{N}^*$. Assume that $\mathbb{E}(X)$ satisfies a margin condition with radius r_0 , and denote by $R_0 = \frac{Br_0}{16\sqrt{2}R}$, $\kappa_0 = \frac{R_0}{R}$. Choose $T = \lceil \frac{\log(n)}{\log(4/3)} \rceil$, and let $\mathbf{c}^{(T)}$ denote the output of Algorithm 1. If $\mathbf{c}^{(0)} \in \mathcal{B}(\mathcal{C}_{opt}, R_0)$, then, for n large enough, with probability $1 - 9e^{-c_1 np_{min}^2 \kappa_0^2 / M^2} - e^{-x}$, where c_1 is a constant, we have*

$$R(\mathbf{c}^{(T)}) - R^* \leq M(\mathbb{E}(X)) \left(\frac{B^2 r_0^2}{512 R^2 n} + C \frac{M^2 R^2 k^2 d \log(k)}{np_{min}^2} (1 + x) \right),$$

for all $x > 0$, where C is a constant.

A proof of Theorem 4 is given in Section 6.1. Combined with (1), Theorem 4 ensures that Algorithm 1 reaches the minimax precision rate in terms of excess distortion after $O(\log(n))$ iterations, provided that the initialization is good enough. Note that Theorem 4 is valid for discrete measures that are supported by a uniformly bounded number of points N_{max} . This assumption is relaxed for Algorithm 2 in Theorem 5.

In the standard quantization case, Theorem 4 might be compared with [23, Theorem 3.1] for instance. In this case, the dependency on the dimension d provided by Theorem 4 is sub-optimal. Slightly anticipating, dimension-free bounds in the mean-measure quantization case exist, for instance by considering the output of Algorithm 2.

In practice, Theorem 4 guarantees that choosing $T = 2 \log(n)$ and repeating several Lloyd algorithms starting from different initializations provides an optimal quantization scheme. Note that combining [25, Theorem 3] or [39] and a deviation inequality for distortions such as in [23] gives an alternative proof of the optimality of Lloyd type schemes, in the sample points case where $X_i = \delta_{X_i^{(1)}}$. Theorem 4 provides in addition an upper bound on the number of iterations needed, as well as an extension of these results to the quantization of mean measure case. Its proof, that may be found in Section 6.1, relies on stochastic gradient techniques in the convex and non-smooth case. Bounds for the single-pass Algorithm 2 might be stated the same way.

Theorem 5. *Let $X \in \mathcal{M}(R, M)$. Assume that $\mathbb{E}(X)$ satisfies a margin condition with radius r_0 , and denote by $R_0 = \frac{Br_0}{16\sqrt{2}R}$, $\kappa_0 = R_0/R$. If (B_1, \dots, B_T) are equally sized mini-batches of length $ckM^2 \log(n)/(\kappa_0 p_{\min})^2$, where c is a positive constant, and $\mathbf{c}^{(T)}$ denotes the output of Algorithm 2, then, provided that $\mathbf{c}^{(0)} \in \mathcal{B}(\mathcal{C}_{\text{opt}}, R_0)$, we have*

$$\mathbb{E} \left(R(\mathbf{c}^{(T)}) - R^* \right) \leq M(\mathbb{E}(X)) \left(Ck^2 M^3 R^2 \frac{\log(n)}{n\kappa_0^2 p_{\min}^3} \right).$$

In the sample point case, the same result holds with the centroid update

$$c_j^{(t+1)} = c_j^{(t)} - \frac{\bar{X}_{B_{t+1}}(du) \bullet \left[(c_j^{(t)} - u) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u) \right]}{(t+1) \bar{X}_{B_{t+1}}(W_j(\mathbf{c}^{(t)}))},$$

that is without splitting the batches.

A proof of Theorem 5 is given in Section 6.2. Note that Theorem 5 does not require the values of X to be finitely supported measures, contrary to Theorem 4. Theorem 5 entails that the resulting codebook of Algorithm 2 has an optimal distortion, up to a $\log(n)$ factor and provided that a good enough initialization is chosen. As for Algorithm 1, in practice, several initializations may be tried and the codebook with the best empirical distortion is chosen. Note that Theorem 5 provides a bound on the expectation of the distortion. Crude deviation bounds can be obtained using for instance a bounded difference inequality (see, e.g., [6, Theorem 6.2]). In the point sample case, more refined bounds can be obtained, using for instance [23, Theorem 4.1, Proposition 4.1]. To investigate whether these kind of bounds still hold in the measure sample case is beyond the scope of the paper. Note also that the bound on the excess distortion provided by Theorem 5 does not depend on the dimension d . This is also the case in [23, Theorem 3.1], where a dimension-free theoretical bound on the excess distortion of an empirical risk minimizer is stated in the sample points case. Interestingly,

this bound also has the correct dependency in n , namely $1/n$. According to Theorem 4 and 5, providing a quantization scheme that provably achieves a dimension-free excess distortion of order $1/n$ in the sample measure case remains an open question.

3. Clustering of measures based on the quantized mean measure

3.1. Vectorization of measures

This section introduces a vectorization method for measures, based on the quantization of the mean measure, that preserves separation between clusters if any. The intuition is the following: for a codebook $\mathbf{c} = (c_1, \dots, c_k)$ and a scale r , we may represent a discrete measure X via the vector of weights $(X(\mathcal{B}(c_1, r)), \dots, X(\mathcal{B}(c_k, r)))$ that encodes the mass that X spreads around every pole c_j . Now, if $X^{(1)}$ and $X^{(2)}$ are measures such that $|X^{(1)}(\mathcal{B}(c_{j_0}, r)) - X^{(2)}(\mathcal{B}(c_{j_0}, r))|$ is large, for some j_0 , then the representations of $X^{(1)}$ and $X^{(2)}$ will be well separated. In practice, convolution with kernels is often preferred to local masses (see, e.g., [36]). To ease computation, we will restrict ourselves to the following class of kernel functions.

Definition 6. For $(p, \delta) \in \mathbb{N}^* \times [0, 1/2]$, a function $\psi : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ is called a (p, δ) -kernel function if

$$\begin{array}{ll} i) & \|\psi\|_\infty \leq 1, \\ iii) & \sup_{|u| > 2p} \psi(u) \leq \delta, \end{array} \quad \begin{array}{ll} ii) & \sup_{|u| \leq 1/p} \psi(u) \geq 1 - \delta, \\ iv) & \psi \text{ is 1-Lipschitz.} \end{array}$$

Note that a (p, δ) -kernel is also a (q, δ) -kernel, for $q > p$. This definition of a kernel function encompasses widely used kernels, such as Gaussian or Laplace kernels. In particular, the function $\psi(u) = \exp(-u)$ that is used in [36] is a $(p, 1/p)$ -kernel for $p \in \mathbb{N}^*$. The 1-Lipschitz requirement is not necessary to prove that the representations of two separated measures will be well-separated. However, it is a key assumption to prove that the representations of two measures from the same cluster will remain close in \mathbb{R}^k . From a theoretical viewpoint, a convenient kernel is $\psi_0 : x \mapsto (1 - ((x - 1) \vee 0)) \vee 0$, which is a $(1, 0)$ -kernel, thus a $(p, 0)$ -kernel for all $p \in \mathbb{N}^*$.

From now on we assume that the kernel ψ is fixed, and, for a k -points codebook \mathbf{c} and scale factor σ , consider the vectorization

$$v_{\mathbf{c}, \sigma} : \begin{cases} \mathcal{M}(R, M) & \rightarrow & [0, M]^k \\ X & \mapsto & (X(du) \bullet \psi(\|u - c_1\|/\sigma), \dots, X(du) \bullet \psi(\|u - c_k\|/\sigma)). \end{cases} \quad (2)$$

Note that the dimension of the vectorization depends on the cardinality of the codebook \mathbf{c} . To guarantee that such a vectorization is appropriate for a classification purpose is the aim of the following section.

3.2. Discrimination and clustering based on the mean measure

In this section we investigate under which conditions the vectorization exposed in the above section provides a representation that is provably suitable for clustering. To this aim, for the sample X_1, \dots, X_n , we introduce $(Z_1, \dots, Z_n) \in \llbracket 1, L \rrbracket^n$ the vector of (hidden) label variables. As well, we let M_1, \dots, M_L be such that, if $Z_i = \ell$, $X_i \in \mathcal{M}(R, M_\ell)$, and denote by $M = \max_{\ell \leq L} M_\ell$. For a given codebook \mathbf{c} , we introduce the following definition of (p, r, Δ) -scattering to quantify how well \mathbf{c} will allow to separate clusters via the related vectorization.

Definition 7. Let $(p, r, \Delta) \in (\mathbb{N}^* \times \mathbb{R}^+ \times \mathbb{R}^+)$. A codebook $\mathbf{c} \in \mathcal{B}(0, R)^k$ is said to (p, r, Δ) -**shatter** X_1, \dots, X_n if, for any $i_1, i_2 \in \llbracket 1, n \rrbracket$ such that $Z_{i_1} \neq Z_{i_2}$, there exists $j_{i_1, i_2} \in \llbracket 1, k \rrbracket$ such that

$$\begin{aligned} X_{i_1}(\mathcal{B}(c_{j_{i_1, i_2}}, r/p)) &\geq X_{i_2}(\mathcal{B}(c_{j_{i_1, i_2}}, 4pr)) + \Delta, \quad \text{or} \\ X_{i_2}(\mathcal{B}(c_{j_{i_1, i_2}}, r/p)) &\geq X_{i_1}(\mathcal{B}(c_{j_{i_1, i_2}}, 4pr)) + \Delta. \end{aligned}$$

In a nutshell, the codebook \mathbf{c} shatters the sample if two different measures from two different clusters have different masses around one of the codepoint of \mathbf{c} , at scale r . Note that, for any i, j , $X_i(\mathcal{B}(c_j, r/p)) \geq X_i(\{c_j\})$, so that a stronger definition of shattering in terms of $X_i(\{c_j\})$'s might be stated, in the particular case where $X_i(\{c_j\}) > 0$. The following Proposition ensures that a codebook which shatters the sample yields a vectorization into separated clusters, provided the kernel decreases fast enough.

Proposition 8. Assume that $\mathbf{c} \in \mathcal{B}(0, R)^k$ shatters X_1, \dots, X_n , with parameters (p, r, Δ) . Then, if Ψ is a (p, δ) -kernel, with $\delta \leq \frac{\Delta}{4M}$, we have, for all $i_1, i_2 \in \llbracket 1, n \rrbracket$ and $\sigma \in [r, 2r]$,

$$Z_{i_1} \neq Z_{i_2} \quad \Rightarrow \quad \|v_{\mathbf{c}, \sigma}(X_{i_1}) - v_{\mathbf{c}, \sigma}(X_{i_2})\|_\infty \geq \frac{\Delta}{2}.$$

A proof of Proposition 8 can be found in Section 7.1. This proposition shed some light on how X_1, \dots, X_n has to be shattered with respect to the parameters of Ψ . Indeed, assume that $\Delta = 1$ (that is the case if the X_i 's are integer-valued measures, such as count processes for instance). Then, to separate clusters, one has to choose δ small enough compared to $1/M$, and thus p large enough if Ψ is non-increasing. Hence, the vectorization will work roughly if the support points of two different counting processes are rp -separated, for some scale r . This scale r will then drive the choice of the bandwidth σ . As shown in the following Section 4.2, this will be the case if the sample measures are persistence diagrams of well separated shapes. If the requirements of Proposition 8 are fulfilled, then a standard hierarchical clustering procedure such as Single Linkage with L_∞ distance will separate the clusters for the scales smaller than $\Delta/2$.

Now, to achieve a perfect clustering of the sample based on our vectorization scheme, we have to ensure that measures from the same cluster are not too far in terms of Wasserstein distance, implying in particular that they have the same total mass. This motivates the following definition.

Definition 9. The sample of measures X_1, \dots, X_n is called w -concentrated if, for all i_1, i_2 in $\llbracket 1, n \rrbracket$ such that $Z_{i_1} = Z_{i_2}$,

$$i) \quad X_{i_1}(\mathbb{R}^d) = X_{i_2}(\mathbb{R}^d), \quad ii) \quad W_1(X_{i_1}, X_{i_2}) \leq w.$$

It now falls under the intuition that well-concentrated and shattered sample measures are likely to be represented in \mathbb{R}^k by well-clusterable points. A precise statement is given by the following Proposition 10.

Proposition 10. Assume that X_1, \dots, X_n is w -concentrated. If Ψ is 1-Lipschitz, then, for all $\mathbf{c} \in \mathcal{B}(0, R)^k$ and $\sigma > 0$, for all i_1, i_2 in $\llbracket 1, n \rrbracket$ such that $Z_{i_1} = Z_{i_2}$,

$$\|v_{\mathbf{c}, \sigma}(X_{i_1}) - v_{\mathbf{c}, \sigma}(X_{i_2})\|_\infty \leq \frac{w}{\sigma}.$$

Therefore, if X_1, \dots, X_n is (p, r, Δ) -shattered by \mathbf{c} , and $(r\Delta/4)$ -concentrated, then, for any (p, δ) -kernel satisfying $\delta \leq \frac{\Delta}{4M}$, we have, for $\sigma \in [r, 2r]$,

$$\begin{aligned} Z_{i_1} = Z_{i_2} &\Rightarrow \|v_{\mathbf{c}, \sigma}(X_{i_1}) - v_{\mathbf{c}, \sigma}(X_{i_2})\|_\infty \leq \frac{\Delta}{4}, \\ Z_{i_1} \neq Z_{i_2} &\Rightarrow \|v_{\mathbf{c}, \sigma}(X_{i_1}) - v_{\mathbf{c}, \sigma}(X_{i_2})\|_\infty \geq \frac{\Delta}{2}. \end{aligned}$$

A proof of Proposition 10 is given in Section 7.2. An immediate consequence of Proposition 10 is that (p, r, Δ) -shattered and $r\Delta/4$ -concentrated sample measures can be vectorized in \mathbb{R}^k into a point cloud that is structured in L clusters. These clusters can be exactly recovered via Single Linkage clustering, with stopping parameter in $]\Delta/4, \Delta/2]$. In practice, tuning the parameter σ is crucial. Some heuristic is proposed in [36] in the special case of i.i.d persistence diagrams. An alternative calibration strategy is proposed in the following Section 4.2.

At last, from Propositions 8 and 10, if an optimal k -codebook of the mean measure shatters well the sample, then we can prove that the output of Algorithm 1 provides a relevant vectorization, with high probability. To properly define the mean measure in this case, we assume that the sample measures X_1, \dots, X_n are drawn from a mixture model X . We let $Z \in \llbracket 1, L \rrbracket$ denote a latent variable, with $\mathbb{P}(Z = \ell) = \pi_\ell$, and we assume that

$$X | \{Z = \ell\} \sim X^{(\ell)},$$

where $X^{(\ell)} \in \mathcal{M}(R, M_\ell)$, or equivalently $X = X^{(Z)}$. We also denote by $\bar{M} = \sum_{\ell=1}^L \pi_\ell M_\ell$, so that $\mathbb{E}(X) \in \mathcal{M}(R, \bar{M})$. In this framework, provided that \mathbf{c}^* shatters well X_1, \dots, X_n , so will $\hat{\mathbf{c}}_n$, where $\hat{\mathbf{c}}_n$ is built with Algorithm 1.

Corollary 11. Assume that $\mathbb{E}(X)$ satisfies the assumption of Theorem 4, and that \mathbf{c}^* provides a (p, r, Δ) shattering of X_1, \dots, X_n , with $p \geq 2$. Let $\hat{\mathbf{c}}_n$ denote the output of Algorithm 1. Then $\hat{\mathbf{c}}_n$ is a $(\lfloor \frac{p}{2} \rfloor, r, \Delta)$ shattering of X_1, \dots, X_n , with probability larger than $1 - \exp \left[-C \left(\frac{nr^2 p_{\min}^2}{p^2 M^2 R^2 k^2 d \log(k)} - \frac{p_{\min}^2 B^2 r_0^2}{M^2 R^4 k^2 d \log(k)} \right) \right]$, where C is a constant.

A proof of Corollary 11 is given in Section 7.3. To fully assess the relevance of our vectorization technique, it remains to prove that k -points optimal codebooks

for the mean measure provide a shattering of the sample measure, with high probability. This kind of result implies more structural assumptions on the components of the mixture X . The following Section 4.1 investigates the case where the sample measures are in fact persistence diagrams from different shapes. In this particular case, we can show that quantization of the mean diagram is a relevant strategy to extract shattering codebooks.

4. Application for persistence diagrams

4.1. Mean measure of persistence diagrams

In this section we investigate the properties of our mean-measure quantization scheme in a particular instance of i.i.d. measure observations. Indeed, we assume that we observe n i.i.d persistence diagrams D_i , that are thought of as discrete measures on the half-plane $H^+ = \{(b, d) \in \mathbb{R}^2 \mid 0 \leq b \leq d\}$ (for a general introduction to persistence diagrams the reader is referred to [5, Section 11.5]). In other words, the observations consist in n discrete measures $D_i = \sum_{j=1}^{n_i} \mu_{i,j} \delta_{x_{i,j}}$, where $x_{i,j} \in H^+$ and $\mu_{i,j}$ are weights that can be tuned beforehand. We will show that, whenever the persistence diagrams are generated from different samplings of the same shape, the mean persistence diagram and its best k -points approximation are relevant topological features. Then, in a mixture of shapes framework, we will show that the mean persistence diagram might be used to build a vectorization of the persistence diagrams that allows a provably correct classification. In this section, a compact d -dimensional submanifold S of \mathbb{R}^D is given, with positive reach τ_S (see, e.g., [31]). The object of interest will be the thresholded persistence diagram generated via the distance to S , denoted by d_S (where the infinite connected component has been removed). Namely, if $D' = \sum_{x \in H^+} n(x) \delta_x$ is the persistence diagram of d_S ($n(x)$ denotes the multiplicity of x), we aim to recover

$$D = \sum_{\{(b,d) \in D \mid d-b \geq s\}} n(b,d) \delta_{(b,d)} := \sum_{j=1}^{k_0} n(m_j) \delta_{m_j},$$

where the m_j 's satisfy $m_j^2 - m_j^1 \geq s$. In general, such a thresholded diagram might have an infinite number of points, that is $k_0 = +\infty$. Whenever S is a compact set of \mathbb{R}^d , the following lemma ensures that k_0 is finite.

Lemma 12. *Let S be a compact subset of \mathbb{R}^d , and D denote the persistence diagram of the distance function d_S . For any $s > 0$, the truncated diagram consisting of the points $m = (m^1, m^2) \in D$ such that $m^2 - m^1 \geq s$ is finite.*

A proof of Lemma 12 is given in Section 9.2. Next, we let P denote a distribution on S that has density f with respect to the Hausdorff measure on S , bounded from below by f_{min} . We generate the sample persistence diagrams as follows: for $i = 1, \dots, n$, \mathbb{Y}_N^i denote an i.i.d N -sample drawn from P . According to Lemma 13 below, the distance to \mathbb{Y}_N^i is a provably good approximation of d_S .

Lemma 13. [1, Lemma B.7] Let $S \subset \mathbb{R}^D$ be a d -dimensional submanifold with positive reach τ_S , and let $\mathbb{Y}_N = Y_1, \dots, Y_N$ be an i.i.d. sample drawn from a distribution that has a density $f(x)$ with respect to the Hausdorff measure of S .

Assume that for all $x \in S$, $0 < f_{\min} \leq f(x)$, and let $h = \left(\frac{C_d k \log(N)}{f_{\min} N}\right)^{\frac{1}{d}}$, where C_d is a constant depending on d . If $h \leq \tau_S/4$, then, with probability larger than $1 - \left(\frac{1}{N}\right)^{\frac{k}{d}}$, we have

$$\|d_M - d_{\mathbb{Y}_N}\|_{\infty} \leq h.$$

For convenience, in what follows we assume that for $i \leq n$, $\|d_S - d_{\mathbb{Y}_N^i}\|_{\infty} \leq h$, where $h = \left(\frac{C_d \log(N)}{f_{\min} N}\right)^{\frac{1}{d}}$, for a constant C_d depending only on d . This occurs with high probability provided N is large enough. Then, for every $i = 1, \dots, n$, if D'_i is the persistence diagram of the sublevel sets of $d_{\mathbb{Y}_N^i}$, we let

$$X_i = \sum_{\{x_{i,j} \in D'_i | x_{i,j}^2 - x_{i,j}^1 \geq s - h\}} \delta_{x_{i,j}}.$$

Note that $s \geq h$ provided N is large enough. This amounts to threshold the points of the persistence diagram D'_i that are close to the diagonal. The following Lemma 14 ensures that X_i and D are close enough, in terms of bottleneck distance.

Lemma 14. [13] If X and Y are compact sets of \mathbb{R}^D , then

$$d_B(D(d_X), D(d_Y)) \leq \|d_X - d_Y\|_{\infty}.$$

This stability result allows us to state a result on the expected persistence diagram $\mathbb{E}(X)$. We recall that the thresholded persistence diagram of d_S is $D = \sum_{j=1}^{k_0} n(m_j) \delta_{m_j}$, and we denote by $\mathbf{m} = (m_1, \dots, m_{k_0})$.

Proposition 15. Let $h = \left(\frac{C_d \log(N)}{f_{\min} N}\right)^{\frac{1}{d}}$. Then, for N large enough, with probability larger than $1 - \left(\frac{1}{N}\right)^{\frac{3}{d}}$, we have

$$\|\mathbf{m} - \mathbf{c}^*\|_{\infty} \leq 8\sqrt{M}h,$$

where \mathbf{c}^* is a k_0 -optimal codebook for $\mathbb{E}(X)$ and $M = \sum_{j=1}^{k_0} n(m_j)$.

The proof of Proposition 15 is given in Section 8.1. If h is chosen small enough, Proposition 15 ensures that quantizing the expected persistence diagram yields a k_0 -points distribution on the half-plane that is provably close to the targeted persistence diagram. This is of particular interest in the following Section 4.2, where we show that the mean persistence diagram provides a relevant feature in a mixture of shapes framework.

4.2. Vectorization and clustering of persistence diagrams

From the mean persistence diagram exposed in Section 4.1, we can build an embedding from the space of persistence diagrams to a finite-dimensional Euclidean space, that we will prove suitable for shape classification. A case of interest for shape classification is when X is a mixture distribution, each component of which being drawn from a shape, as in Section 4.1. To be more precise, we let $L \in \mathbb{N}^*$ denote the number of components, and for $\ell \leq L$, we let $S^{(\ell)}$ denote a compact d_ℓ -submanifold, and $D_{\geq s}^{(\ell)}$ the thresholded persistence diagram built from $d_{S^{(\ell)}}$ (where points that have persistence smaller than s are removed).

As well, we denote by $X^{(\ell)}$ the distribution of the thresholded persistence diagram built from the distance to N_ℓ points drawn on $S^{(\ell)}$, with threshold $s - h_\ell$. Given a latent variable Z on $\llbracket 1, L \rrbracket$, with $\mathbb{P}(Z = \ell) = \pi_\ell$, the mixture distribution X of thresholded persistence diagrams is given by

$$X \mid \{Z = \ell\} \sim X^{(\ell)},$$

or equivalently $X = X^{(Z)}$. To make discrimination between shapes possible, we have to assume that their persistence diagrams differ by at least one point.

Definition 16. *The shapes $S^{(1)}, \dots, S^{(L)}$ are **discriminable at scale s** if for any $1 \leq \ell_1 < \ell_2 \leq L$ there exists $m_{\ell_1, \ell_2} \in H^+$ such that*

$$D_{\geq s}^{(\ell_1)}(\{m_{\ell_1, \ell_2}\}) \neq D_{\geq s}^{(\ell_2)}(\{m_{\ell_1, \ell_2}\}),$$

where the thresholded persistence diagrams are considered as measures.

Note that if m_{ℓ_1, ℓ_2} satisfies the discrimination condition stated above, then $m_{\ell_1, \ell_2} \in D_{\geq s}^{(\ell_1)}$ or $m_{\ell_1, \ell_2} \in D_{\geq s}^{(\ell_2)}$. To discriminate between shapes, we have to ensure that every m_{ℓ_1, ℓ_2} is represented via an optimal codebook. This is the aim of the following Proposition.

Proposition 17. *Let $h_\ell = \left(\frac{C_{d_\ell}(d_\ell^2 + 2) \log(N_\ell)}{f_{\min, \ell} N_\ell} \right)^{1/d_\ell}$, and $h = \max_{\ell \leq L} h_\ell$. Moreover, let $M_\ell = D_{\geq s}^{(\ell)}(H^+)$, $\bar{M} = \sum_{\ell=1}^L \pi_\ell M_\ell$, and $\pi_{\min} = \min_{\ell \leq L} \pi_\ell$.*

Assume that $S^{(1)}, \dots, S^{(L)}$ are discriminable at scale s , and let m_1, \dots, m_{k_0} denote the discrimination points. Let $K_0(h)$ denote

$$\inf \{k \geq 0 \mid \exists t_1, \dots, t_k \quad \bigcup_{\ell=1}^L D_{\geq s}^{(\ell)} \setminus \{m_1, \dots, m_{k_0}\} \subset \bigcup_{s=1}^{K_0(h)} \mathcal{B}_\infty(t_s, h)\}.$$

Let $k \geq k_0 + K_0(h)$, and (c_1^, \dots, c_k^*) denote an optimal k -points quantizer of $\mathbb{E}(X)$. Then, provided that N_ℓ is large enough for all ℓ , we have*

$$\forall j \in \llbracket 1, k_0 \rrbracket \quad \exists p \in \llbracket 1, k \rrbracket \quad \|c_p^* - m_j\|_\infty \leq \frac{5\sqrt{\bar{M}h}}{\sqrt{\pi_{\min}}}.$$

The proof of Proposition 17 is given in Section 8.2. If $\bar{D}_{\geq s}$ denotes the mean persistence diagram $\sum_{\ell=1}^L \pi_{\ell} D_{\geq s}^{(\ell)}$, and $\bar{D}_{\geq s}$ has K_0 points, then it is immediate that $k_0 + K_0(h) \leq K_0$. Moreover, we also have $k_0 \leq \frac{L(L+1)}{2}$. Proposition 17 ensures that the discrimination points are well enough approximated by optimal k -centers of the expected persistence diagram $\mathbb{E}(X)$, provided the shapes $S^{(\ell)}$ are well-enough sampled and k is large enough so that $\bar{D}_{\geq s}$ is well-covered by k balls with radius h . Note that this is always the case if we choose $k = K_0$, but also allows for smaller k 's.

In turn, provided that the shapes $S^{(1)}, \dots, S^{(L)}$ are discriminable at scale s and that k is large enough, we can prove that an optimal k -points codebook \mathbf{c}^* is a (p, r, Δ) -shattering of the sample, with high probability.

Proposition 18. *Assume that the requirements of Proposition 17 are satisfied. Let $\tilde{B} = \min_{i=1, \dots, k_0, j=1, \dots, K_0, j \neq i} \|m_i - m_j\|_{\infty} \wedge s$. Let $\kappa > 0$ be a small enough constant. Then, if N_{ℓ} is large enough for all $\ell \in \llbracket 1, \ell \rrbracket$, X_1, \dots, X_n is $(p, r, 1)$ -shattered by \mathbf{c}^* , with probability larger than $1 - n \max_{\ell \leq L} N_{\ell}^{-\left(\frac{(\kappa \tilde{B})^{d_{\ell}} f_{\min, \ell} N_{\ell}}{C_{\ell} d_{\ell} \log(N_{\ell})}\right)}$, provided that*

- $\frac{r}{p} \geq 2\kappa \tilde{B}$
- $4rp \leq \left(\frac{1}{2} - \kappa\right) \tilde{B}$.

Moreover, on this probability event, X_1, \dots, X_n is $2M\kappa\tilde{B}$ -concentrated.

A proof of Proposition 18 is given in Section 8.3. In turn, Proposition 18 can be combined with Proposition 10 and Corollary 11 to provide guarantees on the output of Algorithm 1 combined with a suitable kernel. We choose to give results for the theoretical kernel $\psi_0 : x \mapsto (1 - ((x - 1) \vee 0)) \vee 0$, and for the kernel used in [36], $\psi_{AT} = x \mapsto \exp(-x)$.

Corollary 19. *Assume that the requirements of Proposition 18 are satisfied. For short, denote by v_i the vectorization of X_i based on the output of Algorithm 1. Then, with probability larger than $1 - \exp\left[-C \left(\frac{nr^2 p_{\min}^2}{p^2 M^2 R^2 k^2 d \log(k)} - \frac{p_{\min}^2 B^2 r_0^2}{M^2 R^4 k^2 d \log(k)}\right)\right] - n \max_{\ell \leq L} N_{\ell}^{-\left(\frac{(\kappa \tilde{B})^{d_{\ell}} f_{\min, \ell} N_{\ell}}{C_{\ell} d_{\ell} \log(N_{\ell})}\right)}$, where κ and C are small enough constants, we have*

$$\begin{aligned} Z_{i_1} = Z_{i_2} &\Rightarrow \|v_{i_1} - v_{i_2}\|_{\infty} \leq \frac{1}{4}, \\ Z_{i_1} \neq Z_{i_2} &\Rightarrow \|v_{i_1} - v_{i_2}\|_{\infty} \geq \frac{1}{2}, \end{aligned}$$

for $\sigma \in [r, 2r]$ and the following choices of p and r :

- If $\Psi = \Psi_{AT}$, $p_{AT} = \lceil 4M \rceil$, and $r_{AT} = \frac{\tilde{B}}{32p_{AT}}$.
- If $\Psi = \Psi_0$, $p_0 = 1$ and $r_0 = \frac{\tilde{B}}{32}$.

A proof of Corollary 19 is given in Section 8.4. Corollary 19 can be turned into probability bounds on the exactness of the output of hierarchical clustering schemes applied to the sample points. For instance, on the probability event described by Corollary 19, Single Linkage with norm $\|\cdot\|_{\infty}$ will provide an exact

clustering. The probability bound in Corollary 19 shed some light on the quality of sampling of each shape that is required to achieve a perfect classification: roughly, for N_ℓ in $\Omega(\log(n))$, the probability of misclassification can be controlled. Note that though the key parameter \tilde{B} is not known, in practice it can be scaled as several times the minimum distance between two points of a diagram.

5. Experimental results

We now provide experiments that showcase the mean measure procedure of this paper. The mini-batch space quantization of Section 2.2 is used in the ATOL procedure (Automatic Topologically-Oriented Learning), [36], to vectorize measures through convolution with an exponential kernel Ψ_{AT} as in Section 3. In this Section our intent is to illustrate the potential of a fast and optimal measure quantization procedure, not to claim methodological superiority on some particular problem type or data. Therefore it is fitting to apply a rather automatic procedure and we use a generic version of ATOL with few to no tuning: for all experiments we use minibatches of size 1000 and the same calibration scheme (use a random 10% of the measures from the training set for learning the space quantization). We use the same kernel Ψ_{AT} , only the ATOL budget k (length of the vectorization) will sometimes vary in the three experiments. We set to survey a variety of modern machine-learning problems: synthetic measure clustering, large-scale graph classification as well as text classification. On these problems, we achieve state-of-the-art performances.

5.1. Measure clustering

In this first experiment we want to directly assess the efficiency of the kmeans-like quantization of the measure space for clustering in a mixture model. We use an i.i.d sample of a mixture of measures subjected to a clustering task, that is we perform measure vectorization via quantization of the mean measure, then perform a standard clustering task on the resulting vectorizations.

We generate synthetic mixture of K measures. We first draw $p - 1$ centers shared by all mixture components on the d -dimensional unit sphere \mathcal{S}_d , and denote them by $\{S_d^i \mid i = 1, \dots, p - 1\}$; then for each mixture component another center is placed at a separate vertex of the d -dimensional unit cube (implying $K \leq 2^d$), labeled $\text{Cube}_{d|k}$ for $k \in [K]$, so that the inner center is the only center that varies amongst mixture components, see instances Figure 1. For given $R > 1$, the *support centers* C^k for the mixture component k is given by

$$C^k = \{R \times S_d^i \mid i = 1, \dots, p - 1\} \cup \text{Cube}_{d|k}. \quad (3)$$

For every mixture component and signal level $r > 0$, we then make N normal simultaneous draws with variance 1 centered around every element of $r \times C^k$, resulting in a point cloud of cardinality $p \times N$ that is interpreted as a measure.

To sum up, the k -th mixture component X^k has distribution

$$X^k = \bigcup_{c \in C^k} \bigcup_{i=1, \dots, N} \{rc + \varepsilon_{c,i}\},$$

where the ε 's are i.i.d standard d -dimensional Gaussian random variables. Finally the space is arbitrarily rotated so as to not favor a specific axis configuration.

We compare ATOL to alternative quantization or clustering procedures, some simple and intuitive to produce clear understanding, some more sophisticated to gain insights. Very close to the ATOL procedure we devise a measure-quantization method that is learnt by randomly choosing points for quantizing the space (labeled "rand" procedure), and another quantization that uses centers of a regular grid (labeled "grid" procedure). For fair comparison we use the same kernel Ψ_{AT} as in ATOL for vectorizing from these two types of quantizations. For broader comparisons we also introduce and compare with two other well known procedures. First a **histogram** quantization that as **grid** does, learns a regular grid for quantizing the measure space, but then vectorizes measure by counting inside the tiles instead of using the ψ_{AT} kernel. Second, a **W2-spectral** clustering method that computes the Wasserstein-2 Gram matrix between every measure pair, and then applies a clustering step on the rows of this matrix - so this procedure is the spectral clustering procedure between measures with the Wasserstein-2 metric. For the final clustering step of all methods we use a standard k-means clustering with 100 initializations.



Fig 1: Synthetic 3-mixture of measures instance (blue, dark brown and pink) and their *support centers* for indication (dark green for the outer centers, yellow, green and brown for the middle centers) with either 4 (left) or 20 (right) *support centers* in dimension 2, $r = 1$ and $R = 10$. The sets of points similarly coloured constitute measures.

We designed the mixtures to exemplify problems where the data are significantly separated (generating points from a different cube edge), but also very similarly noisy by including draws from the same set of centers on the outer sphere that conceals the signal. Therefore in this experiment r represents the strength of the signal separation, and p can be interpreted as a measure of noise.

Empirically we use two different setups for the number of supporting centers p : $p = 4$ or $p = 20$, that we interpret respectively as low and high noise situations, see Figure 1. We generate measures in dimension 2, 3 and 5. We sample each center $N = 25$ times for each measure, we use $R = 10$, we study $K = 3$ mixtures and for each mixture component we produce $n = 20$ i.i.d. measures so that the clustering experiment resolves in clustering 60 measures each supported on $25 \times p$ points from 3 clusters. Note that for the $p = 20$ case, the **W2-spectral** clustering procedure runs takes too long to compute and is not reported. Each experiment is performed identically a hundred times and the resulting average *normalised mutual information* (NMI) with true labels and 95% confidence intervals are presented for each method.

We perform two sets of experiments corresponding to the following two questions.

Q1: at a given signal level $r = 1$, for increasing budget (that is, the size of the vectorizations used in the quantizing process) how accurate are methods at clustering 3-mixtures? Q1 aims at comparing the various method’s potential at capturing the underlying signal with respect to budget.

Results are displayed in Figure 2. The ATOL quantization procedure of this paper is shown to produce the best results in almost all situations, that is, it is the procedure that will most likely cluster the mixture exactly while requiring the least amount of budget for doing so. The grid procedures **grid** and **histogram** naturally suffer from the dimension growth (middle and bottom panels). In dimension 2 the **grid** procedure shows to be very efficient, but for measures in dimension 5 it is always better to select points at random and perform quantization relative to these points, rather than using an instance of regular grid quantization.

Q2: for a given, fixed-size budget $k = 32$ and increasing signal level, how accurate are methods at clustering 3-mixtures? Q2 is practical and shows how the various methods fare with respect to signal strength at a given, low vectorization support length $k = 32$ - the most favorably low budget for regular grid procedures in dimension 5.

Results are shown in Figure 3. ATOL and the **grid** procedure are shown to perform equally well, hinting that given a sufficient budget, the kernel vectorization Ψ_{AT} is a powerful discriminant when complemented with an adequately quantized space. Indeed the synthetic mixture of measures clustering experiment is very favorable to a regular grid quantization provided there is no tile centered on 0_d (see Figure 1) and enough budget for discrimination (see results of Figure 2). Figure 3 also shows that a random space quantization will fare poorly when p increases, and ATOL performs as well as the **W2-spectral** algorithm in the $p = 4$ low noise case, that arguably has optimal behaviour for this problem.

5.2. Large-scale graph classification

We now look at the important problem of large-scale graph classification. ATOL is task-agnostic and not specifically designed for problems involving graphs,

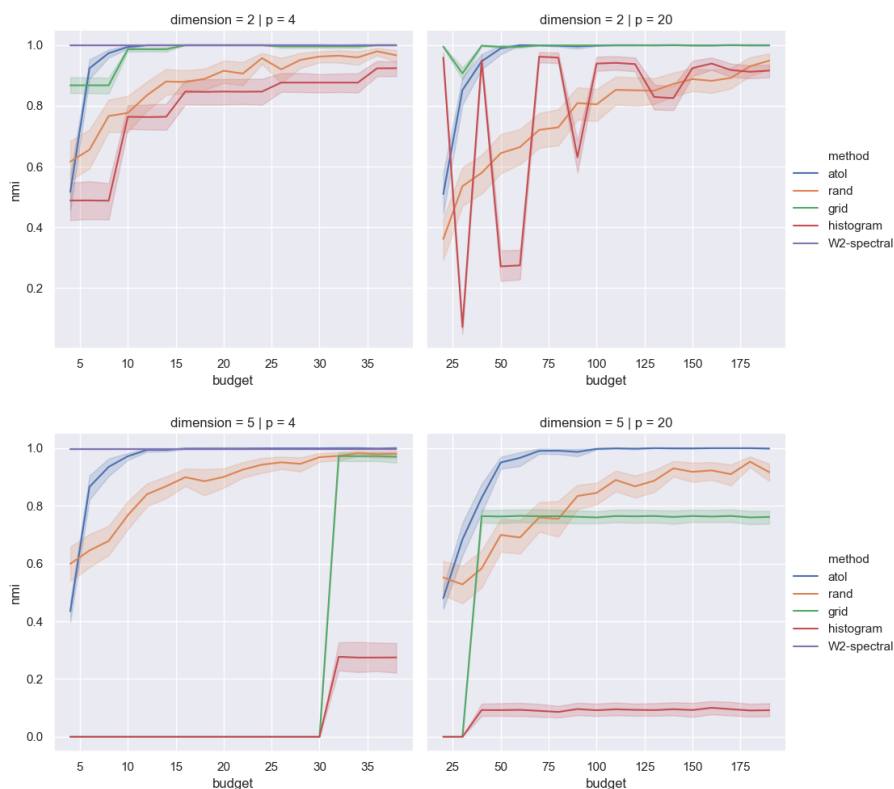


Fig 2: NMI as budget increases, $r = 1$, increasing dimensions along rows, low noise and high noise contexts (left and right columns)

but since the procedure is extremely fast (the quantization step has optimal or near-optimal speed, and the vectorization step is single pass), it has potential for large-scale applications.

There are multiple ways to interpret graphs as measures. In this section we borrow from [7]: for a diffusion time $t > 0$ we compute the Heat Kernel Signatures (HKS_t) for all vertices in a graph, so that each graph $G(V, E)$ is embedded in $\mathbb{R}^{|V|}$ (we refer to [7, Section 2.2]). Then the authors use the extended persistence framework to produce four graph descriptors per diffusion time (see [7, Section 2.1]), that is four types of persistence diagrams (PDs). Schematically for a graph $G(V, E)$ the descriptors are derived as:

$$G(V, E) \xrightarrow[\text{signatures}]{\text{heat kernel}} \text{HKS}_t(G) \in \mathbb{R}^{|V|} \xrightarrow[\text{persistence}]{\text{extended}} \text{PD}(\text{HKS}_t(G)) \in (\mathcal{M}(\mathbb{R}^2))^4. \quad (4)$$

In these experiments we will show that the graph embedding strategy of (4) paired with ATOL can perform up to the state of the art on large-scale graph

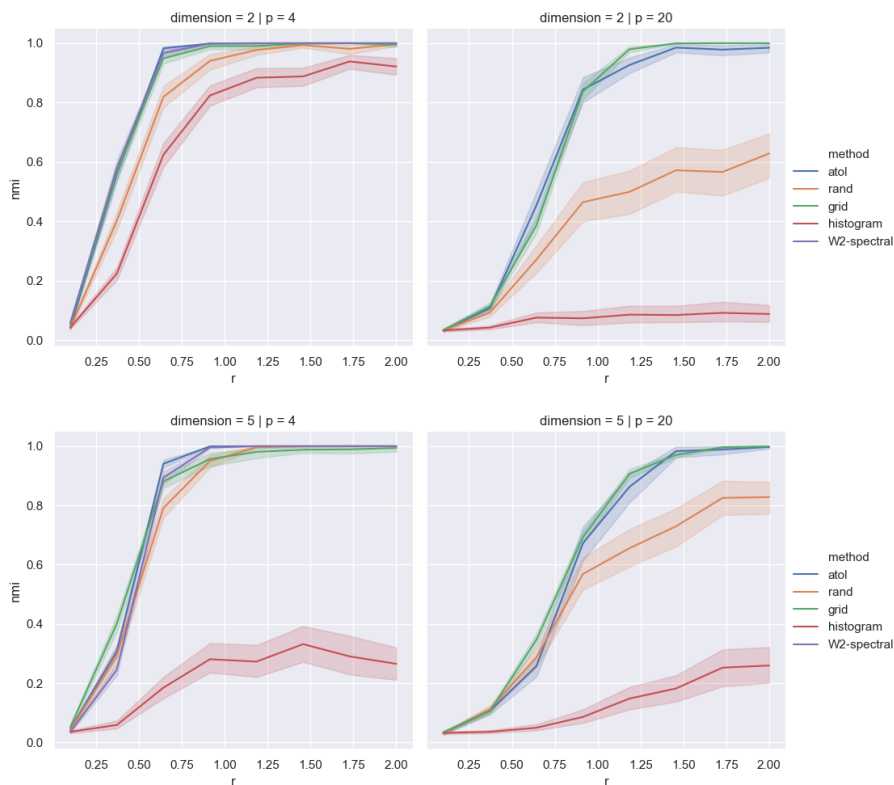


Fig 3: NMI as r increases, budget $k = 32$, increasing dimensions along rows, low noise and high noise contexts (left and right columns)

classification problems. We will also demonstrate that ATOL is well assisted but not dependent on the aforementioned TDA tools.

Large-scale binary classification from [37]

Recently [37] introduces large-scale graph datasets of social or web origin. For each dataset the associated task is binary classification. The authors perform a 80% train/test split of the data and report mean area under the curve (AUC) along with standard errors over a hundred experiments for all the following graph embedding methods. SF from [15] is a simple graph embedding method that extracts the k lowest spectral values from the graph Laplacian, and a standard Random Forest Classifier (RFC) for classification. NetLSD from [40] uses a more refined representation of the graph Laplacian, the heat trace signature (a global variant of the HKS) of a graph using 250 diffusion times, and a 1-layer neural network (NN) for classification. FGSD from [42] computes the biharmonic spectral distance of a graph and uses histogram vectorization with small binwidths that results in featurisation of size [100, 1000000], with a Support Vector Machine (SVM) classifier. GeoScattering from [20] uses graph wavelet

problem	method	size	SF [15]	NetLSD [40]	FGSD [42]	GeoScat [20]	ATOL
reddit	threads	(203K)	81.4±.2	82.7±.1	82.5±.2	80.0±.1	80.7±.1
twitch	egos	(127K)	67.8±.3	63.1±.2	70.5±.3	69.7±.1	69.7±.1
github	stargazers	(12.7K)	55.8±.1	63.2±.1	65.6±.1	54.6±.3	72.3±.4
deezer	ego nets	(9.6K)	50.1±.1	52.2±.1	52.6±.1	52.2±.3	51.0±.6

TABLE 1

Large graph binary classification problems. Mean ROC-AUC and standard deviations.

transform to produce 125 graph embedding features, also with a SVM classifier.

We add our own results for ATOL paired with (4): we use the extended persistence diagrams as input for ATOL computed from the HKS values with diffusion times $t_1 = .1, t_2 = 10$, and vectorize the diagrams with budget $k = 10$ for each diagram type and diffusion time so that the resulting quantization for graph G is $v_{\text{ATOL}}(G) \in \mathbb{R}^{2 \times 4 \times 10}$. We then train a standard RFC (as in [15], we use the implementation from `sklearn` [32] with all default parameters) on the resulting vectorized measures.

The results are shown Table 1. ATOL is close to or over the state-of-the-art for all four datasets. Most of these methods operate directly from graph Laplacians so they are fairly comparable, in essence or as for the dimension of the embedding that is used. The most positive results on `github stargazers` improves on the best method by more than 6 points. Overall, using the ATOL framework to handle quantizing measures on large amounts of graphs proves immediately beneficial, and readily competitive on handling large-scale graph datasets from the measure viewpoint.

A variant of the large-scale graph classification from [36]

The graph classification tasks above were binary classifications. [43] introduced now popular datasets of large-scale graphs associated with multiple classes. These datasets have been tackled with top performant graph methods including the graph kernel methods RetGK from [44], WKPI from [45] and GNTK from [17] (combined with a graph neural network), and the aforementioned graph embedding method FGSD from [42]. PersLay from [7] is not designed for graphs but used (4) as input for a 1-NN classifier. Lastly, in [36], the authors also used (4) and the same diagrams as input data for the ATOL procedure and obtained competitive results.

We now make a variation from this perspective and show that in the case of large-scale graphs, ATOL produces state-of-the-art results that are not dependent on using any specific TDA tools - even though we note that the quantization step of ATOL is inherently topological. Instead we use simpler graph descriptors: we compute four HKS descriptors corresponding to diffusion times $t_1 = .1, t_2 = 1, t_3 = 10, t_4 = 100$ for all vertices in a graph, but this time directly interpret the output as a measure embedding in dimension 4. From there we use ATOL with $k = 80$ budget. Therefore each graph $G(V, E)$ is embedded in $\mathbb{R}^{4|V|}$ seen as $\mathcal{M}(\mathbb{R}^4)$ and our measure vectorization framework is readily applicable from there. To sum-up we now use the point of view:

$$G(V, E) \xrightarrow[\text{signatures}]{\text{heat kernel}} \text{HKS}_{t_1, t_2, t_3, t_4}(G) \in \mathbb{R}^{4|V|} \approx \mathcal{M}(\mathbb{R}^4) \quad (5)$$

As an important comment we make the following point that any type of node or edge embedding, including those that can be efficiently computed on large graphs, could readily be used instead of the HKS embedding employed here. We do not claim that this particular embedding is the correct way to handle graphs in general, much to the contrary: instead we simply show that our methodology can handle all sort of embedding strategies, with good results to support it for the exposed experiments.

method	RetGK	FGSD	WKPI	GNTK	PersLay	ATOL	ATOL
problem	[44]	[42]	[45]	[17]	[7]	with (4) [36]	with (5)
REDDIT (5K, 5 classes)	56.1±.5	47.8	59.5±.6	—	55.6±.3	67.1±.3	66.1±.2
REDDIT (12K, 11 classes)	48.7±.2	—	48.5±.5	—	47.7±.2	51.4±.2	50.7±.3
COLLAB (5K, 3 classes)	81.0±.3	80.0	—	83.6±.1	76.4±.4	88.3±.2	88.5±.1
IMDB-B (1K, 2 classes)	71.9±1.	73.6	75.1±1.1	76.9±3.6	71.2±.7	74.8±.3	73.9±.5
IMDB-M (1.5K, 3 classes)	47.7±.3	52.4	48.4±.5	52.8±4.6	48.8±.6	47.8±.7	47.0±.5

TABLE 2

Mean accuracies and standard deviations for the large multi-classes problems of [43]

On Table 2 we quote results and competitors from [36] and on the right column we add our own experiment with ATOL. The ATOL methodology works very efficiently with the direct HKS embedding as well, although the results tend to be slightly inferior. This may hint at the fact that although PDs are not essential to capturing signal from this dataset, they can be a significant addition for doing so. Overall the ATOL framework is competitive for multiclass classification of large-scale graph datasets. It does not rely solely on specific TDA tools and is adaptable to handle all forms of measure interpretations.

5.3. Text classification with word embedding

In this section we intend to apply our methodology in a high-dimensional framework, namely text classification. Basically, texts are sequences of words and if one forgets about word order, a text can be interpreted as a measure in the (fairly unstructured) space of words. We use the `word2vec` word embedding technique introduced in [30], that uses a two-layer neural network to learn a real-valued vector representation for each word in a dictionary in such a way that distances between words are learnt to reflect the semantic closeness between them, with respect to the corpus. Therefore for a given dimension $E \in \mathbb{N}$ every word w is mapped to the embedding space $v_{\text{word2vec}}(w) \in \mathbb{R}^E$, and we can use word embedding to interpret texts as measures in a given word embedding space:

$$T \in \mathcal{M}(\{\text{words}\}) \xrightarrow[\text{embedding}]{\text{word}} T_{\text{word2vec}} = [v_{\text{word2vec}}(w)]_{w \in T} \in \mathcal{M}(\mathbb{R}^E). \quad (6)$$

In practice we will use the Large Movie Review Dataset from [27] for our text corpus, and learn word embedding on this corpus. To ease the intuition,

let us use a word embedding in dimension 2 and quantize the space of text measures with the minibatch quantization algorithm. Figure 4 shows a visual representation of the quantization centers. Note that this word embedding step does not depend on the classification task that will follow.

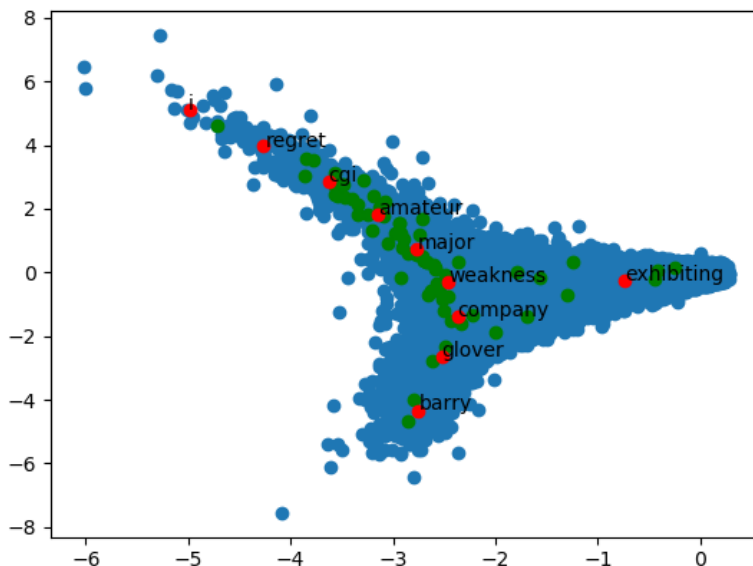


Fig 4: Blue: point cloud embedding in dimension 2 for the words of all reviews; green: point cloud embedding for the words of the first review ("Story of a man who has unnatural feelings for a pig. [...]"); red: centers derived from the mean measure quantization with the text print of their closest corresponding word.

We now turn to the task of classification and use the binary sentiment annotation (positive or negative reviews) from the dataset. For classifying texts with modern machine-learning techniques there are several problems to overcome: important words in a text can be found at almost any place, texts usually have different sizes so that they have to be padded in some way, etc. The measure viewpoint is a direct and simple solution.

The successful way to proceed after a word embedding step is to use some form of deep neural network learning. We learn a 100-dimensional word embedding using the `word2vec` implementation from the `gensim` module, then compare the following classification methods: directly run a recurrent neural network (LSTM with 64 units), against the ATOL vectorization followed by a simple dense layer with 32 units. We measure accuracies through a single 10-fold.

The ATOL vectorization with word embedding in dimension 100, 20 centers, and 1-NN classifier reaches 85.6 accuracy with .95 standard deviation. The

average quantization and vectorization times are respectively 5.5 and 208.3 seconds. The recurrent neural network alternative with word embedding in dimension 100 reaches 89.3 mean accuracy with .44 standard deviation, for an average run time of about 1 hour.

Naturally the results are overall greatly hindered by the fact that we have treated texts as a separate collection of words, forgetting sentence structure when most competitive methods use complex neural networks to analyse n -uplets of words as additional inputs. Additional precision can be also gained using a task-dependent embedding of words, at the price of a larger computation time (see for instance the `kaggle` winner algorithm [12], with precision 99% and run time 10379 seconds).

6. Proofs for Section 2

6.1. Proof of Theorem 4

Throughout this section we assume that $\mathbb{E}(X)$ satisfies a margin condition with radius r_0 , and that $\mathbb{P}(X \in \mathcal{M}_{N_{max}}(R, M)) = 1$. The proof of Theorem 4 is based on the following lemma, which ensures that every step of Algorithm 1 is, up to concentration terms, a contraction towards an optimal codebook. We recall here that $R_0 = \frac{Br_0}{16\sqrt{2}R}$, $\kappa_0 = \frac{R_0}{R}$.

Lemma 20. *Assume that $\mathbf{c}^{(0)} \in \mathcal{B}(\mathbf{c}^*, R_0)$. Then, with probability larger than $1 - 9e^{-c_1 n p_{min}/M} - e^{-x}$, for n large enough, we have, for every t ,*

$$\|\mathbf{c}^{(t+1)} - \mathbf{c}^*\|^2 \leq \frac{3}{4} \|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2 + \frac{K}{p_{min}^2} D_n^2, \quad (7)$$

where $D_n = \frac{CRM}{\sqrt{n}} \left(k\sqrt{d \log(k)} + \sqrt{x} \right)$ and C, K are positive constants.

The proof of Lemma 20 is deferred to Section 9.1.1.

Proof of Theorem 4. Equipped with Lemma 20, the proof of Theorem 4 is straightforward. On the probability event of Lemma 20, using (7) we have that

$$\begin{aligned} \|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2 &\leq \left(\frac{3}{4}\right)^t \|\mathbf{c}^{(0)} - \mathbf{c}^*\|^2 + \left(\sum_{p=0}^{t-1} \left(\frac{3}{4}\right)^p\right) \frac{K}{p_{min}^2} D_n^2 \\ &\leq \left(\frac{3}{4}\right)^t \|\mathbf{c}^{(0)} - \mathbf{c}^*\|^2 + \frac{4K}{p_{min}^2} D_n^2. \end{aligned}$$

□

6.2. Proof of Theorem 5

The proof of Theorem 5 follows the proof of [34, Lemma 1]. Throughout this section we assume that $\mathbb{E}(X)$ satisfies a margin condition with radius r_0 . The

proof of Theorem 5 is based on the following lemma. Recall that $R_0 = \frac{Br_0}{16\sqrt{2}R}$, $\kappa_0 = \frac{R_0}{R}$. We let $\mathbf{c}^{(t)}$ denote the output of Algorithm 2 (or its variant in the sample point case).

Lemma 21. *Assume that $\mathbf{c}^{(0)} \in \mathcal{B}(\mathbf{c}^*, R_0)$, and $n_t \geq c_0 \frac{k^2 M^2}{p_{\min}^2 \kappa_0^2} \log(n)$, for some constant c_0 , with $n \geq k$. Then we have, for any $t = 0, \dots, T-1$,*

$$\mathbb{E} \left(\|\mathbf{c}^{(t+1)} - \mathbf{c}^*\|^2 \right) \leq \left(1 - \frac{2 - K_1}{t+1} \right) \mathbb{E} \left(\|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2 \right) + \frac{16kMR^2}{p_{\min}(t+1)^2}, \quad (8)$$

with $K_1 \leq 0.5$.

The proof of Lemma 21 is deferred to Section 9.1.2.

Proof of Theorem 5. Equipped with Lemma 21, we can prove Theorem 5 using the same method as in the proof of [34, Lemma 1]. Namely, denoting by $a_t = \|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2$, we prove recursively that

$$\mathbb{E}a_t \leq \frac{32kMR^2}{p_{\min}t}.$$

Denote by $G = \frac{16kMR^2}{p_{\min}}$. The case $t = 1$ is obvious. Next, assuming that $\mathbb{E}a_t \leq \frac{2G}{t}$ and using (8) we may write

$$\begin{aligned} \mathbb{E}a_{t+1} &\leq \left(1 - \frac{2}{t+1} \right) \mathbb{E}a_t + \frac{K_1}{t+1} \mathbb{E}a_t + \frac{G}{(t+1)^2} \\ &\leq \frac{G}{t(t+1)} [2t + 2K_1 - 1]. \end{aligned}$$

Since $K_1 \leq \frac{1}{2}$, we get that $\mathbb{E}a_{t+1} \leq 2G/(t+1)$. \square

7. Proofs for Section 3

7.1. Proof of Proposition 8

Assume that X_1, \dots, X_n is (p, r, Δ) -shattered by \mathbf{c} , let i_1, i_2 in $\llbracket 1, n \rrbracket$ be such that $Z_{i_1} \neq Z_{i_2}$, and without loss of generality assume that

$$X_{i_1}(\mathcal{B}(c_1, r/p)) \geq X_{i_2}(\mathcal{B}(c_1, 4rp)) + \Delta.$$

Let Ψ be a (p, δ) -kernel and $\sigma \in [r, 2r]$. We have

$$\begin{aligned} X_{i_1}(du) \bullet \Psi((u - c_1)/\sigma) &\geq X_{i_1}(du) \bullet [\Psi(\|u - c_1\|/\sigma) \mathbb{1}_{\mathcal{B}(c_1, r/p)}(u)] \\ &\geq (1 - \delta) X_{i_1}(\mathcal{B}(c_1, r/p)) \\ &\geq X_{i_1}(\mathcal{B}(c_1, r/p)) - \delta M. \end{aligned}$$

On the other hand, we have that

$$\begin{aligned} X_{i_2}(du) \bullet \Psi(\|u - c_1\|/\sigma) &\leq X_{i_2}(du) \bullet [\Psi(\|u - c_1\|/\sigma) \mathbb{1}_{\mathcal{B}(c_1, 4pr)}] \\ &\quad + X_{i_2}(du) \bullet [\Psi(\|u - c_1\|/\sigma) \mathbb{1}_{(\mathcal{B}(c_1, 4pr))^c}] \\ &\leq X_{i_2}(\mathcal{B}(c_1, 4pr)) + \delta X_{i_2}((\mathcal{B}(c_1, 4pr))^c) \\ &\leq X_{i_1}(\mathcal{B}(c_1, r/p)) - \Delta + \delta M. \end{aligned}$$

We deduce that $\|v_{\mathbf{c}, \sigma}(X_{i_1}) - v_{\mathbf{c}, \sigma}(X_{i_2})\|_\infty \geq \Delta - 2\delta M \geq \frac{\Delta}{2}$ whenever $\delta \leq \frac{\Delta}{4M}$.

7.2. Proof of Proposition 10

Let i_1, i_2 in $\llbracket 1, n \rrbracket$ such that $Z_{i_1} = Z_{i_2}$. Let (Y_1, Y_2) be a random vector such that $Y_1 \sim X_{i_1}$, $Y_2 \sim X_{i_2}$, and $\mathbb{E}(\|Y_1 - Y_2\|) \leq w$. Let $c \in \mathcal{B}(0, R)$, we have

$$\begin{aligned} |X_{i_1}(du) \bullet \Psi(\|u - c\|/\sigma) - X_{i_2}(du) \bullet \Psi(\|u - c\|/\sigma)| \\ \leq |\mathbb{E}[\Psi(\|Y_1 - c\|/\sigma) - \Psi(\|Y_2 - c\|/\sigma)]| \\ \leq \mathbb{E}\left(\frac{\|Y_1 - Y_2\|}{\sigma}\right) \leq \frac{w}{\sigma}, \end{aligned}$$

hence $\|v_{\mathbf{c}, \sigma}(X_{i_1}) - v_{\mathbf{c}, \sigma}(X_{i_2})\|_\infty \leq w/\sigma$. Now if $X_1 \dots, X_n$ is $r\Delta/4$ -concentrated, and $\sigma \in [r, 2r]$, we have $\|v_{\mathbf{c}, \sigma}(X_{i_1}) - v_{\mathbf{c}, \sigma}(X_{i_2})\|_\infty \leq \frac{\Delta}{4}$.

7.3. Proof of Corollary 11

For n large enough, with probability larger than $1 - \exp\left[-C\left(\frac{nr^2 p_{min}^2}{p^2 M^2 R^2 k^2 d \log(k)} - \frac{p_{min}^2 B^2 r_0^2}{M^2 R^4 k^2 d \log(k)}\right)\right]$, we have $\|\hat{\mathbf{c}}_n - \mathbf{c}^*\| \leq \frac{r}{p}$, according to Theorem 4. Let $i_1, i_2 \in \llbracket 1, n \rrbracket$ be such that $Z_{i_1} \neq Z_{i_2}$. Without loss of generality assume that

$$X_{i_1}(\mathcal{B}(c_1^*, r/p)) \geq X_{i_2}(\mathcal{B}(c_1^*, 4pr)) + \Delta.$$

Then $X_{i_1}(\mathcal{B}(\hat{c}_1, 2r/p)) \geq X_{i_1}(\mathcal{B}(\hat{c}_1, r/p))$, combined with $X_{i_2}(\mathcal{B}(\hat{c}_1, 4(p/2)r)) \leq X_{i_2}(\mathcal{B}(c_1^*, 4pr))$ entails that

$$X_{i_1}(\mathcal{B}(\hat{c}_1, 2r/p)) \geq X_{i_2}(\mathcal{B}(\hat{c}_1, 4(p/2)r)) + \Delta.$$

8. Proofs for Section 4

8.1. Proof of Proposition 15

Let D'_1 denote the persistence diagram build from the sublevel sets of $d_{\mathbb{Y}_N}$, where \mathbb{Y}_N is an N -sample drawn on S (without the infinite connected component), and let R denote the diameter of S . Then, every point of D'_1 is in $\mathcal{B}(0, R)$. For short denote by $\alpha_N = (\frac{1}{N})^{d+1/d}$, and we take N large enough so that $\alpha_N \leq \frac{h^2}{R^2} \wedge \frac{1}{2}$. For a positive t , we denote by $D_{\geq t} = \sum_{\{m \in D'_1 | x^2 - x^1 \geq t\}} n(m) \delta_m$, where we recall

that D' denotes the persistence diagram built from the sublevels sets of d_S . Since $D_{\geq \frac{s}{2}}$ is finite, there exists h_0 such that, for every $m \in D_{\geq s-h_0}$, $m \in D_{\geq s}$. At last, denote by $\tilde{B} = \min_{i \neq j} \|m_i - m_j\|_\infty$, where the m_j 's are the points of $D_{\geq s}$, and choose n large enough so that $h \leq \frac{h_0}{2} \wedge \frac{\tilde{B}}{2}$.

For such an h , we have, with probability larger than $1 - \alpha_N$ so that $\|d_{Y_N} - d_S\|_\infty \leq h$, for every $j \in \llbracket 1, k_0 \rrbracket$, $x_{i_1}^{(j)}, \dots, x_{i_{n_j}}^{(j)} \in D_{1, \geq s-h} \cap \mathcal{B}_\infty(m_j, h)$, and $|D_{1, \geq s-h}| = M$. To bound $M(\mathbb{E}(D_{1, \geq s-h}))$, note that, with probability larger than $1 - \alpha_N$, $M(D_{1, \geq s-h}) = M$, and with probability smaller than α_N , $M(D_{1, \geq s-h}) \leq N^d$, so that

$$|M(\mathbb{E}(D_{1, \geq s-h})) - M| \leq \alpha_N (M + N^d).$$

Next, we choose N large enough so that $|M(\mathbb{E}(D_{1, \geq s-h})) - M| \leq \frac{M}{2}$. Denoting by $\mathbf{m} = (m_1, \dots, m_{k_0})$, we have

$$R(\mathbf{m}) \leq 2h^2 M(1 - \alpha_N) + \alpha_N 4R^2 \times 3M/2 \leq 8Mh^2.$$

Now, if there exists j such that, for all $i \in \llbracket 1, k_0 \rrbracket$, $\|c_j - m_i\|_\infty > 8\sqrt{M}h$, then

$$R(\mathbf{c}) > (1 - \alpha_N)16Mh^2 \geq 8Mh^2 \geq R(\mathbf{m}).$$

8.2. Proof of Proposition 17

We let $\alpha_\ell = \left(\frac{1}{N_\ell}\right)^{d_\ell + \frac{2}{d_\ell}}$, and $A = \{\|d_{Y_{N_Z}} - d_{S_Z}\|_\infty > h_Z\}$, so that $\mathbb{P}(A \mid Z = \ell) \leq \alpha_\ell$. Also, let $m_{k_0+1}, \dots, m_{k_0+K_0(h)}$ be such that $\bigcup_{\ell=1}^L D_{\geq s}^{(\ell)} \setminus \{m_1, \dots, m_{k_0}\} \subset \bigcup_{s=1}^{K_0(h)} \mathcal{B}_\infty(m_{k_0+s}, h)$, and $\mathbf{m} = (m_1, \dots, m_{k_0+K_0(h)})$. At last, we let $R = \max_{\ell \leq L} \text{diam}(S_\ell)$. For N_ℓ large enough so that $D_{\geq s-h_\ell}^{(\ell)} = D_{\geq s}^{(\ell)}$ and $s/2 > h_\ell$, we have

$$\begin{aligned} R(\mathbf{m}) &= \mathbb{E} \left(\sum_{\ell=1}^L \mathbb{1}_{Z=\ell} X^{(\ell)}(du) \bullet \min_{j=1, \dots, k_0+K_0(h)} \|u - m_j\|^2 \right) \\ &= \mathbb{E} \left(\sum_{\ell=1}^L \mathbb{1}_{Z=\ell \cap A} X^{(\ell)}(du) \bullet \min_{j=1, \dots, k_0+K_0(h)} \|u - m_j\|^2 \right) \\ &\quad + \mathbb{E} \left(\sum_{\ell=1}^L \mathbb{1}_{Z=\ell \cap A^c} X^{(\ell)}(du) \bullet \min_{j=1, \dots, k_0+K_0(h)} \|u - m_j\|^2 \right), \end{aligned}$$

so that

$$\begin{aligned} R(\mathbf{m}) &\leq \mathbb{E} \left(\sum_{\ell=1}^L \mathbb{1}_{Z=\ell \cap A} 4R^2 N^{d_\ell} \right) + \mathbb{E} \left(\sum_{\ell=1}^L \mathbb{1}_{Z=\ell \cap A^c} M^{(\ell)} 2h_\ell^2 \right) \\ &\leq 2h^2 \bar{M} + 4R^2 \sum_{\ell=1}^L \pi_\ell \alpha_\ell N^{d_\ell}. \end{aligned}$$

For N_ℓ large enough so that $\alpha_\ell N_\ell^{d_\ell} \leq \frac{\bar{M}h_\ell^2}{R^2}$, we have $R(\mathbf{m}) \leq 6h^2\bar{M}$.

On the other hand, let \mathbf{c} be a k -points codebook such that, for every $p \in \llbracket 1, k \rrbracket$, $\|m_1 - c_p\|_\infty > 5\sqrt{\frac{\bar{M}}{\pi_{\min}}}h$. Then we have

$$\begin{aligned} R(\mathbf{c}) &\geq \mathbb{E} \left(\sum_{\ell=1}^L \mathbb{1}_{A^c \cap Z=\ell} X^{(\ell)}(\mathcal{B}_\infty(m_1, h)) \left(5\sqrt{\frac{\bar{M}}{\pi_{\min}}} - 1 \right)^2 \right) h^2 \\ &\geq \mathbb{E} \left(\sum_{\ell=1}^L \mathbb{1}_{A^c \cap Z=\ell} n^{(\ell)}(m_1) \left(5\sqrt{\frac{\bar{M}}{\pi_{\min}}} - 1 \right)^2 \right) h^2. \end{aligned}$$

Now let ℓ_0 be such that $n^{(\ell_0)}(m_1) \geq 1$, and assume that the N_ℓ 's are large enough so that $\alpha_\ell \leq \frac{1}{2}$. It holds

$$R(\mathbf{c}) \geq \left(5\sqrt{\frac{\bar{M}}{\pi_{\min}}} - 1 \right)^2 h^2 \pi_{\ell_0} (1 - \alpha_{\ell_0}) \geq 8\bar{M}h^2 > R(\mathbf{m}),$$

hence the result.

8.3. Proof of Proposition 18

We let $M = \max_{\ell \leq L} M_\ell$, h_0 be such that $\bar{D}_{\geq s-h_0} = \bar{D}_{\geq s}$. Let $\kappa \leq \frac{1}{16} \wedge \frac{h_0}{2\bar{B}}$. Under the assumptions of Proposition 17, we choose N_ℓ , $\ell \leq L$ large enough so that $5\sqrt{\bar{M}}h/(\sqrt{\pi_{\min}}) \leq \kappa\tilde{B}$. Next, denote by $\alpha_\ell = N_\ell^{-\left(\frac{(\kappa\tilde{B})^{d_\ell} f_{\min, \ell} N_\ell}{C_\ell d_\ell \log(N_\ell)}\right)}$. Then we have

$$\begin{aligned} \mathbb{P} \left(\exists i \in \llbracket 1, n \rrbracket \mid d_B(X_i, D_{\geq s}^{Z_i}) > \kappa\tilde{B} \right) &\leq \sum_{i=1}^n \mathbb{P} \left(d_B(X_i, D^{Z_i}) > \kappa\tilde{B} \right) \\ &\leq \sum_{i=1}^n \sum_{\ell=1}^L \pi_\ell \alpha_\ell \leq n \max_{\ell \leq L} \alpha_\ell. \end{aligned}$$

For the remaining of the proof we assume that, for $i = 1, \dots, n$, $d_B(X_i, D_{\geq s}^{Z_i}) \leq \kappa\tilde{B}$, that occurs with probability larger than $1 - n \max_{\ell \leq L} \alpha_\ell$. Let $i_1 \neq i_2$, and assume that $Z_{i_1} = Z_{i_2} = z$. Then $W_\infty(X_{i_1}, X_{i_2}) = d_B(X_{i_1}, X_{i_2}) \leq 2\kappa\tilde{B}$. Hence $W_1(X_{i_1}, X_{i_2}) \leq 2M\kappa\tilde{B}$.

Now assume that $Z_{i_1} \neq Z_{i_2}$, and without loss of generality $m_{Z_{i_1}, Z_{i_2}} = m_1$ with $D_{\geq s}^{Z_{i_1}}(\{m_1\}) \geq D_{\geq s}^{Z_{i_2}}(\{m_1\}) + 1$. Let (p, r) in $\mathbb{N}^* \times \mathbb{R}^+$ be such that $r/p \geq 2\kappa\tilde{B}$ and $4rp \leq (\frac{1}{2} - \kappa)\tilde{B}$. Since $\|c_1^* - m_1\|_\infty \leq \kappa\tilde{B}$ and $d_B(X_{i_1}, D_{\geq s}^{Z_{i_1}}) \leq \kappa\tilde{B} < h_0$, we get

$$X_{i_1} \left(\mathcal{B}(c_1^*, \frac{r}{p}) \right) = D_{\geq s}^{Z_{i_1}}(\{m_1\}).$$

On the other hand, since $4rp \leq (\frac{1}{2} - \kappa)\tilde{B}$, we also have $X_{i_2}(\mathcal{B}(c_1^*, 4rp)) = D_{\geq s}^{Z_{i_2}}(\{m_1\})$. Thus X_1, \dots, X_n is $(p, r, 1)$ -shattered by \mathbf{c}^* .

8.4. Proof of Corollary 19

In the case where $\Psi = \Psi_{AT}$, we have that Ψ_{AT} is a $(p, 1/p)$ kernel. The requirement $1/p \leq \frac{1}{4M}$ of Proposition 8 is thus satisfied for $p_{AT} = \lceil 4M \rceil$. On the other hand, choosing $r_{AT} = \frac{\tilde{B}}{32p_{AT}}$ ensures that $8r_{AT}p_{AT} \leq (1/2 - \kappa)\tilde{B}$ and $\frac{r_{AT}}{2p_{AT}} \geq 2\kappa\tilde{B}$, for κ small enough. Thus, the requirements of Proposition 18 are satisfied: \mathbf{c}^* is a $(2p_{AT}, r, 1)$ shattering of X_1, \dots, X_n . At last, using Corollary 11, we have that $\hat{\mathbf{c}}_n$ is a $(p_{AT}, r_{AT}, 1)$ shattering of X_1, \dots, X_n , on the probability event described by Corollary 11. It remains to note that $2\kappa\tilde{B} \leq \frac{r_{AT}}{4}$ for κ small enough to conclude that X_1, \dots, X_n is $\frac{r_{AT}}{4}$ -concentrated on the probability event described in Proposition 18. Thus Proposition 10 applies.

The case $\Psi = \Psi_0$ is simpler. Since Ψ_0 is a $(1, 0)$ -kernel, we obviously have that $0 \leq \frac{1}{2M}$, so that the requirement of Proposition 18 is satisfied. With $p_0 = 1$ and $r_0 = \frac{\tilde{B}}{16}$ we immediatly get that $r_0/(2p_0) \geq 2\kappa\tilde{B}$ and $8r_0p_0 \leq (1/2 - \kappa)\tilde{B}$, for κ small enough, so that $\hat{\mathbf{c}}$ is a $(p_0, r_0, 1)$ shattering of X_1, \dots, X_n . As well, $2M\kappa\tilde{B} \leq \frac{r_0}{4}$, for κ small enough. Thus Proposition 10 applies.

9. Technical proofs

9.1. Proofs for Section 6

A key ingredient of the proofs of Lemma 20 and 21 is the following Lemma 22, ensuring that around optimal codebooks the expected gradients of Algorithms 1 and 2 are almost Lischitz.

Lemma 22. *Assume that $\mathbb{E}(X) \in \mathcal{M}(R, M)$ satisfies a margin condition with radius r_0 , and denote by $R_0 = \frac{Br_0}{16\sqrt{2}R}$. Let $\mathbf{c}^* \in \mathcal{C}_{opt}$, and \mathbf{c} such that $\|\mathbf{c} - \mathbf{c}^*\| \leq R_0$. Then*

- $\sum_{j=1}^k |p_j(\mathbf{c}) - p_j(\mathbf{c}^*)| \leq \frac{p_{min}}{64}$,
- $\sum_{j=1}^k \|\mathbb{E}(X)(du)((u - c_j)\mathbb{1}_{W_j(\mathbf{c})}(u)) - p_j(\mathbf{c}^*)(c_j^* - c_j)\| \leq \frac{p_{min}}{8\sqrt{2}}\|\mathbf{c} - \mathbf{c}^*\|$.

The proof of Lemma 22 follows from [24, Section A.3].

9.1.1. Proof of Lemma 20

We adopt the following notation: for any $\mathbf{c} \in \mathcal{B}(0, R)^k$, we denote by $\hat{p}_j(\mathbf{c}) = \bar{X}_n(W_j(\mathbf{c}))$, as well as $p_j(\mathbf{c}) = \mathbb{E}(X)(W_j(\mathbf{c}))$. Moreover, we denote by $\hat{m}(\mathbf{c})$ (resp. $m(\mathbf{c})$) the codebooks satisfying, for $j \in \llbracket 1, k \rrbracket$,

$$\hat{m}(\mathbf{c})_j = \frac{\bar{X}_n(du)(u\mathbb{1}_{W_j(\mathbf{c})}(u))}{\hat{p}_j(\mathbf{c})}, \quad m(\mathbf{c})_j = \frac{\mathbb{E}(X)(du)(u\mathbb{1}_{W_j(\mathbf{c})}(u))}{p_j(\mathbf{c})},$$

if $\hat{p}_j(\mathbf{c}) > 0$ (resp. $p_j(\mathbf{c}) > 0$), and $\hat{m}(\mathbf{c})_j = 0$ (resp. $m(\mathbf{c})_j = 0$) if $\hat{p}_j(\mathbf{c}) = 0$ (resp. $p_j(\mathbf{c}) = 0$). The proof of Lemma 20 will make use of the following concentration lemma.

Lemma 23. *With probability larger than $1 - 8e^{-x}$, for all $\mathbf{c} \in \mathcal{B}(0, R)^k$,*

$$\begin{aligned}\hat{p}_j(\mathbf{c}) &\leq p_j(\mathbf{c}) + \sqrt{\frac{4Mc_0kd \log(k) \log(2nN_{max})}{n}} + \frac{4Mx}{n} \sqrt{p_j(\mathbf{c})} \\ \hat{p}_j(\mathbf{c}) &\geq p_j(\mathbf{c}) - \frac{4Mc_0kd \log(k) \log(2nN_{max})}{n} - \frac{4Mx}{n} \\ &\quad - \sqrt{\frac{4Mc_0kd \log(k) \log(2nN_{max})}{n}} + \frac{4Mx}{n} \sqrt{p_j(\mathbf{c})},\end{aligned}$$

where c_0 is an absolute constant. Moreover, with probability larger than $1 - e^{-x}$, we have

$$\begin{aligned}\sup_{\mathbf{c} \in \mathcal{B}(0, R)^k} &\| ((\bar{X}_n - \mathbb{E}(X))(du) \bullet [(c_j - u) \mathbb{1}_{W_j(\mathbf{c})}(u)])_{j=1, \dots, k} \| \\ &\leq \frac{CRM}{\sqrt{n}} \left(k\sqrt{d \log(k)} + \sqrt{x} \right),\end{aligned}$$

where C is a constant.

The proof of Lemma 23 is given in Section 9.1.3, and is based on empirical processes theory.

Proof of Lemma 20. Let $\mathbf{c} \in \mathcal{B}(\mathbf{c}^*, R_0)$, and

$$D_n = \sup_{\mathbf{c} \in \mathcal{B}(0, R)^k} \| ((\bar{X}_n - \mathbb{E}(X)) \bullet [(c_j - x) \mathbb{1}_{W_j(\mathbf{c})}(x)])_{j=1, \dots, k} \|.$$

We decompose $\|\hat{m}(\mathbf{c}) - \mathbf{c}^*\|^2$ as follows.

$$\|\hat{m}(\mathbf{c}) - \mathbf{c}^*\|^2 = \|\mathbf{c} - \mathbf{c}^*\|^2 + 2 \langle \hat{m}(\mathbf{c}) - \mathbf{c}, \mathbf{c} - \mathbf{c}^* \rangle + \|\hat{m}(\mathbf{c}) - \mathbf{c}\|^2. \quad (9)$$

Next, we bound the first term of (9).

$$\begin{aligned}2 \langle \hat{m}(\mathbf{c}) - \mathbf{c}, \mathbf{c} - \mathbf{c}^* \rangle &= 2 \sum_{j=1}^k \frac{1}{\hat{p}_j(\mathbf{c})} \langle \bar{X}_n(du) ((u - c_j) \mathbb{1}_{W_j(\mathbf{c})}(u)), c_j - c_j^* \rangle \\ &\leq 2 \sum_{j=1}^k \frac{1}{\hat{p}_j(\mathbf{c})} \langle \mathbb{E}(X)(du) ((u - c_j) \mathbb{1}_{W_j(\mathbf{c})}(u)), c_j - c_j^* \rangle \\ &\quad + 2D_n \sqrt{\sum_{j=1}^k \frac{\|c_j - c_j^*\|^2}{\hat{p}_j(\mathbf{c})^2}} \\ &\leq 2 \sum_{j=1}^k \frac{1}{\hat{p}_j(\mathbf{c})} \langle p_j(\mathbf{c}^*)(c_j^* - c_j), c_j - c_j^* \rangle \\ &\quad + \frac{2p_{min}}{8\sqrt{2}} \|\mathbf{c} - \mathbf{c}^*\| \sqrt{\sum_{j=1}^k \frac{\|c_j - c_j^*\|^2}{\hat{p}_j(\mathbf{c})^2}} + 2D_n \sqrt{\sum_{j=1}^k \frac{\|c_j - c_j^*\|^2}{\hat{p}_j(\mathbf{c})^2}},\end{aligned}$$

where the last line follows from Lemma 22. Now, using Lemma 23 with $x = c_1 n p_{min}/M$, for c_1 a small enough absolute constant, entails that, with probability larger than $1 - 8e^{c_1 n p_{min}/M}$, for n large enough and every $\mathbf{c} \in \mathcal{B}(\mathbf{c}^*, R_0)$,

$$\begin{aligned}\hat{p}_j(\mathbf{c}) &\geq \frac{63}{64}p_j(\mathbf{c}) - \frac{p_{min}}{64} \geq \frac{31}{32}p_{min} \\ \hat{p}_j(\mathbf{c}) &\leq \frac{33}{32}p_j(\mathbf{c}^*),\end{aligned}$$

according to Lemma 22. Therefore

$$\begin{aligned}2 \langle \hat{m}(\mathbf{c}) - \mathbf{c}, \mathbf{c} - \mathbf{c}^* \rangle &\leq -2 \sum_{j=1}^k \frac{p_j(\mathbf{c}^*)}{\hat{p}_j(\mathbf{c})} \|c_j - c_j^*\|^2 + \frac{32}{124\sqrt{2}} \|\mathbf{c} - \mathbf{c}^*\|^2 \\ &\quad + K_1 \|\mathbf{c} - \mathbf{c}^*\|^2 + K_1^{-1} \frac{32^2}{31^2 p_{min}^2} D_n^2, \quad (10)\end{aligned}$$

where $K_1 > 0$ is to be fixed later. Then, the second term of (9) may be bounded as follows.

$$\begin{aligned}\|\hat{m}(\mathbf{c}) - \mathbf{c}\|^2 &= \sum_{j=1}^k \frac{\|\bar{X}_n(du)((u - c_j)\mathbb{1}_{W_j(\mathbf{c})}(u))\|^2}{\hat{p}_j(\mathbf{c})^2} \\ &= \sum_{j=1}^k \frac{\|p_j(\mathbf{c}^*)(c_j - c_j^*) + \Delta_j(\mathbf{c}) + \Delta_{n,j}(\mathbf{c})\|^2}{\hat{p}_j(\mathbf{c})^2},\end{aligned}$$

where

$$\Delta_j(\mathbf{c}) = \mathbb{E}(X)(du) \bullet [(u - c_j)\mathbb{1}_{W_j(\mathbf{c})}(u) - (u - c_j^*)\mathbb{1}_{W_j(\mathbf{c}^*)}(u)],$$

so that $\sum_{j=1}^k \|\Delta_j(\mathbf{c})\| \leq \frac{p_{min}}{8\sqrt{2}} \|\mathbf{c} - \mathbf{c}^*\|$, according to Lemma 22, and

$$\Delta_{n,j}(\mathbf{c}) = (\bar{X}_n - \mathbb{E}(X))(du) \bullet ((u - c_j)\mathbb{1}_{W_j(\mathbf{c})}(u)),$$

so that $\sum_{j=1}^k \|\Delta_{n,j}\|^2 \leq D_n^2$. Thus,

$$\begin{aligned}\|\hat{m}(\mathbf{c}) - \mathbf{c}\|^2 &\leq (1 + K_2 + K_3) \sum_{j=1}^k \frac{p_j(\mathbf{c}^*)^2}{\hat{p}_j(\mathbf{c})^2} \|c_j - c_j^*\|^2 + (1 + K_2^{-1} + K_4) \sum_{j=1}^k \frac{\|\Delta_j(\mathbf{c})\|^2}{\hat{p}_j(\mathbf{c})^2} \\ &\quad + (1 + K_3^{-1} + K_4^{-1}) \sum_{j=1}^k \frac{\|\Delta_{n,j}(\mathbf{c})\|^2}{\hat{p}_j(\mathbf{c})^2} \\ &\leq (1 + K_2 + K_3) \sum_{j=1}^k \frac{p_j(\mathbf{c}^*)^2}{\hat{p}_j(\mathbf{c})^2} \|c_j - c_j^*\|^2 + (1 + K_2^{-1} + K_4) \frac{32^2}{31^2 \times 128} \|\mathbf{c} - \mathbf{c}^*\|^2 \\ &\quad + (1 + K_3^{-1} + K_4^{-1}) \frac{32^2}{31^2 p_{min}^2} D_n^2, \quad (11)\end{aligned}$$

wherer K_2 , K_3 and K_4 are positive constants to be fixed later. Combining (10) and (11) yields that

$$\begin{aligned} \|\hat{m}(\mathbf{c}) - \mathbf{c}^*\|^2 &\leq \|\mathbf{c} - \mathbf{c}^*\|^2 \left(1 + K_1 + \frac{32}{124\sqrt{2}} + \frac{32^2}{31^2 \times 128} (1 + K_2^{-1} + K_4) \right) \\ &\quad - 2 \sum_{j=1}^k \frac{p_j(\mathbf{c}^*)}{\hat{p}_j(\mathbf{c})} \|c_j - c_j^*\|^2 + (1 + K_2 + K_3) \sum_{j=1}^k \frac{p_j(\mathbf{c}^*)^2}{\hat{p}_j(\mathbf{c})^2} \|c_j - c_j^*\|^2 \\ &\quad + D_n^2 \frac{32^2}{31^2 p_{min}^2} (1 + K_1^{-1} + K_3^{-1} + K_4^{-1}). \end{aligned}$$

Taking $K_2 = \frac{1}{32}$ gives, through numerical computation,

$$\begin{aligned} \|\hat{m}(\mathbf{c}) - \mathbf{c}^*\|^2 &\leq \|\mathbf{c} - \mathbf{c}^*\|^2 \left(0.62 + K_1 + K_3 \frac{32^2}{31^2} + K_4 \frac{32^2}{31^2 \times 128} \right) \\ &\quad + D_n^2 \frac{32^2}{31^2 p_{min}^2} (1 + K_1^{-1} + K_3^{-1} + K_4^{-1}) \\ &\leq \frac{3}{4} \|\mathbf{c} - \mathbf{c}^*\|^2 + \frac{K}{p_{min}^2} D_n^2, \end{aligned}$$

for K_1 , K_3 and K_4 small enough. Now, according to Lemma 23, it holds

$$\frac{K}{p_{min}^2} D_n^2 \leq \frac{R_0^2}{4},$$

with probability larger than $1 - e^{-c_1 n p_{min}^2 \kappa_0^2 / M^2}$, for some constant c_1 small enough.

Recalling that, for any t , $\mathbf{c}^{(t+1)} = \hat{m}(\mathbf{c}^{(t)})$, a straightforward recursion entails that, on a global probability event that has probability larger than $1 - 9e^{-cn\kappa_0^2 p_{min}^2 / M^2} - e^{-x}$, for c small enough, provided that $\mathbf{c}^{(0)} \in \mathcal{B}(\mathbf{c}^*, R_0)$, we have for any $t \geq 0$ $\mathbf{c}^{(t)} \in \mathcal{B}(\mathbf{c}^*, R_0)$ and

$$\begin{aligned} \|\mathbf{c}^{(t+1)} - \mathbf{c}^*\|^2 &\leq \frac{3}{4} \|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2 + \frac{K}{p_{min}^2} D_n^2 \\ &\leq \frac{3}{4} \|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2 + \frac{K}{p_{min}^2} \frac{C^2 R^2 M^2}{n} \left(k \sqrt{d \log(k)} + \sqrt{x} \right)^2. \end{aligned}$$

□

9.1.2. Proof of Lemma 21

The proof of Lemma 21 will make use of the following deviation bounds.

Lemma 24. *Let $\mathbf{c} \in \mathcal{B}(0, R)^k$. Then, with probability larger than $1 - 2ke^{-x}$, we have, for all $j = 1, \dots, k$,*

$$|\hat{p}_j(\mathbf{c}) - p_j(\mathbf{c})| \leq \sqrt{\frac{2M p_j(\mathbf{c}) x}{n}} + \frac{Mx}{n}.$$

Moreover, with probability larger than $1 - e^{-x}$, we have,

$$\left\| (\bar{X}_n - \mathbb{E}(X))(du) \bullet ((c_j - u) \mathbb{1}_{W_j(\mathbf{c})}(u))_{j=1, \dots, k} \right\| \leq \frac{4RM\sqrt{k}}{\sqrt{n}} (1 + \sqrt{x}).$$

A proof of Lemma 24 is given in Section 9.1.4.

Proof of Lemma 21. Assume that $n \geq k$, and let $n_t = |B_t|/2 \geq \frac{CM}{p_{\min}} \log(n)$, for C large enough to be fixed later. For a given $t \leq T$, denote by $\hat{p}_j^{(t)} = \bar{X}_{B_t^{(1)}}(W_j(\mathbf{c}^{(t)}))$, and by $A_{t,1}$ and $A_{t,2}$ the events

$$\begin{aligned} A_{t,1} &= \left\{ \forall j = 1, \dots, k \quad |\hat{p}_j^{(t)} - p_j^{(t)}| \leq \frac{p_{\min} + \sqrt{p_j^{(t)} p_{\min}}}{256} \right\}, \\ A_{t,2} &= \left\{ \forall j = 1, \dots, k \quad \left\| (\bar{X}_{B_t^{(2)}} - \mathbb{E}(X))(du) \bullet ((c_j^{(t)} - u) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u))_j \right\| \leq 8R\sqrt{\frac{Mkp_{\min}}{C}} \right\}. \end{aligned}$$

According to Lemma 24 with $x = 4 \log(2n)$, we have $\mathbb{P}(A_{t,j}^c) \leq k/(2n^4)$, for $j = 1, 2$. We let also $A_{\leq t}$ denote the event $\cap_{r \leq t} A_{r,1} \cap A_{r,2}$, that has probability larger than $1 - kt/n^4$. First we prove that if $\mathbf{c}^{(0)} \in \mathcal{B}(\mathbf{c}^*, R_0)$, then, on $A_{\leq t}$, for all $r \leq t$, $\mathbf{c}^{(r)} \in \mathcal{B}(\mathbf{c}^*, R_0)$. We proceed recursively, assuming that $\mathbf{c}^{(t)} \in \mathcal{B}(\mathbf{c}^*, R_0)$. Then, on $A_{\leq t+1}$, applying Lemma 22 yields that $\frac{33}{32}p_j^* \geq \hat{p}_j^t \geq \frac{31}{32}p_j^*$. Denoting by $a_t = \|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2$ and $g_{t+1} = \left(\frac{\bar{X}_{B_{t+1}^{(2)}}(du) \bullet (c_j^{(t)} - u) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u)}{\hat{p}_j^{t+1}} \right)_j$, the recursion equation entails that

$$\begin{aligned} a_{t+1} &= \|\pi_{B(0,R)^k} \left(\mathbf{c}^{(t)} - \frac{g_{t+1}}{t+1} \right) - \mathbf{c}^*\|^2 \\ &\leq \|\mathbf{c}^{(t)} - \frac{g_{t+1}}{t+1} - \mathbf{c}^*\|^2 = a_t - \frac{2}{t+1} \langle g_{t+1}, \mathbf{c} - \mathbf{c}^* \rangle + \frac{1}{(t+1)^2} \|g_{t+1}\|^2. \end{aligned} \tag{12}$$

As in the proof of Lemma 20, denote by

$$\begin{aligned} \Delta_j^t &= \mathbb{E}(X)(du) \bullet \left((u - c_j^{(t)}) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u) \right) - p_j^*(c_j^* - c_j^{(t)}) \\ \Delta_{n,j}^{t+1} &= (\bar{X}_{B_{t+1}^{(2)}} - \mathbb{E}(X))(du) \bullet (u - c_j^{(t)}) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u) \\ D_n^{t+1} &= \sqrt{\sum_{j=1}^k \|\Delta_{n,j}^{t+1}\|^2}. \end{aligned}$$

We have that

$$\begin{aligned}
-\frac{2}{t+1} \langle g_{t+1}, \mathbf{c} - \mathbf{c}^* \rangle &\leq -\frac{2}{t+1} \sum_{j=1}^k \left(\frac{p_j^*}{\hat{p}_j^{t+1}} \|c_j^{(t)} - c_j^*\|^2 - \frac{\|\Delta_{j,n}^{t+1}\| \|c_j^{(t)} - c_j^*\|}{\hat{p}_j^{t+1}} \right. \\
&\quad \left. - \frac{\|c_j^{(t)} - c_j^*\| \|\Delta_j^t\|}{\hat{p}_j^{t+1}} \right) \\
&\leq -2 \frac{32}{33(t+1)} \|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2 + \frac{64}{31p_{\min}(t+1)} \|\mathbf{c}^{(t)} - \mathbf{c}^*\| D_n^{t+1} \\
&\quad + \frac{64}{8\sqrt{2} \times 31(t+1)} \|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2 \\
&\leq \|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2 \left(\frac{-64}{33(t+1)} + \frac{K_4}{t+1} + \frac{64}{8\sqrt{2} \times 31(t+1)} \right) + K_4^{-1} \left(\frac{32}{31p_{\min}} D_n^{t+1} \right)^2,
\end{aligned}$$

according to Lemma 22, where K_4 denotes a constant. Next, the second term in (12) may be bounded by

$$\begin{aligned}
\|g_{t+1}\|^2 &\leq \sum_{j=1}^k \frac{1}{(\hat{p}_j^{t+1})^2} (p_j^*)^2 \|c_j^{(t)} - c_j^*\|^2 (1 + K_1 + K_2) \\
&\quad + \frac{p_{\min}^2}{128 \min_j (\hat{p}_j^{t+1})^2} \|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2 (1 + K_2^{-1} + K_3) + \frac{1}{\min_j (\hat{p}_j^{t+1})^2} (1 + K_1^{-1} + K_3^{-1}) (D_n^{t+1})^2 \\
&\leq \frac{32^2}{31^2} \|\mathbf{c}^{(t)} - \mathbf{c}^*\|^2 \left(1 + K_1 + K_2 + \frac{1 + K_2^{-1} + K_3}{128} \right) + (D_n^{t+1})^2 \frac{32^2(1 + K_1^{-1} + K_3^{-1})}{31^2 p_{\min}^2},
\end{aligned}$$

where K_1 , K_2 and K_3 are constants to be fixed later. Combining pieces and using $t+1 \geq 1$ leads to

$$\begin{aligned}
a_{t+1} &\leq a_t + \frac{a_t}{t+1} \left(\frac{-64}{33} + \frac{64}{8\sqrt{2} \times 31} + K_4 + \frac{32^2}{31^2} \left(1 + K_1 + K_2 + \frac{1 + K_2^{-1} + K_3}{128} \right) \right) \\
&\quad + (D_n^{t+1})^2 \left(\frac{32^2}{31^2 p_{\min}^2} K_4^{-1} + \frac{32^2(1 + K_1^{-1} + K_3^{-1})}{31^2 p_{\min}^2} \right).
\end{aligned}$$

Choosing $K_2 = \frac{1}{32}$ entails that

$$\begin{aligned}
\left(\frac{-64}{33} + \frac{64}{8\sqrt{2} \times 31} + K_4 + \frac{32^2}{31^2} \left(1 + K_1 + K_2 + \frac{1 + K_2^{-1} + K_3}{128} \right) \right) \\
\leq -0.38 + K_4 + \frac{32^2}{31^2} \left(K_1 + \frac{K_3}{128} \right),
\end{aligned}$$

so that, for K_1 , K_3 and K_4 small enough, we have

$$a_{t+1} \leq 0.8a_t + \frac{K}{p_{\min}^2} (D_n^{t+1})^2.$$

Now, if $n_t \geq c_0 \frac{k^2 M^2}{p_{\min}^2 \kappa_0^2} \log(n)$, $n \geq k$, where c_0 is an absolute constant, on $A_{\leq t+1}$ we have

$$a_{t+1} \leq 0.8a_t + 0.2R_0^2 \leq R_0^2.$$

Thus, provided that $\mathbf{c}^{(0)} \in \mathcal{B}(\mathbf{c}^*, R_0)$, on $A_{\leq t}$ we have $\mathbf{c}^{(p)} \in \mathcal{B}(\mathbf{c}^*, R_0)$, for $p \leq t$.

Next, if \mathcal{F}_t denotes the sigma-algebra corresponding to the observations of the t first mini-batches B_1, \dots, B_t , and E_t denotes the conditional expectation with respect to \mathcal{F}_t . We will show that

$$\mathbb{E}a_{t+1} \leq \left(1 - \frac{2 - K_1}{t+1}\right) \mathbb{E}a_t + \frac{16kMR^2}{p_{\min}(t+1)^2},$$

where $K_1 < 0.5$. First, we may write

$$\mathbb{E}a_{t+1} = \mathbb{E}(a_{t+1} \mathbb{1}_{A_{\leq t}} \mathbb{1}_{A_{t+1,1}}) + R_1,$$

with $R_1 \leq (4k^2 R^2)/n^3 \leq 4kMR^2/(p_{\min}(t+1)^2)$, since $p_{\min} \leq M/k$ and $t+1 \leq T \leq n$. Then, using (12) entails

$$\begin{aligned} \mathbb{E}(a_{t+1} \mathbb{1}_{A_{\leq t} \cap A_{t+1,1}}) &\leq \mathbb{E}a_t - \frac{2}{t+1} \mathbb{E}\left(\langle g_{t+1}, \mathbf{c}^{(t)} - \mathbf{c}^* \rangle \mathbb{1}_{A_{\leq t} \cap A_{t+1,1}}\right) \\ &\quad + \frac{1}{(t+1)^2} \mathbb{E}(\|g_{t+1}\|^2 \mathbb{1}_{A_{\leq t} \cap A_{t+1,1}}). \end{aligned}$$

Next, we bound the scalar product as follows.

$$\begin{aligned} &\mathbb{E}\left(\langle -g_{t+1}, \mathbf{c}^{(t)} - \mathbf{c}^* \rangle \mathbb{1}_{A_{\leq t} \cap A_{t+1,1}}\right) \\ &= \mathbb{E}\left(\mathbb{1}_{A_{\leq t}} \sum_{j=1}^k E_t \left(\frac{\left\langle \bar{X}_{B_{t+1}^{(2)}}(du) \bullet (u - c_j^{(t)}) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u), c_j^{(t)} - c_j^* \right\rangle}{\hat{p}_j^{t+1}} \mathbb{1}_{A_{t+1,1}} \right)\right), \end{aligned}$$

where, for any $j \in \llbracket 1, k \rrbracket$, we have

$$\begin{aligned} &E_t \left(\frac{\left\langle \bar{X}_{B_{t+1}^{(2)}}(du) \bullet (u - c_j^{(t)}) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u), c_j^{(t)} - c_j^* \right\rangle}{\hat{p}_j^{t+1}} \mathbb{1}_{A_{t+1,1}} \right) \\ &= E_t \left(\left\langle \bar{X}_{B_{t+1}^{(2)}}(du) \bullet (u - c_j^{(t)}) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u), c_j^{(t)} - c_j^* \right\rangle \right) E_t \left(\frac{1}{\hat{p}_j^{t+1}} \mathbb{1}_{A_{t+1,1}} \right). \end{aligned}$$

The first term may be bounded by

$$\begin{aligned} E_t \left(\left\langle \bar{X}_{B_{t+1}^{(2)}}(du) \bullet (u - c_j^{(t)}) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u), c_j^{(t)} - c_j^* \right\rangle \right) \mathbb{1}_{A_{\leq t}} &\leq -p_j^* \|c_j^{(t)} - c_j^*\|^2 \mathbb{1}_{A_{\leq t}} \\ &\quad + \|\Delta_{j,t}\| \|c_j^{(t)} - c_j^*\|, \end{aligned}$$

and the second term by

$$\frac{32}{33p_j^*} \mathbb{1}_{A_{\leq t}} \leq E_t \left(\frac{1}{\hat{p}_j^{t+1}} \mathbb{1}_{A_{t+1,1}} \right) \mathbb{1}_{A_{\leq t}} \leq \frac{32}{31p_j^*}.$$

This gives

$$\begin{aligned} \mathbb{E} \left(\left\langle -g_{t+1}, \mathbf{c}^{(t)} - \mathbf{c}^* \right\rangle \mathbb{1}_{A_{\leq t} \cap A_{t+1,1}} \right) &\leq -\frac{32}{33} \mathbb{E} (a_t \mathbb{1}_{A_{\leq t}}) + \frac{32}{31p_{\min}} \mathbb{E} \left(\sum_{j=1}^k \|\Delta_{j,t}\| \|c_j^{(t)} - c_j^*\| \mathbb{1}_{A_{\leq t}} \right) \\ &\leq -\frac{32}{33} \mathbb{E}(a_t) + \frac{32}{31 \times 8\sqrt{2}} \mathbb{E}(a_t) + \frac{32}{33} \frac{4k^2 R^2}{n^3}, \end{aligned}$$

according to Lemma 22. At last, the bound on $\|g_{t+1}\|^2$ writes as follows.

$$\begin{aligned} \mathbb{E} (\|g_{t+1}\|^2 \mathbb{1}_{A_{\leq t} \cap A_{t+1,1}}) &= \mathbb{E} (\mathbb{1}_{A_{\leq t}} E_t (\|g_{t+1}\|^2 \mathbb{1}_{A_{t+1,1}})) \\ &\leq \frac{32}{31} \frac{4kMR^2}{p_{\min}}. \end{aligned}$$

Gathering all pieces leads to

$$\mathbb{E}a_{t+1} \leq \left(1 - \frac{2 - K_1}{t+1}\right) \mathbb{E}a_t + \frac{16kMR^2}{p_{\min}(t+1)^2},$$

with $K_1 \leq 0.5$.

At last, in the point sample case where we observe n points in \mathbb{R}^d X_1, \dots, X_n i.i.d with distribution X , recall that we take

$$\mathbf{c}^{(t+1)} = \mathbf{c}^{(t)} - \frac{g_{t+1}}{t+1}, \quad \text{with} \quad g_{t+1} = \frac{\bar{X}_{B_{t+1}}(du) \bullet (c_j^{(t)} - u) \mathbb{1}_{W_j(\mathbf{c}^{(t)})(u)}}{\hat{p}_j^{t+1}}.$$

With a slight abuse of notation we denote by $A_{\leq t}$ the event onto which the concentration inequalities of Lemma 24 are satisfied (with $B_t^{(1)} = B_t^{(2)} = B_t$). The first step of the proof is the same: if $n_t \geq c_0 \frac{k}{p_{\min}^2 \kappa_0^2}$ and $n \geq k$, then, on $A_{\leq t}$, for all $j \leq t$, $a_j \leq R_0$. It remains to prove the recursion inequality

$$\mathbb{E}a_{t+1} \leq \left(1 - \frac{2 - K_1}{t+1}\right) \mathbb{E}a_t + \frac{16kR^2}{p_{\min}(t+1)^2}.$$

We proceed as before, writing $\mathbb{E}(a_{t+1}) = \mathbb{E}(a_{t+1} \mathbb{1}_{A_{\leq t}}) + R_1$, with $R_1 \leq 4kR^2/(p_{\min}(t+1)^2)$, and

$$\mathbb{E}(a_{t+1} \mathbb{1}_{A_{\leq t}}) \leq \mathbb{E}a_t + \frac{1}{(t+1)^2} \mathbb{E}(\|g_{t+1}\|^2) - \frac{2}{t+1} \mathbb{E} \left(\left\langle g_{t+1}, \mathbf{c}^{(t)} - \mathbf{c}^* \right\rangle \mathbb{1}_{A_{\leq t}} \right).$$

Note that $\|g_{t+1}\|^2 \leq 4kR^2$, so that the second term might be bounded by $4kR^2/(t+1)^2$. To bound the scalar product, we proceed as follows. Let $j \in [1, k]$,

and, for $i \in B_{t+1}$, denote by $U_{i,j}$ the random variable $\mathbb{1}_{W_j(\mathbf{c}^{(t)})}(X_i)$. We have

$$\begin{aligned}
& \mathbb{E} \left(\left\langle \frac{\bar{X}_{B_{t+1}}(du) \bullet (u - c_j^{(t)}) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u), c_j^{(t)} - c_j^*}{\hat{p}_j^{t+1}} \mathbb{1}_{A_{\leq t}} \right\rangle \right) \\
&= \mathbb{E} \left(\frac{\mathbb{1}_{A_{\leq t}}}{\hat{p}_j^{t+1}} \left\langle \mathbb{E} \left[\bar{X}_{B_{t+1}}(du) \bullet (u - c_j^{(t)}) \mathbb{1}_{W_j(\mathbf{c}^{(t)})}(u) \mid \mathcal{F}_t, (U_{i,j})_{i \in B_{t+1}} \right], c_j^{(t)} - c_j^* \right\rangle \right) \\
&= \mathbb{E} \left(\frac{\mathbb{1}_{A_{\leq t}}}{n_{t+1} \hat{p}_j^{t+1}} \sum_{i \in B_{t+1}} U_{i,j} \left[-\frac{p_j^*}{p_j^t} \|c_j^{(t)} - c_j^*\|^2 + \frac{\langle \Delta_{j,t}, c_j^{(t)} - c_j^* \rangle}{p_j^t} \right] \right) \\
&\leq -\frac{32}{33} \mathbb{E}(\|c_j^* - c_j\|^2 \mathbb{1}_{A_{\leq t}}) + \frac{32}{31 p_{\min}} \mathbb{E}(\|\Delta_{j,t}\| \|c_j^t - c_j^*\| \mathbb{1}_{A_{\leq t}}).
\end{aligned}$$

The remaining of the proof is the same as for the sample measure case. \square

9.1.3. Proof of Lemma 23

Let Z_1 denote the process

$$Z_1 = \sup_{\mathbf{c} \in \mathcal{B}(0,R)^k, j=1, \dots, k} \left| \left(\frac{\bar{X}_n}{M} - \frac{\mathbb{E}(X)}{M} \right) \mathbb{1}_{W_j(\mathbf{c})} \right|.$$

Note that the VC dimensions of Voronoi cells in a k -points Voronoi diagram is at most $c_0 k d \log(k)$ ([41, Theorem 1.1]). We first use a symmetrization bound.

Lemma 25. *Let \mathcal{F} denote a class of functions taking values in $[0, 1]$, and $X_1, \dots, X_n, X'_1, \dots, X'_n$ i.i.d random variables drawn from P . Denote by P_n and P'_n the empirical distributions associated to the X_i 's and X'_i 's. If $nt^2 \geq 1$, then*

$$\begin{aligned}
\mathbb{P} \left(\sup_{f \in \mathcal{F}} \frac{(P - P_n)f}{\sqrt{P_n f}} \geq 2t \right) &\leq 2\mathbb{P} \left(\sup_{f \in \mathcal{F}} \frac{(P'_n - P_n)f}{\sqrt{(P'_n f + P_n f)/2}} \geq t \right) \\
\mathbb{P} \left(\sup_{f \in \mathcal{F}} \frac{(P_n - P)f}{\sqrt{P_n f}} \geq 2t \right) &\leq 2\mathbb{P} \left(\sup_{f \in \mathcal{F}} \frac{(P_n - P'_n)f}{\sqrt{(P'_n f + P_n f)/2}} \geq t \right).
\end{aligned}$$

For the sake of completeness a proof of Lemma 25 is given in Section 9.1.5. Next, introducing $\sigma_1, \dots, \sigma_n$ independent Rademacher variables, we get

$$\begin{aligned}
\mathbb{P} \left(\sup_{f \in \mathcal{F}} \frac{(P'_n - P_n)f}{\sqrt{(P'_n f + P_n f)/2}} \geq t \right) &\leq \mathbb{P} \left(\sup_{f \in \mathcal{F}} \frac{\frac{1}{n} \sum_{i=1}^n \sigma_i (f(X_i) - f(X'_i))}{\sqrt{(P'_n f + P_n f)/2}} \geq t \right) \\
&\leq \mathbb{E}_{X_1, \dots, X_n, X'_1, \dots, X'_n} \left(\mathbb{P}_\sigma \left(\sup_{f \in \mathcal{F}} \frac{\frac{1}{n} \sum_{i=1}^n \sigma_i (f(X_i) - f(X'_i))}{\sqrt{(P'_n f + P_n f)/2}} \geq t \right) \right).
\end{aligned}$$

For a set of functions \mathcal{F} and elements $x_1, \dots, x_q \in \mathcal{M}(R)$ we denote by $S_{\mathcal{F}}(x_1, \dots, x_q)$ the cardinality of the set $\{(f(x_1), \dots, f(x_q)) \mid f \in \mathcal{F}\}$. Let \mathcal{F}_1 denote the sets of

functions $\{X \in \mathcal{M}(R, M) \mapsto X(W)/M \mid W = \bigcap_{j=1}^k H_j, H_j \text{ half-space}\}$. Since, for every $i \in \llbracket 1, n \rrbracket$, $X_i = \sum_{j=1}^{n_i} \mu_{i,j} \delta_{x_j^{(i)}}$, we have

$$\begin{aligned} S_{\mathcal{F}_1}(X_1, \dots, X_n, X'_1, \dots, X'_n) &\leq |\{(\mathbb{1}_W(x_j^{(i)}))_{i=1, \dots, 2n, j=1, \dots, n_i} \mid W = \bigcap_{j=1}^k H_j, H_j \text{ half-space}\}| \\ &\leq \left(2 \left(\sum_{i=1}^n n_i + n'_i \right) \right)^{c_0 k d \log(k)}, \end{aligned}$$

using [29, Theorem 1], and [41, Theorem 1] to bound the VC-dimension of the sets W 's. On the other hand, for any $f \in \mathcal{F}_1$, it holds

$$\frac{\sum_{i=1}^n (f(X'_i) - f(X_i))^2}{\sum_{i=1}^n (f(X_i) + f(X'_i))} \leq 1.$$

Thus, combining Hoeffding's inequality and a plain union bound yields

$$\left(\mathbb{P}_\sigma \left(\sup_{f \in \mathcal{F}} \frac{\frac{1}{n} \sum_{i=1}^n \sigma_i (f(X_i) - f(X'_i))}{\sqrt{(P'_n f + P_n f)/2}} \geq t \right) \right) \leq \left(2 \sum_{i=1}^n (n_i + n'_i) \right)^{c_0 k d \log(k)} e^{-nt^2},$$

hence, since for $i = 1, \dots, n$, $X_i \in \mathcal{M}_{N_{max}}(R, M)$,

$$\mathbb{P} \left(\sup_{f \in \mathcal{F}} \frac{(P'_n - P_n) f}{\sqrt{(P'_n f + P_n f)/2}} \geq t \right) \leq (4nN_{max})^{c_0 k d \log(k)} e^{-nt^2},$$

that proves the second inequality of Lemma 23. The first inequality of Lemma 23 derives the same way from the second inequality of Lemma 25.

We turn to the third inequality of Lemma 23. Let Z denote the process

$$Z = \sup_{\mathbf{c} \in \mathcal{B}(0, R)^k, \|\mathbf{t}\| \leq 1} \left\langle \left(\frac{\bar{X}_n}{M} - \frac{\mathbb{E}(X)}{M} \right) \bullet [(c_j - u) \mathbb{1}_{W_j(\mathbf{c})}(u)]_{j=1, \dots, k}, \mathbf{t} \right\rangle,$$

and, for $j = 1, \dots, k$,

$$Z_j = \sup_{\mathbf{c} \in \mathcal{B}(0, R)^k, \|t_j\| \leq 1} \left\langle \frac{1}{M} (\bar{X}_n - \mathbb{E}(X)) \bullet [(c_j - u) \mathbb{1}_{W_j(\mathbf{c})}(u)], t_j \right\rangle,$$

so that $Z \leq \sqrt{\sum_{j=1}^k Z_j^2}$. According to the bounded differences inequality ([6, Theorem 6.2]), we have

$$\mathbb{P} \left(Z_j \geq \mathbb{E}(Z_j) + \sqrt{\frac{8R^2}{n} x} \right) \leq e^{-x}.$$

Using symmetrization we get

$$\mathbb{E} Z_j \leq \frac{2}{n} \mathbb{E}_{X_1, \dots, X_n} \mathbb{E}_\sigma \sup_{\mathbf{c} \in \mathcal{B}(0, R)^k, \|t_j\| \leq 1} \sum_{i=1}^n \sigma_i \left\langle \frac{X_i}{M} \bullet [(c_j - \cdot) \mathbb{1}_{W_j(\mathbf{c})}(\cdot)], t_j \right\rangle,$$

where $\sigma_1, \dots, \sigma_n$ are i.i.d Rademacher variables. Now assume that X_1, \dots, X_n is fixed and $j = 1$. For a set \mathcal{F} of real-valued functions we denote by $\mathcal{N}(\mathcal{F}, \varepsilon, \|\cdot\|)$ its ε -covering number with respect to the norm $\|\cdot\|$. Denoting by Γ_0, Γ_1 and Γ_2 the following sets

$$\begin{aligned}\Gamma_0 &= \left\{ \gamma_{(\mathbf{c}, t_1)}^{(0)} : X \mapsto \frac{X}{M} \bullet \left[\frac{\langle c_1 - \cdot, t_1 \rangle}{2R} \mathbb{1}_{W_1(\mathbf{c})}(\cdot) \right] \mid \mathbf{c} \in \mathcal{B}(0, R)^k, t_1 \in \mathcal{B}(0, 1) \right\}, \\ \Gamma_1 &= \left\{ \gamma_{(c_1, t_1)}^{(1)} : x \mapsto \frac{\langle c_1 - x, t_1 \rangle}{2R} \mid c_1 \in \mathcal{B}(0, R), t_1 \in \mathcal{B}(0, 1) \right\}, \\ \Gamma_2 &= \left\{ \gamma_{\mathbf{c}'}^{(2)} : x \mapsto \mathbb{1}_{W_1(\mathbf{c})}(x) \mid \mathbf{c} \in \mathcal{B}(0, R)^k \right\},\end{aligned}$$

so that, for every $(\mathbf{c}, t_1), (\mathbf{c}', t_1') \in (\mathcal{B}(0, R)^k \times \mathcal{B}(0, 1))^2$,

$$\gamma_{(\mathbf{c}, t_1)}^{(0)}(X_i) - \gamma_{(\mathbf{c}', t_1')}^{(0)}(X_i) = \frac{X_i}{M} \bullet \left[\gamma_{(c_1, t_1)}^{(1)}(\cdot) \gamma_{\mathbf{c}}^{(2)}(\cdot) - \gamma_{(c_1', t_1')}^{(1)}(\cdot) \gamma_{\mathbf{c}'}^{(2)}(\cdot) \right].$$

Let $\varepsilon > 0$. If $\|\gamma_{(c_1, t_1)}^{(1)} - \gamma_{(c_1', t_1')}^{(1)}\|_\infty \leq \varepsilon$, we may write

$$\left(\gamma_{(\mathbf{c}, t_1)}^{(0)}(X_i) - \gamma_{(\mathbf{c}', t_1')}^{(0)}(X_i) \right)^2 \leq \left(\varepsilon + \frac{X_i}{M} \bullet \left[|\gamma_{\mathbf{c}}^{(2)} - \gamma_{\mathbf{c}'}^{(2)}| \right] \right)^2.$$

Thus,

$$\begin{aligned}\|\gamma_{(\mathbf{c}, t_1)}^{(0)} - \gamma_{(\mathbf{c}', t_1')}^{(0)}\|_{L_2(P_n)}^2 &\leq 2\varepsilon^2 + \frac{2}{n} \sum_{j=1}^n \|\gamma_{\mathbf{c}}^{(2)} - \gamma_{\mathbf{c}'}^{(2)}\|_{L_2(X_j/M)}^2 \\ &\leq 2\varepsilon^2 + 2\|\gamma_{\mathbf{c}}^{(2)} - \gamma_{\mathbf{c}'}^{(2)}\|_{L_2(\bar{X}_n/M)}^2 \\ &\leq 2\varepsilon^2 + 2\|\gamma_{\mathbf{c}}^{(2)} - \gamma_{\mathbf{c}'}^{(2)}\|_{L_2(\bar{X}_n/M(\bar{X}_n))}^2.\end{aligned}$$

We deduce

$$\mathcal{N}(\Gamma_0, \varepsilon, L_2(P_n)) \leq \mathcal{N}(\Gamma_1, \varepsilon/2, \|\cdot\|_\infty) \times \mathcal{N}(\Gamma_2, \varepsilon/2, L_2(\bar{X}_n/M(\bar{X}_n))),$$

for every $\varepsilon > 0$. According to [29, Theorem 1], we may write

$$\begin{aligned}\mathcal{N}\left(\Gamma_1, \frac{\varepsilon}{2}, \|\cdot\|_\infty\right) &\leq \left(\frac{4}{\varepsilon}\right)^{K(d+1)} \\ \mathcal{N}\left(\Gamma_2, \frac{\varepsilon}{2}, L_2(\bar{X}_n/M(\bar{X}_n))\right) &\leq \left(\frac{4}{\varepsilon}\right)^{c_0 K k d \log(k)},\end{aligned}$$

where K is a constant and $\varepsilon < 2$. Thus, for every $\varepsilon < 2$,

$$\mathcal{N}(\Gamma_0, \varepsilon, L_2(P_n)) \leq \left(\frac{4}{\varepsilon}\right)^{C k d \log(k)}.$$

Using Dudley's entropy integral (see, e.g., [6, Corollary 13.2]) yields, for $k \geq 2$,

$$\mathbb{E}_\sigma Z_j \leq CR \sqrt{\frac{k d \log(k)}{n}},$$

hence the result.

9.1.4. Proof of Lemma 24

The first bound of Lemma 24 follows from Bernstein's inequality. To prove the second inequality, we first bound the expectation as follows.

$$\begin{aligned}
& \mathbb{E} \left(\left\| (\bar{X}_n - \mathbb{E}(X))(du) \bullet ((c_j - u)\mathbb{1}_{W_j(\mathbf{c})}(u))_{j=1,\dots,k} \right\| \right) \\
& \leq \sqrt{\mathbb{E} \left\| (\bar{X}_n - \mathbb{E}(X))(du) \bullet ((c_j - u)\mathbb{1}_{W_j(\mathbf{c})}(u))_{j=1,\dots,k} \right\|^2} \\
& \leq \sqrt{\frac{1}{n^2} \sum_{i=1}^n \mathbb{E} \left(\left\| (X_i - \mathbb{E}(X)) \bullet ((c_j - u)\mathbb{1}_{W_j(\mathbf{c})}(u))_{j=1,\dots,k} \right\|^2 \right)} \\
& \leq \sqrt{\frac{(4RM)^2 k}{n}} = \frac{4RM\sqrt{k}}{\sqrt{n}}
\end{aligned}$$

A bounded difference inequality (see, e.g., [6, Theorem 6.2]) entails that, with probability larger than $1 - e^{-x}$,

$$\left\| (\bar{X}_n - \mathbb{E}(X))(du) \bullet ((c_j - u)\mathbb{1}_{W_j(\mathbf{c})}(u))_{j=1,\dots,k} \right\| \leq \frac{4RM\sqrt{k}}{\sqrt{n}} + \sqrt{\frac{8kR^2M^2x}{n}},$$

hence the result.

9.1.5. Proof of Lemma 25

We follow the proof of [4, Theorem 1]. Let $t > 0$, and assume that $Pf - P_n f > 2t\sqrt{Pf}$, as well as $P'_n f \geq Pf - t\sqrt{Pf} \geq 0$. Let $g_a : \mathbb{R}^+ \rightarrow \mathbb{R}$ be defined as $g_a(x) = \frac{x-a}{\sqrt{x+a}}$, for $a \geq 0$. Then g_a is nondecreasing on \mathbb{R}^+ . With $a = P_n f$, $0 \leq x_2 = Pf - t\sqrt{Pf} \leq P'_n f = x_1$, we have $g_a(x_2) \leq g_a(x_1)$, so that

$$\frac{P'_n f - P_n f}{\sqrt{\frac{1}{2}(P'_n f + P_n f)}} \geq \frac{Pf - t\sqrt{Pf} - P_n f}{\sqrt{\frac{1}{2}(P_n f + Pf - t\sqrt{Pf})}}.$$

Since $P_n f + Pf - t\sqrt{Pf} \leq 2Pf$, we deduce that

$$\frac{P'_n f - P_n f}{\sqrt{\frac{1}{2}(P'_n f + P_n f)}} \geq \frac{Pf - P_n f - t\sqrt{Pf}}{\sqrt{Pf}} \geq t.$$

Thus,

$$\begin{aligned}
& \mathbb{P} \left(\sup_{f \in \mathcal{F}} \frac{P'_n f - P_n f}{\sqrt{\frac{1}{2}(P'_n f + P_n f)}} \right) \\
& \geq \mathbb{P} \left(\exists f_0 \in \mathcal{F} \mid Pf_0 - P_n f_0 > 2t\sqrt{Pf_0} \text{ and } P'_n f_0 \geq Pf_0 - t\sqrt{Pf_0} \right).
\end{aligned}$$

Let $A = \{\exists f_0 \in \mathcal{F} \mid Pf_0 - P_n f_0 > 2t\sqrt{Pf_0}\}$. The previous inequality may be written as

$$\begin{aligned} & \mathbb{P}\left(\exists f_0 \in \mathcal{F} \mid Pf_0 - P_n f_0 > 2t\sqrt{Pf_0} \text{ and } P_n' f_0 \geq Pf_0 - t\sqrt{Pf_0}\right) \\ & \geq \mathbb{E}\left(\mathbb{1}_A \mathbb{P}\left(\bigcup_{\{f \mid Pf - P_n f > 2t\sqrt{Pf}\}} \{P_n' f \geq Pf - t\sqrt{Pf}\} \mid X_1, \dots, X_n\right)\right), \end{aligned}$$

with, for a fixed $f \in \mathcal{F}$, using Cantelli's inequality,

$$\mathbb{P}\left(P_n' f - Pf < -2t\sqrt{Pf}\right) \leq \frac{\frac{1}{n} \text{Var}(f)}{\frac{1}{n} \text{Var}(f) + t^2 Pf}.$$

Since, for any $f \in \mathcal{F}$, $\|f\|_\infty \leq 1$, we have $\text{Var}(f) \leq Pf^2 \leq Pf$, thus

$$\mathbb{P}\left(P_n' f - Pf < -t\sqrt{Pf}\right) \leq \frac{1}{2},$$

provided that $nt^2 \geq 1$. Thus

$$\mathbb{P}\left(\sup_{f \in \mathcal{F}} \frac{P_n' f - P_n f}{\sqrt{\frac{1}{2}(P_n' f + P_n f)}} \geq t\right) \geq \frac{1}{2} \mathbb{P}\left(\frac{Pf - P_n f}{\sqrt{Pf}} \geq 2t\right).$$

The other inequality proceeds from the same reasoning, considering f such that $P_n f - Pf > 2t\sqrt{P_n f}$ and $P_n' f \leq Pf + t\sqrt{P_n f}$, and $g_a : \mathbb{R}^+ \rightarrow \mathbb{R}$ defined by $g_a(x) = \frac{a-x}{\sqrt{a+x}}$, that is nonincreasing for $a \geq 0$. Choosing $a = P_n f$, $0 \leq x_1 = P_n' f \leq Pf + t\sqrt{P_n f} = x_2$ leads to

$$\frac{P_n f - P_n' f}{\sqrt{\frac{1}{2}(P_n' f + P_n f)}} \geq \frac{P_n f - Pf - t\sqrt{P_n f}}{\sqrt{\frac{1}{2}(Pf + t\sqrt{P_n f} + P_n f)}} \geq \frac{P_n f - Pf - t\sqrt{P_n f}}{\sqrt{P_n f}} \geq t,$$

since $Pf + t\sqrt{P_n f} \leq P_n f$. Using Cantelli's inequality again leads to the result.

9.2. Proof of Lemma 12

The lemma follows from standard arguments in geometric inference and persistent homology theory.

First, the definition of generalized gradient of d_S - see [9] or [5, Section 9.2] - implies that the critical points of d_S are all contained in the convex hull of S . As a consequence, they are all contained in the sublevel set $d_S^{-1}([0, 2\text{diam}(S)])$. It follows from the Isotopy Lemma - [5, Theorem 9.5] - that all the sublevel sets $d_S^{-1}([0, t])$, $t > 2\text{diam}(S)$ have the same homology. As a consequence, no point in D has a larger coordinate than $2\text{diam}(S)$ and D is contained in $[0, 2\text{diam}(S)]^2$.

Since S is compact, the persistence module of the filtration defined by the sublevel sets of d_S is q -tame ([10, Corollary 3.35]). Equivalently, this means that for any $b_0 < d_0$, the intersection of D with the quadrant $Q_{(b_0, d_0)} = \{(b, d) : b < b_0 \text{ and } d_0 < d\}$ is finite. Noting that the intersection of $[0, 2\text{diam}(S)]^2$ with the half-plane $\{(b, d) : d \geq b + s\}$ can be covered by a finite union of quadrants $Q_{(b, b+\frac{s}{2})}$ concludes the proof of the lemma.

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