STRONG CONSISTENCY FOR A CLASS OF ADAPTIVE CLUSTERING PROCEDURES

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Abstract. We introduce a class of clustering procedures which includes $k$-means and $k$-medians, as well as variants of these where the domain of the cluster centers can be chosen adaptively (for example, $k$-medoids) and where the number of cluster centers can be chosen adaptively (for example, according to the elbow method). In the non-parametric setting and assuming only the finiteness of certain moments, we show that all clustering procedures in this class are strongly consistent under IID samples. Our method of proof is to directly study the continuity of various deterministic maps associated with these clustering procedures, and to show that strong consistency simply descends from analogous strong consistency of the empirical measures. In the adaptive setting, our work provides a strong consistency result that is the first of its kind. In the non-adaptive setting, our work strengthens Pollard’s classical result by dispensing with various unnecessary technical hypotheses, by upgrading the particular notion of strong consistency, and by using the same methods to prove further limit theorems.

1. Introduction

A fundamental task in unsupervised learning is that of clustering, namely, partitioning a set of data into a finite number of groups where elements within a group are similar (and, typically, elements between distinct groups are dissimilar). Among the most common clustering methods is $k$-means clustering \cite{KMeans}: For data points $Y_1, \ldots, Y_n$ in a metric space $(X, d)$ and any $k \in \mathbb{N} := \{1, 2, \ldots\}$, the set of $k$-means cluster centers is any solution to the set-indexed optimization problem

\begin{equation}
\begin{aligned}
\text{minimize} & \quad \frac{1}{n} \sum_{i=1}^{n} \min_{x \in S} d^2(x, Y_i) \\
\text{subject to} & \quad S \subseteq X \text{ and } 1 \leq \#S \leq k.
\end{aligned}
\end{equation}

(1.1)

Intuitively speaking, a set of $k$-means cluster centers for these data points is a set of points $S_n$ in $X$ to at least one of which all data are optimally close; the $k$-means clusters are then the sets

$$\{Y_i : d(x, Y_i) \leq d(x', Y_i) \text{ for all } x' \in S_n\}$$

indexed by $x \in S_n$. The simplicity of $k$-means makes it appealing, but there are many known drawbacks and many variant procedures which have been proposed

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and analyzed to overcome these; see the surveys [34, 14] for further information on the vast world of clustering.

The basic theoretical justification for $k$-means is Pollard [23] in which strong consistency is shown for a wide class of non-parametric models; that is, if $Y_1, Y_2, \ldots$ is an IID sequence of random variables in an abstract metric space $(X, d)$, and if a number of technical hypotheses hold, then the sequence of solutions $S_1, S_2, \ldots$ to the optimization problems above has a limit almost surely, in a sense which we will soon make precise. Moreover, the limit is a solution to the set-indexed optimization problem

\[
\begin{align*}
\text{minimize} & \quad \int_X \min_{x \in S} d^2(x, y) \, d\mu(y) \\
\text{subject to} & \quad S \subseteq X \text{ and } 1 \leq \#S \leq k.
\end{align*}
\]

The arguments therein rely on delicate calculations which combine uniform laws of large numbers with some recursive structure that relates the $k$-means cluster centers to the $(k-1)$-means cluster centers.

While this strong consistency result is applicable in a small number of settings, it is lacking in several important ways. First of all, the requisite technical hypotheses (which we have not attempted to state) are in many cases difficult to verify or actually false. Second, the proof is not at all amenable to establishing the analogous strong consistency for a number of more complicated clustering procedures of interest. Third, the proof establishes a strong consistency result but provides no avenue for establishing further limit theorems. In the present work we introduce a new perspective on clustering which, still in the non-parametric setting, resolves all of these issues.

Our approach, generally speaking, is motivated by the following observations: First, we notice that (1.2) generalizes (1.1) since one can always takes $\mu$ to be the empirical measure $\bar{\mu}_n := \frac{1}{n} \sum_{i=1}^{n} \delta_{Y_i}$ of the first $n \in \mathbb{N}$ data points; in other words, the empirical $k$-means cluster centers are just plug-in estimators for the population $k$-means cluster centers. Second, we recall that the empirical measures of IID samples have $\bar{\mu}_n \to \mu$ almost surely, for many interesting senses of convergence of probability measures. Therefore, we notice that an alternative proof of strong consistency would be to show that the (deterministic) map sending $\mu$ to the solution set of (1.2) is “continuous” in a suitable sense. Indeed this is the case, and the method of proof is robust enough to overcome the aforementioned challenges to the classical proof of strong consistency for $k$-means.

The remainder of this introduction is divided into further subsections. In Subsection 1.1 we define several adaptive clustering procedures which are of interest in statistics and machine learning but which heretofore lack theoretical justification in the form of strong consistency. In Subsection 1.2 we precisely state our main results. In Subsection 1.3 we review some literature related to the present work. The remainder of the paper is dedicated to the proofs of our main results.

1.1. Adaptive Clustering Procedures. In this subsection we precisely define a few adaptive clustering procedures which are of great practical interest but which have not been substantiated by many or any theoretical guarantees. Our later work will unify these procedures into a common class for which strong consistency can be easily proved.
Throughout this subsection, let \((X, d)\) be a metric space; while the primary setting of interest is \(X = \mathbb{R}^m\) for \(m \in \mathbb{N}\) with its usual Euclidean metric, most of the results in this paper are stated in the abstract setting. Also let \(Y_1, Y_2, \ldots\) be a sequence of points in \(X\) and \(\bar{\mu}_n := \frac{1}{n} \sum_{i=1}^{n} \delta_{Y_i}\) their empirical distributions for all \(n \in \mathbb{N}\).

The first of these procedures is a slight generalization of \(k\)-means.

**Restricted \((k, p)\)-means.** Fix \(k \in \mathbb{N}\), \(p \geq 1\), and \(R \subseteq X\). Then consider

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{n} \sum_{i=1}^{n} \min_{x \in S} d^p(x, Y_i) \\
\text{subject to} & \quad S \subseteq R \text{ and } 1 \leq \#S \leq k.
\end{align*}
\]

When \(R = X\), the case of \(p = 2\) is exactly \(k\)-means clustering, and the case of \(p = 1\) is exactly \(k\)-medians clustering. In general, increasing \(p\) results in monotonically increasing the sensitivity of the cluster centers to outliers in the data. As such, \(p = 1\) is the most robust clustering procedure in this class and “\(p = \infty\)" is the least robust. Moreover, the set \(R\) provides a uniform way to restrict the feasible set of cluster centers. Such considerations might arise, for example, in scientific settings where a priori domain knowledge dictates that cluster centers must lie in a “meaningful region”, or in engineering settings where physical constraints dictate that cluster centers must lie in an “attainable region”.

Although the setting of restricted \((k, p)\)-means is slightly different from the class of procedures considered by Pollard in [23], the methods therein can be easily modified to show strong consistency under the analogous technical hypotheses; the limit of any sequence of solutions turns out to be, as expected, a solution to the analogous population problem. In the setting above we call \(k\) the number of clusters and \(R\) the domain of the cluster centers.

By an adaptive clustering procedure we mean one where at least one of the number of clusters \(k\) or the domain of the cluster centers \(R\) is not fixed but rather is taken to be a measurable function of the data. One can also let \(p\) be chosen adaptively, but this appears to be less interesting and will not be pursued in the present work. Let us now review some important adaptive clustering procedures.

**(k, p)-medoids.** Fix \(k \in \mathbb{N}\) and \(p \geq 1\), and consider

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{n} \sum_{i=1}^{n} \min_{x \in S} d^p(x, Y_i) \\
\text{subject to} & \quad S \subseteq \{Y_1, \ldots Y_n\} \text{ and } 1 \leq \#S \leq k.
\end{align*}
\]

By constraining the domain of the clusters centers in this way, we force the cluster centers to be bona fide data points rather than abstract points in the space \(X\); such procedures are particularly important in interpretable machine learning. For example, if data points represent users of some system, it may be desirable that each cluster center be an actual user who serves as a prototype for the whole cluster.

**Elbow-method \((k, p)\)-means.** Fix \(p \geq 1\). For each \(k \in \mathbb{N}\), set

\[
m_{k,p} := \inf_{S \subseteq X \atop 1 \leq \#S \leq k} \frac{1}{n} \sum_{i=1}^{n} \min_{x \in S} d^p(x, y).
\]
Then for \( k \geq 2 \) define \( \Delta^2 m_{k,p} := m_{k+1,p} + m_{k-1,p} - 2m_{k,p} \), and also define \( \Delta^2 m_{1,p} := m_{2,p} - 2m_{1,p} \) by taking the convention that \( m_{0,p} = 0 \). Finally, set
\[
k^\text{elb}_p := \min\{\arg\max\{\Delta^2 m_{k,p} : k \in \mathbb{N}\}\},
\]
and consider
\[
\minimize 1/n \sum_{i=1}^{n} \min_{x \in S} d^p(x, Y_i)
\]
subject to \( S \subseteq X \) and \( \#S \leq k^\text{elb}_p \).

This is a naive formalism of the well-known method for choosing \( k \), where one inspects the graph of \( \{m_{k,p}\}_{k \in \mathbb{N}} \) and chooses the value of \( k \) for which the added model complexity experiences maximally diminishing returns. Such procedures are ubiquitous in exploratory data science, where the number of clusters is not known and fixed ahead of time, but rather must itself be estimated.

Even under IID samples, adaptive clustering procedures like the ones we have outlined appear difficult to analyze, since the domain and the number of clusters have some non-obvious dependency structure with the data itself. This global interaction compromises the usefulness of the independence of the data points and prevents one from using the standard approaches like uniform laws of large numbers. Thus, new tools are needed for establishing any kind of limit theorems like strong consistency.

Finally, we make a remark on a particular piece of terminology used throughout the paper. While we will always discuss clustering procedures, some authors prefer to discuss clustering algorithms. To make things concrete for this paper, a procedure will always refer to the setting in which one has oracle access to the solution set of each optimization problem. Likewise, an algorithm always refers to a particular method of computing such optimizers (or near-optimizers). With a few exceptions, we will only consider procedures in this work, although the algorithmic questions related to clustering are themselves highly non-trivial.

1.2. Statement of Results. In this subsection we detail the specific mathematical setting of our work and precisely state our main results.

We begin by “lifting” the clustering operation from \( X \) to \( \mathcal{P}(X) \); here, and throughout, \((X,d)\) is a fixed metric space and \( \mathcal{P}(X) \) is the space of Borel probability measures on \( X \). Indeed, choose any real \( p \geq 1 \), any distribution \( \mu \in \mathcal{P}(X) \) with \( \int_X d^p(x,y) \, d\mu(y) < \infty \) for some (equivalently, all) \( x \in X \), any integer \( k \in \mathbb{N} \), and any closed set \( R \subseteq X \). Then we consider the problem of choosing the best set of cluster centers \( S \subseteq R \) with \( 1 \leq \#S \leq k \), as quantified by the loss
\[
\int_X \min_{x \in S} d^p(x, y) \, d\mu(y).
\]

More precisely, we write \( C_p(\mu, k, R) \) for the set of all \( S \subseteq R \) with \( 1 \leq \#S \leq k \) satisfying
\[
\int_X \min_{x \in S} d^p(x, y) \, d\mu(y) = \inf_{S' \subseteq R} \int_X \min_{1 \leq \#S' \leq k} d^p(x, y) \, d\mu(y) =: m_{k,p}(\mu).
\]

Note that \( C_p(\mu, k, R) \) is, in general, a set of subsets of \( X \). Under mild conditions it can be shown to be non-empty.
Now let us observe that this framework unifies all of the clustering procedures of Subsection 1.1. Indeed, $C_{k,p}(\mu) := C_p(\mu,k,X)$ is exactly the set of sets of (unrestricted) $(k,p)$-means cluster centers, $C_{k,p}^{\text{med}}(\mu) := C_p(\mu,k,\text{supp}(\mu))$ is exactly the set of sets of $(k,p)$-medoids cluster centers, and $C_{p}^{\text{elb}}(\mu) := C_p(\mu,k^{\text{elb}}(\mu),X)$ is exactly the set of sets of $(k,p)$-means cluster centers when $k$ is chosen adaptively according to the elbow method.

The next step is to address certain notions of convergence of subsets of a given metric space. One notion is the relatively well-known Hausdorff metric. More specifically, for compact sets $A,A' \subseteq X$, define

$$d_H(A,A') := \inf \left\{ r \geq 0 : A \subseteq \bigcup_{x \in A'} \bar{B}_r^d(x) \text{ and } A' \subseteq \bigcup_{x \in A} \bar{B}_r^d(x) \right\},$$

where $\bar{B}_r^d(x) := \{ y \in X : d(x,y) \leq r \}$ is the closed ball of radius $r \geq 0$ around $x \in X$. In words, $d_H(A,A')$ is the smallest radius $r \geq 0$ for which the $r$-thickening of $A$ contains $A'$ and such that the $r$-thickening of $A'$ contains $A$. Another notion is the lesser-known Kuratowski convergence. More specifically, for $\{R_n\}_{n \in \mathbb{N}}$ and $R$ closed subsets of $X$, we write $\lim_{n \in \mathbb{N}} R_n = R$ to mean

- if $x \in R$, then for sufficiently large $n \in \mathbb{N}$ there exist $x_n \in R_n$ such that $x_n \to x$, and
- if $\{n_j\}_{j \in \mathbb{N}}$ is any subsequence and $x_j \in R_{n_j}$ are any points with $x_j \to x \in X$, then $x \in R$.

Observe in particular that if $\{A_n\}_{n \in \mathbb{N}}$ and $A$ are compact subsets of $X$, then $d_H(A_n,A) \to 0$ implies $\lim_{n \in \mathbb{N}} A_n = A$; the converse is not true in general. We will carefully develop further properties of these notions of convergence and the relationships between them in Subsection 2.2.

Now we can give the primary statistical setting of interest. Let $(X,d)$ be an abstract metric space, and fix some $\mu \in \mathcal{P}(X)$. Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space on which is defined an IID sequence $Y_1,Y_2,\ldots$ of $X$-valued random variables with common distribution $\mu$, and write $\hat{\mu}_n := \frac{1}{n} \sum_{i=1}^{n} \delta_{Y_i}$ for the empirical probability measure of the first $n \in \mathbb{N}$ samples.

The first of our main results can now be stated as follows. Recall that by a random closed set we mean a measurable map from $\Omega$ to the space of closed subsets of $X$ endowed with the Effros $\sigma$-algebra.

**Theorem 1.1.** If $(X,d)$ is separable and if $\int_X d^p(x,y) \, d\mu(y) < \infty$ holds for some (equivalently, all) $x \in X$, then for any random closed sets $\{R_n\}_{n \in \mathbb{N}}$ and $R$ of $X$ and any random positive integers $\{k_n\}_{n \in \mathbb{N}}$ and $k$, we have

$$\bigcap_{n \in \mathbb{N}} \bigcup_{m \in \mathbb{N}} C_p(\hat{\mu}_m,k_m,R_m) \subseteq C_p(\mu,k,R)$$

almost surely on

$$\{k_n \neq k \text{ finitely often}\} \cap \{\lim_{n \in \mathbb{N}} R_n = R\}.$$

In words, the result guarantees that any subsequential $d_H$-limit of the sets $\{C_p(\hat{\mu}_n,k_n,R_n)\}_{n \in \mathbb{N}}$ must lie in $C_p(\mu,k,R)$. Roughly speaking, this means any set of cluster centers appearing frequently at the level of empirical cluster centers must itself be a set of population cluster centers. This is the same sense in which Pollard proved strong consistency of $k$-means, but under many further assumptions.
While this result is extremely general and quite easy to prove, it turns out that we can say slightly more in most settings of interest.

Recall that when we say that \((X, d)\) has the Heine-Borel property we mean that all \(d\)-closed balls are compact. This is a sort of finite-dimensionality condition which holds in many statistical settings, for example \(X = \mathbb{R}^m\) for some \(m \in \mathbb{N}\) with its usual (Euclidean) metric, \(X\) being a finite-dimensional Riemannian with its metric tensor, or \(X\) any finite set with any metric. Most examples of spaces lacking the Heine-Borel property are infinite-dimensional, like spaces of functions or spaces of measures. Under this assumption on the ambient space, we have our second main result.

**Theorem 1.2.** If \((X, d)\) has the Heine-Borel property and if \(\int_X d^p(x, y) \, d\mu(y) < \infty\) holds for some (equivalently, all) \(x \in X\), then for any random closed sets \(\{R_n\}_{n \in \mathbb{N}}\) and \(R\) of \(X\) and any random positive integers \(\{k_n\}_{n \in \mathbb{N}}\) and \(k\), we have

\[
\max_{S_n \in C_{k, p}(\bar{\mu}_n, k, R)} \min_{S \in C_{p}(\mu, R)} d_H(S_n, S) \to 0
\]

almost surely on

\[
\{k_n \neq k \text{ finitely often}\} \cap \{\text{Lt}_{n \in \mathbb{N}} R_n = R\} \cap \{k \leq \#(R \cap \text{supp}(\mu))\}.
\]

This result can be viewed as a uniform version of the preceding result, since it guarantees that the distance from any set of empirical cluster centers to some set of population cluster centers goes to zero uniformly. This strengthened form of strong consistency is slightly more difficult to prove than the first result.

Let us now consider some particular consequences of Theorem 1.2, in the setting of \(X = \mathbb{R}^m\) for some \(m \in \mathbb{N}\) with the metric induced by the usual \(\ell_2\) norm \(\| \cdot \|\). Indeed, suppose that the population distribution \(\mu\) satisfies \(\#\text{supp}(\mu) = \infty\), which is certainly the case in most applications where clustering is relevant (for example, if \(\mu\) has a density with respect to the Lebesgue measure). Let us also suppose that \(p \geq 1\) is such that we have \(\int_{\mathbb{R}^m} \|y\|^p \, d\mu(y) < \infty\). Then, we have the following:

(i) Taking \(R_n = R = \mathbb{R}^d\) and \(k_n = k\) for all \(n \in \mathbb{N}\), yields

\[
\max_{S_n \in C_{k, p}(\bar{\mu}_n, k, R)} \min_{S \in C_{p}(\mu, R)} d_H(S_n, S) \to 0
\]

almost surely. In words, this says that \((k, p)\)-means is strongly consistent.

(ii) Take \(R = \text{supp}(\mu)\), as well as \(R_n = \text{supp}(\bar{\mu}_n)\) and \(k_n = k\) for all \(n \in \mathbb{N}\). Then note [11, Proposition 4.2] which shows that we have \(\text{Lt}_{n \in \mathbb{N}} \text{supp}(\bar{\mu}_n) = \text{supp}(\mu)\) almost surely. Thus, we get

\[
\max_{S_n \in C_{k, p}^{\text{med}}(\bar{\mu}_n)} \min_{S \in C_{p}(\mu, R)} d_H(S_n, S) \to 0
\]

almost surely. In words, this establishes that \((k, p)\)-medoids is strongly consistent.

(iii) Take \(R_n = \mathbb{R}^d\) and \(k_n = k^\text{elb}(\bar{\mu}_n)\) for all \(n \in \mathbb{N}\), as well as \(R = \mathbb{R}^d\) and \(k = k^\text{elb}(\mu)\). Let us further suppose \(\# \arg \max \{\Delta^2 k_{p, \mu} : k \in \mathbb{N}\} = 1\), which by Lemma 3.14 implies \(k^\text{elb}(\bar{\mu}_n) \neq k^\text{elb}(\mu)\) finitely often almost surely. Hence,

\[
\max_{S_n \in C_{p}^{\text{elb}}(\bar{\mu}_n)} \min_{S \in C_{p}(\mu)} d_H(S_n, S) \to 0
\]
almost surely. In words, $(k, p)$-means, where $k$ is chosen adaptively according to the elbow method, is strongly consistent provided that $\mu$ has a uniquely-defined number of clusters in the sense of the elbow method.

These results essentially follow immediately from Theorem 1.2 and some auxiliary results.

Importantly, our method of proof for Theorem 1.1 and Theorem 1.2 is novel and has many advantages over existing methods. To see this, write $C(X)$ for the space of $d$-closed subsets of $X$ and $K(X)$ for the space of non-empty $d$-compact subsets of $X$; in particular, we write $C(K(X))$ for the space of $d_H$-closed subsets of $K(X)$ and $K(K(X))$ for the space of non-empty $d_H$-compact subsets of $K(X)$. While previous approaches involved studying probabilistic aspects of the random optimization problems determining $C_p(\bar{\mu}_n, k_n, R_n)$, we take a more abstract perspective and show directly that these spaces can be “topologized” such that

$$C_p : \mathcal{P}(X) \times \mathbb{N} \times C(K(X)) \to K(K(X))$$

is “continuous”. To be slightly more precise, this result states that $C_p$ maps “convergent” sequences to “convergent” sequences, where the respective senses of “convergence” are meaningful and explicit but may not correspond to convergence in any topology.

By this continuity perspective, we see that the strong consistency for clustering procedures is merely descended down from an analogous strong law of large numbers for empirical measures of IID samples. Moreover, through this lens it is easy to see that there is nothing special about our apparent focus on strong limit theorems; we can actually descend many types of limit theorems for empirical measures down to analogous limit theorems for clustering procedures. We conclude this subsection by describing two examples of this, which we will carefully prove and analyze at the end of the paper.

One example of particular interest is the notion of descending a large deviations principle, since this establishes the asymptotic rate of decay of the tail probabilities associated to certain clustering events. For such a result, we limit our attention to the case of non-adaptive $(k, p)$-means. While this result is an interesting starting point for understanding concentration of measure for clustering procedures, there are many natural questions which remain to be answered; we address some of these at the end of Subsection 4.2.

**Theorem 1.3.** If $(X, d)$ has the Heine-Borel property and if $\int_X \exp(\alpha d^p(x, y)) \, d\mu(y) < \infty$ holds for all $\alpha > 0$ and some (equivalently, all) $x \in X$, then, for all $k \leq \#\text{supp}(\mu)$ and $\varepsilon > 0$, we have

$$\limsup_{n \to \infty} \frac{1}{n} \log \mathbb{P}\left( \max_{S_n \in C_{k,n}^p(\bar{\mu}_n)} \min_{S \in C_{k}^p(\mu)} d_H(S_n, S) \geq \varepsilon \right) \leq -c_{k,p}(\mu, \varepsilon),$$

for some $c_{k,p}(\mu, \varepsilon) > 0$.

Another example is the notion of applying clustering procedures to data coming from a Markov chain (MC). In this setting, we show that a naive application of $(k, p)$-medoids can fail to be strongly consistent. Nonetheless, the tools developed in this paper easily lead one to a slight adaptation of $(k, p)$-medoids which we show is strongly consistent. We detail the precise statement of this result in Subsection 4.3 when some further preliminaries have been established.
1.3. Related Literature. In this subsection we briefly review some research, both classical and modern, which is related to the results in the present paper.

Among all clustering procedures, $k$-means has certainly received the most attention. A typical reference for the initial theoretical study of $k$-means is usually taken to be [20], but it is known [7] that the procedure has a rich prehistory under many different names. The primary theoretical justification for $k$-means (as well as $k$-medians) is [23] in which strong consistency is shown. Our Theorem 1.2 is a strengthening of this, in the sense that we upgrade the particular notion of strong consistency and that we dispense some of the unnecessary technical hypotheses. Our Theorem 1.3 also provides what appear to be the first large deviations upper bound for these procedures in a wide non-parametric setting. One of the major drawbacks of $k$-means is its computational difficulty, owing to the fact that the optimization problem (1.1) is non-convex. In fact, it is known [1] that this problem is NP-hard, and that iterative methods like the ubiquitous Lloyd-Forgy algorithm [19, 12] can become stuck in local optima which are globally suboptimal.

Much subsequent research has focused on alternatives to $k$-means whose theoretical or computational properties are more desirable. Examples include spectral clustering, Bayesian and Bayesian non-parametric clustering, hierarchical clustering, and a wide range of others; see [14, 34] for surveys of this large class of procedures. Despite this interest, the adaptive $k$-means procedures of Subsection 1.1 seem to lack theoretical justification.

The most important adaptive clustering procedure for which our results are novel appears to be $k$-medians, which was introduced in [16] and has since become a staple of interpretable machine learning. (Note that some authors reserve $k$-medoids to refer to the case of $p = 1$, while we use the term for all such $p \geq 1$.) In this realm, the primary interest is in computational questions. Indeed, there exist randomized algorithms [2, 3] which can provably identify $k$-medoids clustering centers with high probability at a low runtime.

The other class of clustering procedures for which our results are novel are variants of $k$-means and $k$-medians where $k$ is chosen adaptively. While there is substantial literature proposing and experimentally analyzing various adaptive choices of $k$ (see [13] for a small selection), there does not appear to be much that has been rigorously proved about the consistency of such procedures. Hence, our results providing strong consistency under an adaptive choice of $k$ according to the elbow method, are novel. We believe that it would be interesting to dedicate future work to studying strong consistency under an adaptive choice of $k$ according to, say, the gap statistic [28] or the silhouette statistic.

Another aspect of clustering procedures which is relevant to the present work is the notion of stability, which is known, at least at the level of some formal similarities, to be closely related to the notion of continuity. In this sense our results are quite similar to those of [18, 26], except that we prove a slightly weaker asymptotic statement in a far more general setting. In this realm there is also the observation [24, 31, 25] that a good clustering procedure should have the property that it is relatively stable under perturbations of the data, so some authors [17, 5] have proposed stability-based methods as a starting point for adaptively choosing the number of clusters $k$. However, this approach was later shown to have some crucial drawbacks [32]. Our results, which show that $k$-means and its offspring
are always continuous hence stable in a very concrete sense, provide a possible explanation of this phenomenon.

Finally, we point out that the most closely-related literature to the present is the author’s own work on Fréchet means [11]. Indeed, the notion of the Fréchet $p$-mean of a probability distribution is equivalent to the $(k, p)$-means cluster centers when fixing $k = 1$. That earlier work already contains the core idea of the present work: It was observed that the strong law of large numbers for Fréchet means merely “descend” from analogous strong laws of large numbers for the empirical measures, by showing that a certain deterministic map is suitably continuous. The primary difficulty in extending that work to cover the case of general $k \in \mathbb{N}$ is that one must go “two levels deep” into set-valued topologies and work with the spaces $C(K(X))$ and $K(K(X))$.

The remainder of the paper is structured as follows. In Section 2 we review some preliminary topological concepts related to metric spaces, spaces of subsets of a given metric space, and spaces of probability measures on a given metric space. In Section 3 we study the clustering map itself, and we show that it is, in several suitable senses, continuous. Finally, we have Section 4 in which we prove our main probabilistic results.

2. Preliminaries

In this section we develop the basic results which will combine in the next sections to prove various limit theorems for a wide class of clustering procedures. Unless otherwise stated, we always assume that $(X, d)$ is a metric space and that $1 \leq p < \infty$.

2.1. Metric Spaces. By a slight abuse of notation, we write $d$ for both the metric on $X$ and also for the topology on $X$ generated by this metric. When we say that $(X, d)$ is locally compact we mean that for every point $x \in X$ there is some $r > 0$ such that the closed ball $B_d^r(x) := \{ y \in X : d(x, y) \leq r \}$ is compact; when we say that $(X, d)$ has the Heine-Borel property we mean that the closed ball $B_d^r(x)$ is compact for all $x \in X$ and $r \geq 0$.

We now give two inequalities for a general metric space $(X, d)$ that will be essential for our work. The first is that for any $p \geq 1$, we have

$$d^p(x', y) \leq 2^{p-1}(d^p(x', x'') + d^p(x'', y))$$

for all $x', x'', y \in X$. The second is a quantitative version of the above which states that, for any $p \geq 1$ and $\varepsilon > 0$, there exists some constant $c_{p, \varepsilon} > 0$ such that we have

$$d^p(x', y) \leq c_{p, \varepsilon}d^p(x', x'') + (1 + \varepsilon)d^p(x'', y)$$

for all $x', x'', y \in X$. The latter inequality is sometimes called the “Rob Peter to pay Paul inequality” since it shows that one can make either coefficient of (2.1) arbitrarily close to 1 at the cost of increasing the other. Proofs of these facts can be found in [11, Equation (2.3) and Lemma 2.3], respectively.

Also, unless stated otherwise, we let any subset of the real numbers be endowed with the topology induced by the usual Euclidean metric, and we let $\mathbb{N} \cup \{\infty\}$ be given the topology of the one-point-compactification of the discrete topology on $\mathbb{N}$. 

2.2. **Spaces of Subsets.** Write $C(X, d)$ for the collection of all $d$-closed subsets of $X$ and $K(X, d)$ for the collection of all non-empty $d$-compact subsets of $X$; we simply write $C(X)$ and $K(X)$, respectively, if $d$ is clear from the context. In this subsection we introduce some notions of convergence for elements of $C(X)$ and $K(X)$ and establish some basic properties that we will later need.

To begin we introduce and review some basic properties of “Kuratowski convergence”, sometimes called the “Kuratowski-Painlevé convergence”. We do not need the full generality of this theory, but we direct the interested reader to [4, Chapter 5] for more information. In particular, our work is simplified since we are only interested in metric spaces rather than general topological spaces and since we are only interested in sequences rather than general nets. At any rate, we define, for $\{C_n\}_{n \in \mathbb{N}}$ in $C(X)$, the sets

$$
L_s \quad C_n := \left\{ x \in X : \text{for all open neighborhoods } U \text{ of } x, \quad U \cap C_n \neq \emptyset \text{ for infinitely many } n \in \mathbb{N} \right\}
$$

$$
L_i \quad C_n := \left\{ x \in X : \text{for all open neighborhoods } U \text{ of } x, \quad U \cap C_n \neq \emptyset \text{ for large enough } n \in \mathbb{N} \right\}
$$
called the Kuratowski upper limit and Kuratowski lower limit, respectively. More concretely, for a point $x \in X$, we have $x \in L_s_{n \in \mathbb{N}}C_n$ if and only if there exists some subsequence $\{n_j\}_{j \in \mathbb{N}}$ and some $x_j \in C_{n_j}$ for each $j \in \mathbb{N}$ such that $x_j \to x$, and we have $x \in L_i_{n \in \mathbb{N}}C_n$ if and only if for any subsequence $\{n_j\}_{j \in \mathbb{N}}$ there exists a further subsequence $\{j_i\}_{i \in \mathbb{N}}$ and some $x_i \in C_{n_{j_i}}$ for each $i \in \mathbb{N}$ with $x_i \to x$. It is also straightforward to show that $L_s_{n \in \mathbb{N}}C_n$ and $L_i_{n \in \mathbb{N}}C_n$ are both closed.

If $\{C_n\}_{n \in \mathbb{N}}$ and $C$ in $C(X)$ are such that $L_s_{n \in \mathbb{N}}C_n \subseteq C$, then we say that $\{C_n\}_{n \in \mathbb{N}}$ converges in the Kuratowski upper sense to $C$, and if they are such that $L_i_{n \in \mathbb{N}}C_n \supseteq C$, then we say that $\{C_n\}_{n \in \mathbb{N}}$ converges in the Kuratowski lower sense to $C$. Note the inclusions rather than exact equality here. If $\{C_n\}_{n \in \mathbb{N}}$ satisfies $L_s_{n \in \mathbb{N}}C_n = L_i_{n \in \mathbb{N}}C_n$, then we write $C := L_{n \in \mathbb{N}}C_n$ for their common value, called the Kuratowski (full) limit, and in this case we say that $\{C_n\}_{n \in \mathbb{N}}$ converges in the Kuratowski (full) sense to $C$ or that the Kuratowski limit exists and equals $C$.

It is known that convergence in the Kuratowski full sense coincides with convergence in a topology $\tau$ on $C(X)$ if and only if $(X, d)$ is locally compact, in which case $\tau$ is exactly the Fell topology (see [4, Theorem 5.2.6] and the remarks thereafter). Contrarily, we do not know when convergence in the Kuratowski upper and lower senses correspond to convergence in suitable topologies. Our later results will establish that certain functions map Kuratowski-convergent sequences to Kuratowski-convergent sequences, but, because of this issue of possible non-topologizability, we will not say that such functions are continuous; instead, we will say that they are “continuous”. It is possible, in the locally compact setting, that these “continuity” statements become bona fide continuity statements, but we will not concern ourselves with such technicalities in this work.

Next, we introduce and review some basic properties of “Hausdorff convergence”, and we note that a more comprehensive account of this theory can be found in [9, Section 7.3]. That is, for $x \in X$ and $S' \in K(X)$, write

$$
d(x, S') := \min_{x' \in S'} d(x, x')
$$

for the shortest distance from the point $x$ to the set $S'$. Observe that $S'$ being compact and $d$ being continuous implies that the min is in fact achieved. Now for
$S, S' \in K(X)$, write

$$\tilde{d}_H(S, S') := \max_{x \in S} d(x, S') = \max_{x \in S} \min_{x' \in S'} d(x, x')$$

for the largest possible shortest distance from a point in $S$ to the set $S'$. As before, it is easy to show by the compactness of $S$ and the continuity of $x \mapsto d(x, S')$ that the max and min are both achieved. Although $\tilde{d}_H$ is not a metric (it is not symmetric), it is easy to show that it satisfies the following triangle inequality

$$(2.3) \quad \tilde{d}_H(S, S'') \leq \tilde{d}_H(S, S') + \tilde{d}_H(S', S'')$$

for $S, S', S'' \in K(X)$. We also have an immediate extension of (2.2) to the set-valued setting, where, for any $r \geq 0$ and any $\varepsilon > 0$, there exists a constant $c_{r, \varepsilon} > 0$ such that we have

$$(2.4) \quad d^r(y, S') \leq c_{r, \varepsilon}(\tilde{d}_H(S', S''))^r + (1 + \varepsilon)d^r(y, S'')$$

for all $S', S'' \in K(X)$ and $y \in X$.

If $\{C_n\}_{n \in \mathbb{N}}$ and $C$ in $K(X)$ are such that $\tilde{d}_H(C_n, C) \to 0$, then we say that $\{C_n\}_{n \in \mathbb{N}}$ converges in the Hausdorff upper sense to $C$, and if they are such that $\tilde{d}_H(C, C_n) \to 0$, then we say that $\{C_n\}_{n \in \mathbb{N}}$ converges in the Hausdorff lower sense to $C$. As before, we will not discuss these as topological notions (although we believe, in contrast to the Kuratowski convergences, that the Hausdorff convergences are always topologizable).

**Remark 2.1.** By replacing the maximum with a supremum and the minimum with an infimum, we can extend our definition of $\tilde{d}_H$ to cover the case that $C, C' \in C(X)$ are assumed only to be non-empty; in this case we set

$$\tilde{d}_H(C, C') := \sup_{x \in C} \inf_{x' \in C'} d(x, x'),$$

which takes values in the extended real half-line, $[0, \infty]$. Thus, if $\{C_n\}_{n \in \mathbb{N}}$ and $C$ in $C(X)$ are assumed only to be non-empty then the expression

$$\lim_{n \to \infty} \tilde{d}_H(C_n, C) = 0$$

is taken to mean that $\tilde{d}_H(C_n, C)$ is finite for sufficiently large $n \in \mathbb{N}$ and that it converges to zero as $n \to \infty$.

Now, for $S, S' \in K(X)$, write

$$d_H(S, S') := \max \{\tilde{d}_H(S, S'), \tilde{d}_H(S', S)\}.$$ 

This is a well-studied object called the Hausdorff metric, and it is, as the name suggests, a bona fide metric on $K(X)$. Write $\tau_H$ for the topology on $K(X)$ such that $\{S_n\}_{n \in \mathbb{N}}$ and $S$ in $K(X)$ have $\lim_{n \to \infty} S_n = S$ in $\tau_H$ if and only if $\lim_{n \to \infty} d_H(S_n, S) = 0$; this is called the Hausdorff topology. Equivalently, $\tau_H$ is the weakest topology on $K(X)$ such that $d_H(\cdot, S), \tilde{d}_H(\cdot, S) : K(X) \to [0, \infty)$ are continuous for all $S \in K(X)$.

Our next goal is to develop some useful results about these notions of convergence, with a particular focus on the lower senses of convergence. These will be heavily used in the remaining parts of the paper. The first such result concerns the relationship between the Kuratowski and the Hausdorff lower senses of convergence, and can be seen as a sharpening of [11, Lemma 2.9].
Lemma 2.2. For any \{S_n\}_{n \in \mathbb{N}} and \(S \in K(X)\), we have \(\tilde{d}_H(S, S_n) \to 0\) if and only if \(S \subseteq \text{Lim}_{n \in \mathbb{N}}S_n\).

Proof. First suppose \(\tilde{d}_H(S, S_n) \to 0\) and consider any \(x \in S\). For each \(n \in \mathbb{N}\) there is some \(x_n \in S_n\) with \(d(x, x_n) = d(x, S_n) \leq d_H(S, S_n) \to 0\), hence \(x_n \to x\). Thus, \(x \in \text{Lim}_{n \in \mathbb{N}}S_n\), as claimed. For the second direction, suppose \(S \subseteq \text{Lim}_{n \in \mathbb{N}}S_n\). Take arbitrary \(\varepsilon > 0\) and use compactness to get \(S' = \{x^1, \ldots, x^k\}\) points in \(S\) such that \(\tilde{d}_H(S, S') < \varepsilon\). For each \(1 \leq i \leq k\) there exists some \(N_i\) such that for \(n \geq N_i\) there is \(x_n \in S_n\) such that \(x_n \to x^i\) as \(n \to \infty\). Consequently, \(\tilde{d}_H(S', S_n) \to 0\). Thus:

\[
\limsup_{n \to \infty} \tilde{d}_H(S, S_n) \leq \tilde{d}_H(S, S') + \lim_{n \to \infty} \tilde{d}_H(S', S_n) \leq \varepsilon,
\]

so taking \(\varepsilon \to 0\) shows \(\tilde{d}_H(S, S_n) \to 0\). \(\square\)

The next result relates the Kuratowski lower sense of convergence to the cardinalities of the constituent sets. Combining it with the above shows that the same consequence is true if one assumes the stronger hypothesis of Hausdorff lower convergence.

Lemma 2.3. For \(\{S_n\}_{n \in \mathbb{N}}\) and \(S \in C(X)\), we have that \(S \subseteq \text{Lim}_{n \in \mathbb{N}}S_n\) implies \#S \leq \text{lim inf}_{n \to \infty} \#S_n\).

Proof. There is nothing to prove if \(\text{lim inf}_{n \to \infty} \#S_n = \infty\), so we assume \(k := \text{lim inf}_{n \to \infty} \#S_n < \infty\). Then there is a subsequence \(\{n_j\}_{j \in \mathbb{N}}\) such that \(\#S_{n_j} = k\) for all \(j \in \mathbb{N}\). Assume for the sake of contradiction that \(\#S > k\). Then get \(S' \subseteq S\) with \(\#S' = k + 1\), and write \(\varepsilon := \min\{d(x, x') : x, x' \in S', x \neq x'\} > 0\). For each \(x \in S'\) there is some \(J_x \in \mathbb{N}\) such that \(j \geq J_x\) implies that \(B^{d}(x, \varepsilon/2) \cap S_{n_j} \neq \emptyset\). Thus, taking \(j \geq J := \max\{J_x : x \in S'\}\) shows that for \(j \geq J\) we can construct a function \(\phi_j : S' \to S_{n_j}\) sending each \(x \in S'\) to a point \(\phi_j(x) \in S_{n_j}\) with \(d(x, \phi_j(x)) < \varepsilon/2\). Observe that all \(\phi_j\) must be injective, since \(x, x' \in S'\) with \(\phi_j(x) = \phi_j(x')\) implies \(d(x, x') = d(x, \phi_j(x)) + d(x', \phi_j(x')) < \varepsilon\) whence \(x = x'\) by the minimality of \(\varepsilon\). This means we have \(k + 1 \leq \#S' \leq \#S_{n_j} = k\) for all sufficiently large \(j \in \mathbb{N}\), and this is a contradiction. \(\square\)

In light of the above, it is natural to guess that the “dual” statement of \(L_{\text{Lim}_{n \in \mathbb{N}}S_n} \subseteq S\) implying \(\text{lim sup}_{n \to \infty} \#S_n \leq \#S\) may be true. It turns out that this fails in general, as can be seen by considering \(X = \mathbb{R}\) with its usual metric, \(S_n = \{-\frac{1}{n}, \frac{1}{n}\}\) for \(n \in \mathbb{N}\), and \(S = \{0\}\). In fact, this example shows that neither \(\tilde{d}_H(S_n, S) \to 0\) nor \(S_n \to S\) in \(d_H\) even implies \(\text{lim sup}_{n \to \infty} \#S_n \leq \#S\).

Another important result concerning cardinalities and lower senses of convergence is the following. In words, it states that a priori information about cardinalities allows one to upgrade Hausdorff lower convergence to convergence in the (full) Hausdorff metric.

Lemma 2.4. If \(\{S_n\}_{n \in \mathbb{N}}\) and \(S \in K(X)\) all have the same finite cardinality then we have \(\tilde{d}_H(S_n, S) \to 0\) if and only if \(S_n \to S\) in \(d_H\).

Proof. Since \(S_n \to S\) in \(d_H\) implies \(\tilde{d}_H(S_n, S) \to 0\), we only need to show the converse. That is, suppose \(\tilde{d}_H(S_n, S) \to 0\), and write \(\varepsilon := \min\{d(x, x') : x, x' \in S, x \neq x'\} > 0\). Note that there is some \(N \in \mathbb{N}\) such that \(n \geq N\) implies \(\tilde{d}_H(S_n, S) < \varepsilon/2\), and, in particular, that there is a map \(\phi_n : S \to S_n\) defined by sending \(x \in S\) to some \(\phi_n(x) \in S_n\) such that \(d(x, \phi_n(x)) < \varepsilon/2\). Of course, if \(\phi_n(x) = \phi_n(x')\) for
Proof. Let \( S \subseteq K(X) \) and \( r \geq 0 \) be arbitrary. Then write \( \text{diam}(S) := \max \{d(x, x') : x, x' \in S\} \), choose any \( a \in S \), and note that we have

\[
\overline{B}^d_r(a) = \overline{B}^d_{r + \text{diam}(S)}(a).
\]

Of course, \( \overline{B}^d_{r + \text{diam}(S)}(a) \) is compact by the Heine-Borel property of \( (X, d) \), hence the right side is compact by Blaschke’s theorem \cite[Theorem 7.3.8]{Klee}. Since the left side is closed, it is also compact. Thus, we have shown that all closed balls are compact, whence the claim. \( \square \)

**Lemma 2.6.** Let \( (X, d) \) be a Heine-Borel space and suppose that \( \{S_n\}_{n \in \mathbb{N}} \) in \( K(X) \) have \( \limsup_{n \to \infty} d(o, S_n) < \infty \) for some \( o \in X \). Then, there is a subsequence \( \{n_j\}_{j \in \mathbb{N}} \) and \( S \subseteq K(X) \) with \( \overline{d}_H(S, S_{n_j}) \to 0 \).

Proof. There exists some \( r > 0 \) such that \( \{S_n\}_{n \in \mathbb{N}} \) intersect \( \overline{B}^d_r(o) \) for all sufficiently large \( n \in \mathbb{N} \). The ball \( \overline{B}^d_r(o) \) is compact by the Heine-Borel property of \( (X, d) \), hence there exists a subsequence \( \{n_j\}_{j \in \mathbb{N}} \) such that \( L_{j \in \mathbb{N}} S_{n_j} \) is non-empty. Then for \( S \) any non-empty compact subset of \( L_{j \in \mathbb{N}} S_{n_j} \), Lemma 2.2 gives \( \overline{d}_H(S, S_{n_j}) \to 0 \) as \( j \to \infty \), as needed. \( \square \)

We conclude this subsection with a remark about a potential cause for confusion. At the present level of generality, the perspective of working with spaces of subsets should not be too difficult. However, the situation will become more complicated in the next parts of the paper when we venture “two levels deep” into spaces of subsets. In particular, we will soon need to consider Kuratowski and Hausdorff senses of convergence on the space \( (K(X), d_H) \). We will attempt to keep the reader on track by adding “in \( C(K(X)) \)” or “in \( K(K(X)) \)” to the ends of statements where we anticipate that difficulty may arise. Of course, \( C(K(X)) \) and \( K(K(X)) \) are shorthand for \( C(K(X), d) \) and \( K(K(X), d) \), respectively. It should also be understood that \( K(X) \) is always endowed with the metric \( d_H \).

### 2.3 Spaces of Measures

Write \( \mathcal{P}(X, d) \) to denote the space of Borel probability measures on \( (X, d) \) which we endow with the topology of weak convergence \( \tau_w \); we write \( \mathcal{P}(X) \) if the metric \( d \) is clear from context. Then write \( \mathcal{P}_p(X) \subseteq \mathcal{P}(X) \) for
the subspace of all Borel probability measures which satisfy \( \int_X d^p(x, y) \, d\mu(y) < \infty \) for some \( x \in X \). By (2.1), we have \( \mu \in \mathcal{P}_p(X) \) if and only if \( \int_X d^p(x, y) \, d\mu(y) < \infty \) for all \( x \in X \).

Next define the function \( W_p : K(X) \times \mathcal{P}_p(X) \to [0, \infty) \) via

\[
W_p(S, \mu) := \int_X d^p(y, S) \, d\mu(y) = \int_X \min_{z \in \mathcal{S}} d^p(x, y) \, d\mu(y).
\]

As a consequence of (2.4), we immediately get that, for any \( \mu \in \mathcal{P}_p(X) \) and any \( \varepsilon > 0 \), there exists a constant \( c_{p, \varepsilon} > 0 \) such that

\[
W_p(S', \mu) = c_{p, \varepsilon}(\bar{d}_H(S', S''))^p + (1 + \varepsilon)W_p(S'', \mu).
\]

Of course, this inequality is true trivially, with both sides equalling infinity, whenever we have \( \mu \in \mathcal{P}(X) \setminus \mathcal{P}_p(X) \).

Now define a topology \( \tau_{\bar{d}_H}^p \) on \( \mathcal{P}_p(X) \) such that \( \{\mu_n\}_{n \in \mathbb{N}} \) and \( \mu \in \mathcal{P}_p(X) \) have \( \lim_{n \to \infty} \mu_n = \mu \) in \( \tau_{\bar{d}_H}^p \) if and only if we have \( \int_X d^p(x, y) \, d\mu_n(y) \to \int_X d^p(x, y) \, d\mu(y) \) as \( n \to \infty \) for some \( x \in X \). This is called the \( p \)-Wasserstein topology and is closely related to many aspects of optimal transport [30]. It turns out that this condition for convergence in \( \tau_{\bar{d}_H}^p \) is equivalent the following, which at first appears to be stronger.

**Lemma 2.7.** For \( 1 \leq p < \infty \), the measures \( \{\mu_n\}_{n \in \mathbb{N}} \) and \( \mu \in \mathcal{P}_p(X) \) have \( \mu_n \to \mu \) in \( \tau_{\bar{d}_H}^p \) if and only if for all \( S \in K(X) \) we have \( W_p(S, \mu_n) \to W_p(S, \mu) \).

**Proof.** The “if” direction is obvious since \( \{x\} \in K(X) \) for each \( x \in X \). For the “only if” direction, let \( S \in K(X) \) be arbitrary. Then let \( \{Y_n\}_{n \in \mathbb{N}} \) and \( Y \) be \( X \)-random elements such that \( Y_n \) has law \( \mu_n \) for each \( n \in \mathbb{N} \), that \( Y \) has law \( \mu \). It follows by the continuous mapping theorem [15, Theorem 4.27] that we have \( d^p(Y_n, S) \to d^p(Y, S) \) in distribution as \( n \to \infty \). Now let \( x \in S \) be such that we have \( \mathbb{E}[d^p(x, Y_n)] \to \mathbb{E}[d^p(x, Y)] \) as \( n \to \infty \). Hence, \( \{d^p(x, Y_n)\}_{n \in \mathbb{N}} \) is uniformly integrable by [15, Theorem 4.11], and, since we have \( d^p(Y_n, S) \leq d^p(x, Y_n) \) for all \( n \in \mathbb{N} \), this implies \( \{d^p(Y_n, S)\}_{n \in \mathbb{N}} \) is uniformly integrable, also by [15, Theorem 4.11]. Thus we have \( \mathbb{E}[d^p(Y_n, S)] \to \mathbb{E}[d^p(Y, S)] \) as \( n \to \infty \), as desired. \( \square \)

**Lemma 2.8.** The function \( W_p : (K(X) \times \mathcal{P}_p(X), d_H \times \tau_{\bar{d}_H}^p) \to [0, \infty) \) is continuous.

**Proof.** Suppose \( \{(S_n, \mu_n)\}_{n \in \mathbb{N}} \) and \( (S, \mu) \) in \( K(X) \times \mathcal{P}_p(X) \) have \( (S_n, \mu_n) \to (S, \mu) \) in \( d_H \times \tau_{\bar{d}_H}^p \), and let \( \varepsilon > 0 \) be arbitrary. Then use (2.5) and Lemma 2.7 to get

\[
\limsup_{n \to \infty} W_p(S_n, \mu_n) \leq \limsup_{n \to \infty} \left( c_{p, \varepsilon}(\bar{d}_H(S_n, S))^p + (1 + \varepsilon)W_p(S, \mu_n) \right)
= (1 + \varepsilon) \limsup_{n \to \infty} W_p(S, \mu_n)
= (1 + \varepsilon)W_p(S, \mu)
\]

and

\[
W_p(S, \mu) = \liminf_{n \to \infty} W_p(S, \mu_n)
\leq \liminf_{n \to \infty} \left( c_{p, \varepsilon}(\bar{d}_H(S, S_n))^p + (1 + \varepsilon)W_p(S_n, \mu_n) \right)
= (1 + \varepsilon) \liminf_{n \to \infty} W_p(S_n, \mu_n).
\]
Combining these inequalities and taking \( \varepsilon \downarrow 0 \) gives
\[
\limsup_{n \to \infty} W_p(S_n, \mu_n) \leq W_p(S, \mu) \leq \liminf_{n \to \infty} W_p(S_n, \mu_n),
\]
as claimed. \( \square \)

3. The Clustering Map

In this section, we show that various natural maps used in the construction of clustering algorithms are continuous with respect to various topologies of spaces of measures, space of sets, and on spaces of sets of sets. In particular, we show Proposition 3.3 which gives “continuity” of the clustering map in Kuratowski upper sense and Proposition 3.13 which gives “continuity” of the clustering map in the Hausdorff upper sense. We also have Lemma 3.14 which provides sufficient conditions for the continuity of the adaptive choice of \( k \) arising in the elbow-method.

To begin we give the basic notions of the clustering operations of interest.

**Definition 3.1.** For \( \mu \in \mathcal{P}_p(X) \), \( k \in \mathbb{N} \), and \( R \in C(X) \), set
\[
m_{k, p}(\mu, R) := \inf_{S \subseteq R} \{ \min_{1 \leq \#S' \leq k} W_p(S', \mu) \},
\]
and also set \( C_p(\mu, k, R) \) to be the set of all \( S \subseteq R \) with \( 1 \leq \#S \leq k \) satisfying
\[
W_p(S, \mu) \leq m_{k, p}(\mu, R).
\]
If a set \( S \subseteq X \) has \( S \subseteq R \) and \( 1 \leq \#S \leq k \) it is called feasible and if it achieves \( 3.2 \) it is called optimal. Note that \( C_p(\mu, k, R) \) is empty if there are no optimal sets or if \( R \) is empty. We refer to \( C_p(\mu, k, R) \) as the set of sets of Fréchet clustering centers.

In order to apply the natural set-valued notions of convergence to this map \( C \), one needs to verify that it takes values in a suitably nice space of subsets of \( K(X) \). In other words, we need to establish some basic regularity in order for notions of convergence of sets to be well-defined.

**Lemma 3.2.** For \( (\mu, k, R) \in \mathcal{P}_p(X) \times \mathbb{N} \times C(X) \), we have \( C_p(\mu, k, R) \in C(K(X)) \).

**Proof.** Suppose \( \{S_n \}_{n \in \mathbb{N}} \) in \( C_p(\mu, k, R) \) have \( d_H(S_n, S) \to 0 \) for \( S \in K(X) \). For any \( x \in S \) there must exist \( x_n \in S_n \subseteq R \) for all \( n \in \mathbb{N} \) with \( x_n \to x \), so \( R \) being closed implies \( x \in R \), hence \( S \subseteq R \). Moreover, Lemma 2.3 implies \( \#S = \lim_{n \to \infty} \#S_n \leq k \). Thus, \( S \) is feasible. Finally, by Lemma 2.8 we have
\[
W_p(S, \mu) = \lim_{n \to \infty} W_p(S_n, \mu) \leq m_{k, p}(\mu, R),
\]
so \( S \) is optimal. Therefore, \( S \in C_p(\mu, k, R) \). \( \square \)

Now we have the first of our main “continuity” results.

**Proposition 3.3.** If \( \{ (\mu_n, k_n, R_n) \}_{n \in \mathbb{N}} \) and \( (\mu, k, R) \) in \( \mathcal{P}_p(X) \times \mathbb{N} \times C(X) \) satisfy
(i) \( \mu_n \to \mu \) in \( \tau_{\mathbb{N}}^\mu \),
(ii) \( k_n \neq k \) for finitely many \( n \in \mathbb{N} \), and
(iii) \( \text{Lt}_{n \in \mathbb{N}} R_n = R \) in \( C(X) \),
then we have
\[
\text{Lt}_{n \in \mathbb{N}} C_p(\mu_n, k_n, R_n) \subseteq C_p(\mu, k, R) \subseteq C(K(X))
\]
Proof. Take any $S \in \text{Ls}_{n \in \mathbb{N}} C(\mu_n, k_n, R_n)$ so that there exists \( \{n_j\}_{j \in \mathbb{N}} \) and \( S_j \in C_p(\mu_{n_j}, k_{n_j}, R_{n_j}) \) for each \( j \in \mathbb{N} \) satisfying \( S_j \to S \) in \( d_H \). First we show that \( S \) is feasible. Indeed, for each \( x \in S \), there exist points \( x_j \in S_j \subseteq R_{n_j} \) for all \( j \in \mathbb{N} \) with \( x_j \in x \), hence \( x \in \text{Ls}_{j \in \mathbb{N}} R_{n_j} \subseteq \text{Ls}_{n \in \mathbb{N}} R_n \subseteq R \). Likewise, Lemma 2.3 implies \( \#S = \lim_{j \to \infty} \#S_j \leq k \). Thus, we have \( S \subseteq R \) with \( 1 \leq \#S \leq k \), so \( S \) is feasible.

Next, take arbitrary \( S' \subseteq R \) with \( 1 \leq \#S' \leq k \). Since \( R \subseteq \text{Ls}_{n \in \mathbb{N}} R_n \), one can get a further subsequence \( \{j_i\}_{i \in \mathbb{N}} \) and some \( S'_{j_i} \subseteq R_{n_{j_i}} \) with \( \#S'_{j_i} \leq k \) for each \( i \in \mathbb{N} \) satisfying \( S'_{j_i} \to S' \) in \( d_H \). Then for \( \varepsilon > 0 \) we can use (2.5) and Lemma 2.7 to bound:

\[
W_p(S, \mu) = \lim_{i \to \infty} W_p(S_{j_i}, \mu_{n_{j_i}}) \\
\leq \liminf_{i \to \infty} (W_p(S'_{j_i}, \mu_{n_{j_i}})) \\
\leq \liminf_{i \to \infty} (c_{p, \varepsilon} (d_H(S'_{j_i}, S'))^p + (1 + \varepsilon) W_p(S', \mu_{n_{j_i}})) \\
= (1 + \varepsilon) \liminf_{i \to \infty} W_p(S', \mu_{n_{j_i}}) \\
= (1 + \varepsilon) W_p(S', \mu).
\]

Now take \( \varepsilon \to 0 \) and the infimum over all feasible \( S' \) to get

\[
W_p(S, \mu) \leq m_{k, p}(\mu, R).
\]

This shows that \( S \) is optimal. Therefore, \( S \in C_p(\mu, k, R) \), as claimed.

The preceding result shows that the clustering operation \( C \) is “continuous” when its codomain is endowed with the Kuratowski upper sense of convergence; already this will be enough to recover the result of Pollard and a few important extensions. Nonetheless, it is natural to push this idea further. That is, we wonder whether \( C \) is “continuous” when its codomain is endowed with the upper Hausdorff sense of convergence. More concretely, we wonder which further hypotheses need to be added to the setting of Proposition 3.3 in order to guarantee

\[
\text{(3.4)} \quad \tilde{d}_H(C_p(\mu_n, k_n, R_n), C_p(\mu, k, R)) \to 0.
\]

If true, this would provide a more quantitative notion of convergence.

Of course, some regularity beyond that of Lemma 3.2 must be established in order for (3.4) to be well-defined. First of all, we need \( C_p(\mu, k, R) \) and \( C_p(\mu_n, k_n, R_n) \) for \( n \in \mathbb{N} \) be non-empty. Second, while it appears that we need \( C_p(\mu, k, R) \) and \( C_p(\mu_n, k_n, R_n) \) for \( n \in \mathbb{N} \) to be \( d_H \)-compact, we observed in Remark 2.1 that one can make sense of the expressions as taking values in \( [0, \infty] \) in the general case; thus, all that is truly needed is that \( C_p(\mu_n, k_n, R_n) \) is compact for sufficiently large \( n \in \mathbb{N} \). We will show, through a series of intermediate results, that these regularity conditions are satisfied under very mild assumptions.

First we concern ourselves with the question of non-emptiness. It turns out that a natural setting for this question is that in which \( (X, d) \) is a Heine-Borel space. The following pair of results, which are closely related but slightly different, will be used many times throughout the remainder of this paper.

**Lemma 3.4.** Take a Heine-Borel space \( (X, d) \) and any \( \{\text{(}\mu_n, k_n, R_n\text{)}\}_{n \in \mathbb{N}} \) and \( (\mu, k, R) \) in \( \mathcal{P}_p(X) \times \mathbb{N} \times C(X) \) such that \( R \) is non-empty, and

\begin{align*}
\text{(i)} & \quad \mu_n \to \mu \text{ in } \tau^*_p, \\
\text{(ii)} & \quad k_n \neq k \text{ for finitely many } n \in \mathbb{N}, \text{ and} \\
\text{(iii)} & \quad \text{Lt}_{n \in \mathbb{N}} R_n = R \text{ in } C(X).
\end{align*}
Then, for any \( \{S_n\}_{n \in \mathbb{N}} \) in \( K(X) \) with \( S_n \in C_p(\mu_n, k_n, R_n) \) for all \( n \in \mathbb{N} \), there exists a subsequence \( \{n_j\}_{j \in \mathbb{N}} \) and some \( S \in C_p(\mu, k, R) \) such that \( \bar{d}_H(S, S_{n_j}) \to 0 \).

**Proof.** Take any \( o \in R \), and compute:

\[
\left( \bar{d}_H(\{o\}, S_n) \right)^p = \min_{x \in S_n} d^p(o, x_n) \\
\leq 2^{p-1} \left( \int_X d^p(o, y) d\mu_n(y) + \int_X \min_{x_n \in S_n} d^p(x_n, y) d\mu_n(y) \right) \\
= 2^{p-1} \left( W_p(\{o\}, \mu_n) + W_p(S_n, \mu_n) \right).
\]

Since \( o \in R \subseteq \bigcup_{n \in \mathbb{N}} R_n \), we can get \( o_n \in R_n \) for sufficiently large \( n \in \mathbb{N} \) such that \( o_n \to o \). Then applying the optimality of \( S_n \) for \( n \in \mathbb{N} \), taking \( n \to \infty \), and applying Lemma 2.8, we get:

\[
\limsup_{n \to \infty} \left( \bar{d}_H(\{o\}, S_n) \right)^p \leq 2^{p-1} \limsup_{n \to \infty} \left( W_p(\{o\}, \mu_n) + W_p(S_n, \mu_n) \right) \\
\leq 2^{p-1} \limsup_{n \to \infty} \left( W_p(\{o\}, \mu_n) + W_p(\{o_n\}, \mu_n) \right) \\
\leq 2^p W_p(\{o\}, \mu).
\]

Since the right side above is finite, we use Lemma 2.6 to get some subsequence \( \{n_j\}_{j \in \mathbb{N}} \) and some \( S \in K(X) \) with \( \bar{d}_H(S, S_{n_j}) \to 0 \) as \( j \to \infty \). Since \( S_{n_j} \subseteq R_{n_j} \) for all \( j \in \mathbb{N} \), this implies \( S \subseteq \bigcup_{j \in \mathbb{N}} R_{n_j} \subseteq R \). Also, Lemma 2.3 implies \( \#S \leq \liminf_{j \to \infty} \#S_{n_j} = k \). Thus, \( S \) is feasible. In fact, for any \( \varepsilon > 0 \) we can use (2.5) and Lemma 2.7 to bound:

\[
W_p(S, \mu) \leq \liminf_{j \to \infty} (c_{p, \varepsilon}(\bar{d}_H(S, S_{n_j}))^p + (1 + \varepsilon) W_p(S_{n_j}, \mu) \\
= (1 + \varepsilon) \liminf_{j \to \infty} W_p(S_{n_j}, \mu) \\
= (1 + \varepsilon) m_{k,p}(\mu, R).
\]

So, taking \( \varepsilon \to 0 \) gives that \( S \) is optimal. This gives \( S \in C_p(\mu, k, R) \), as needed. \( \Box \)

**Lemma 3.5.** Take any Heine-Borel space \( (X, d) \) and any \( \mu \in \mathcal{P}_p(X) \), \( k \in \mathbb{N} \), and non-empty \( R \in C(X) \). If \( \{S_n\}_{n \in \mathbb{N}} \) in \( K(X) \) have \( S_n \subseteq R \) and \( 1 \leq \#S_n \leq k \) for \( n \in \mathbb{N} \), as well as

\[
W_p(S_n, \mu) \to m_{k,p}(\mu, R),
\]

then there exists a subsequence \( \{n_j\}_{j \in \mathbb{N}} \) and \( S \in C_p(\mu, k, R) \) with \( \bar{d}_H(S, S_{n_j}) \to 0 \).

**Proof.** For any \( o \in R \) we compute:

\[
\left( \bar{d}_H(\{o\}, S_n) \right)^p = \min_{x_n \in S_n} d^p(o, x_n) \\
\leq 2^{p-1} \left( \int_X d^p(o, y) d\mu(y) + \int_X \min_{x_n \in S_n} d^p(x_n, y) d\mu(y) \right) \\
= 2^{p-1} \left( W_p(\{o\}, \mu) + W_p(S_n, \mu) \right).
\]

Thus taking \( n \to \infty \) yields

\[
\limsup_{n \to \infty} \left( \bar{d}_H(\{o\}, S_n) \right)^p \leq 2^{p-1} \left( W_p(\{o\}, \mu) + \lim_{n \to \infty} W_p(S_n, \mu) \right) \\
= 2^{p-1} \left( W_p(\{o\}, \mu) + m^k_p(\mu, R) \right) \\
\leq 2^p W_p(\{o\}, \mu).
\]
Since the right side above is finite, we use Lemma 2.6 to get some subsequence \( \{n_j\}_{j \in \mathbb{N}} \) and some \( S \in K(X) \) with \( d_H(S,S_{n_j}) \to 0 \) as \( j \to \infty \). Since \( S_{n_j} \subseteq R \) for all \( j \in \mathbb{N} \) and \( R \) is closed, this implies \( S \subseteq R \). Also, Lemma 2.3 implies \( \#S \leq \liminf_{j \to \infty} \#S_{n_j} \leq k \). Thus, \( S \) is feasible. In fact, for any \( \varepsilon > 0 \) we can use (2.5) and Lemma 2.7 to bound:

\[
W_p(S, \mu) \leq \liminf_{j \to \infty} c_{p,\varepsilon}(\delta_H(S,S_{n_j}))^p + (1 + \varepsilon)W_p(S_{n_j}, \mu) \\
= (1 + \varepsilon)\liminf_{j \to \infty} W_p(S_{n_j}, \mu) \\
= (1 + \varepsilon)m_{k,p}(\mu, R)
\]

So, taking \( \varepsilon \to 0 \) gives that \( S \) is optimal. This gives \( S \in C_p(\mu, k, R) \), as needed. \( \square \)

**Lemma 3.6.** For \((X,d)\) a Heine-Borel space and \( \mu \in \mathcal{P}_p(X) \), \( k \in \mathbb{N} \), and non-empty \( R \in C(X) \), we have that \( C_p(\mu, k, R) \) is non-empty.

**Proof.** Take \( \{S_n\}_{n \in \mathbb{N}} \) in \( K(X) \) such that we have \( S_n \subseteq R \) and \( \#S_n \leq k \) for all \( n \in \mathbb{N} \), as well as

\[
W_p(S_n, \mu) \to m_{k,p}(\mu, R).
\]

By Lemma 3.5, there exists \( S \in C_p(\mu, k, R) \), so \( C_p(\mu, k, R) \) is non-empty. \( \square \)

Next we need to verify \( d_H \)-compactness. To see that it is not always satisfied, we have the following pathological but illustrative example.

**Example 3.7.** Take \( X := \mathbb{R} \) with its usual metric, \( p \geq 1 \) arbitrary, \( \mu := \delta_0 \), and \( k := 2 \). Then, for any \( x \in \mathbb{R} \) the set \( S_x := \{0, x\} \) is an optimal set of cluster centers, that is, it lies in \( C_{2,p}(\delta_0) \). Note \( d_H(S_0, S_n) \to \infty \) as \( n \to \infty \). This means the family \( \{S_x\}_{x \in \mathbb{R}} \) is not \( d_H \)-bounded. By Lemma 2.5 and Lemma 3.2, we know that \( d_H \)-compactness is equivalent to \( d_H \)-boundedness in \( K(\mathbb{R}) \), hence \( C_{2,p}(\delta_0) \) is not \( d_H \)-compact.

The root cause of the pathology in the preceding example is that we have \( m_{k,p}(\mu, R) = m_{k',p}(\mu, R) \) for some \( k' < k \). Pollard already identified this issue in [22], at least for the case of \( R = X \), stating “In that case the whole theorem falls apart, because at least one cluster center is free to wander where it will.” He goes on to explain that the problem in this case is that there is necessarily non-uniqueness of the set of optimal cluster centers. While there indeed is non-uniqueness, this is not really an issue; note that we have already proved Proposition 3.3 under no assumptions about uniqueness. Instead, we proffer that the undesirable issue in this case is that the set of optimal sets of cluster centers is not \( d_H \)-compact. Towards removing this pathology, we consider the following.

**Definition 3.8.** We say that \( (\mu, k, R) \in \mathcal{P}_p(X) \times \mathbb{N} \times C(X) \) is non-singular if \( m_{1,p}(\mu, R) < m_{2,p}(\mu, R) < \ldots < m_{k,p}(\mu, R) \) and singular otherwise.

**Lemma 3.9.** If \((X,d)\) is a Heine-Borel space and \( (\mu, k, R) \in \mathcal{P}_p(X) \times \mathbb{N} \times C(X) \) is non-singular, then we have \( C_p(\mu, k, R) \in K(K(X)) \).

**Proof.** By Lemma 2.5, Lemma 3.2, and Lemma 3.6, it suffices to show that \( C_p(\mu, k, R) \) is \( d_H \)-bounded. Towards a contradiction, assume that there were a sequence \( \{S_n\}_{n \in \mathbb{N}} \) in \( C_p(\mu, k, R) \) such that for some (equivalently, all) \( S' \in K(X) \) we have \( d_H(S', S_n) \to \infty \). By non-singularity, we have \( \#S_n = k \) for all \( n \in \mathbb{N} \). By Lemma 3.6, there is some \( \{n_j\}_{j \in \mathbb{N}} \) and some \( S \in C_p(\mu, k, R) \) such that we
have \( d_H(S, S_n) \to 0 \). Applying non-singularity again, we have \( \#S = k \). Finally, Lemma 2.4 upgrades \( d_H(S, S_{n_j}) \to 0 \) to \( d_H(S, S_n) \to 0 \), and this contradicts the assumption that we have \( d_H(S', S_n) \to \infty \) for all \( S' \in K(X) \). Therefore, \( C_p(\mu, k, R) \) is indeed \( d_H \)-bounded.

\[ \]

**Lemma 3.10.** If \( (X, d) \) is a Heine-Borel space and if \( \{(\mu_n, R_n)\}_{n \in \mathbb{N}} \) in \( \mathcal{P}_p(X) \times C(X) \) and \((\mu, k, R)\) in \( \mathcal{P}_p(X) \times \mathbb{N} \times C(X) \) are such that \((\mu, k, R)\) is non-singular and

\begin{align*}
(i) & \quad \mu_n \to \mu \text{ in } \tau^*_u, \text{ and} \\
(ii) & \quad \lim_{n \in \mathbb{N}} R_n = R \text{ in } C(X),
\end{align*}

then \( m_{k', p}(\mu_n, R_n) \to m_{k', p}(\mu, R) \) for all \( 1 \leq k' \leq k \).

**Proof.** Let us show that any subsequence of \( \{m_{k', p}(\mu_n, R_n)\}_{n \in \mathbb{N}} \) has a further subsequence converging to \( m_{k', p}(\mu, R) \). Indeed, take arbitrary \( \{n_j\}_{j \in \mathbb{N}} \) and, for each \( j \in \mathbb{N} \) use Lemma 3.6 to get \( S_j \subseteq C_{k', p}(\mu_n, R_n) \). That is, we have \( S_j \subseteq R_{n_j} \), \( 1 \leq \#S_j \leq k' \), and \( W_p(S_j, \mu_{n_j}) = m_{k', p}(\mu_{n_j}, R_{n_j}) \) for all \( j \in \mathbb{N} \). By Lemma 3.4, there exist \( \{n_j\} \subseteq \mathbb{N} \) and \( S \subseteq C_{k', p}(\mu, R) \) with \( d_H(S, S_{n_j}) \to 0 \) as \( i \to \infty \). By Lemma 2.3, we have \( \#S \leq \liminf_{i \to \infty} \#S_j \leq k' \), and also \( W_p(S, \mu) = m_{k', p}(\mu, R) \), hence \( \#S = k' \) by non-singularity. In particular, we have \( \#S_{n_j} = k \) for sufficiently large \( i \in \mathbb{N} \). Thus, Lemma 2.4 implies \( d_H(S, S_{n_j}) \to 0 \) as \( i \to \infty \). Finally, by Lemma 2.8 we have

\[ m_{k', p}(\mu_{n_j}, R_{n_j}) = W_p(S_{j_n}, \mu_{n_j}) \to W_p(S, \mu) = m_{k', p}(\mu, R) \]

as \( i \to \infty \).

We now give two simple results for demonstrating non-singularity.

**Lemma 3.11.** If \( (X, d) \) has the Heine-Borel property and \((\mu, k, R)\) in \( \mathcal{P}_p(X) \times \mathbb{N} \times C(X) \) satisfy \( k \leq \#(R \cap \supp(\mu)) \), then \((\mu, k, R)\) is non-singular.

**Proof.** Take any \( 1 < k' \leq k \), and, by Lemma 3.6, get some \( S' \subseteq C_p(\mu, k' - 1, R) \). That is, we get some \( S' \in K(X) \) with \( S' \subseteq R, 1 \leq \#S' < k' \), and \( W_p(S', \mu) = m_{k', p}(\mu, R) \). Now take any \( x' \in (R \cap \supp(\mu)) \setminus S' \), and set \( S := S' \cup \{x'\} \). Assume for the sake of contradiction that we have \( W_p(S, \mu) \geq W_p(S', \mu) \). Since we obviously have

\[ \min_{x \in S} d^p(x, y) \leq \min_{x \in S'} d^p(x, y) \]

for all \( y \in X \), this implies

\[ \min_{x \in S} d^p(x, y) = \min_{x \in S'} d^p(x, y) \]

for \( \mu \)-almost all \( y \in X \). Now choose \( r > 0 \) small enough so that for all \( y \in B^d_r(x') \) we have

\[ \min_{x \in S} d^p(x, y) = d^p(x', y) \]

hence

\[ \min_{x \in S} d^p(x, y) < \min_{x \in S'} d^p(x, y). \]

But \( \mu(B^d_r(x')) > 0 \) since \( x' \in \supp(\mu) \), and this is a contradiction. Thus we have

\[ m_{k', p}(\mu, R) \leq W_p(S, \mu) < W_p(S', \mu) = m_{k'-1, p}(\mu, R), \]

and this proves the claim.
Lemma 3.12. If \((X, d)\) is a Heine-Borel space and if \(\{(\mu_n, k_n, R_n)\}_{n \in \mathbb{N}}\) and \((\mu, k, R)\) in \(\mathcal{P}_p(X) \times \mathbb{N} \times C(X)\) are such that \((\mu, k, R)\) is non-singular and

(i) \(\mu_n \to \mu\) in \(\tau_{\mu}^p\),
(ii) \(k_n \neq k\) for finitely many \(n \in \mathbb{N}\), and
(iii) \(\lim_{n \to \infty} R_n = R\) in \(C(X)\)

then \((\mu_n, k_n, R_n)\) is non-singular for sufficiently large \(n \in \mathbb{N}\).

Proof. Set \(\varepsilon := \min\{m_{k',p}(\mu, R) - m_{k-1,p}(\mu, R) : 1 < k' \leq k\}\), which is strictly positive by \((\mu, k, R)\) being non-singular. By Lemma 3.10, we can take \(n \in \mathbb{N}\) sufficiently large to get \(|m_{k',p}(\mu_n, R_n) - m_{k-1,p}(\mu, R)| < \varepsilon/2\), and for such \(n\) we have \(m_{1,p}(\mu_n, R_n) < \cdots < m_{k,p}(\mu_n, R_n)\), hence \((\mu_n, k_n, R_n)\) is non-singular. \(\square\)

Having carefully studied these notions, we prove the following continuity-type result, under the Heine-Borel and non-singularity assumptions.

Proposition 3.13. Take a Heine-Borel space \((X, d)\), and any \(\{(\mu_n, k_n, R_n)\}_{n \in \mathbb{N}}\) and \((\mu, k, R)\) in \(\mathcal{P}_p(X) \times \mathbb{N} \times C(X)\) such that \((\mu, k, R)\) is non-singular, and

(i) \(\mu_n \to \mu\) in \(\tau_{\mu}^p\),
(ii) \(k_n \neq k\) for finitely many \(n \in \mathbb{N}\), and
(iii) \(\lim_{n \to \infty} R_n = R\) in \(C(X)\).

Then we have

\[
\tilde{d}_H(C_p(\mu_n, k_n, R_n), C_p(\mu, k, R)) \to 0
\]

in \(K(K(X))\).

Proof. First, note that Lemma 3.9 implies \(C_p(\mu, k, R) \in K(K(X))\) and that Lemma 3.12 implies \(C_p(\mu_n, k_n, R_n) \in K(K(X))\) for sufficiently large \(n \in \mathbb{N}\). Thus, (3.5) is finite for sufficiently large \(n \in \mathbb{N}\). (See Remark 2.1.) Now we show \(\tilde{d}_H(C_p(\mu_n, k_n, R_n), C_p(\mu, k, R)) \to 0\) by showing that any subsequence of \(\{\tilde{d}_H(C_p(\mu_n, k_n, R_n), C_p(\mu, k, R))\}_{n \in \mathbb{N}}\) has a further subsequence converging to zero. Indeed, this follows immediately from Lemma 3.4. \(\square\)

Finally, we study the continuity of the adaptive choice of \(k\) arising in the elbow method. To do this, we let \(\mu \in \mathcal{P}_p(X)\) be arbitrary, and we define

\[
\Delta^2 m_{k,p}(\mu) := k_{k+1,p}(\mu) + m_{k-1,p}(\mu) - 2m_{k,p}(\mu)
\]

for \(k \geq 2\) as well as \(\Delta^2 m_{1,p}(\mu) := m_{2,p}(\mu) - 2m_{1,p}(\mu)\). This is equivalent to taking the convention \(m_{0,p}(\mu) = 0\), but other choices are, of course, possible. Then we define the function \(k_{p}^{elb}(\mu) : \mathcal{P}_p(X) \to \mathbb{N} \cup \{\infty\}\) via

\[
k_{p}^{elb}(\mu) := \min\{\arg\max\{\Delta^2 m_{k,p}(\mu) : k \in \mathbb{N}\}\}
\]

for \(\mu \in \mathcal{P}_p(X)\). Now we have the following.

Lemma 3.14. Suppose that \((X, d)\) is a Heine-Borel space and that \(\mu \in \mathcal{P}_p(X)\) satisfies \#supp(\(\mu\)) = \(\infty\) and \#arg\max(\{\Delta^2 m_{k,p}(\mu) : k \in \mathbb{N}\}) = 1. Then, the function \(k_{p}^{elb} : \mathcal{P}_p(X) \to \mathbb{N}\) is continuous at \(\mu\).

Proof. First, note that we have \(m_{k,p}(\mu) \to 0\) as \(k \to \infty\), hence \(\Delta^2 m_{k,p}(\mu) \to 0\) as \(k \to \infty\). In particular, the value \(M := \max\{\Delta^2 m_{k,p}(\mu) : k \in \mathbb{N}\}\) is finite, and, by assumption, there is a unique \(k_* \in \mathbb{N}\) such that \(M = \Delta^2 m_{k_*,p}(\mu)\).
Now suppose that \( \{\mu_n\}_{n \in \mathbb{N}} \) have \( \mu_n \to \mu \) in \( \tau_w^p \), and fix any \( o \in X \). A well-known property of the Wasserstein topology (see Definition 6.8(iii)[30], or apply uniform integrability) is that we can choose \( R \geq 0 \) large enough so that

\[
\limsup_{n \to \infty} \int_{X \setminus B_R(o)} d^p(o, y) \, d\mu_n(y) \leq \frac{M}{16}. \tag{3.6}
\]

Now let \( K_0 \) be an \( (M/16)^{1/p} \)-net of \( B_R(o) \), and set \( K := K_0 \cup \{o\} \). Also, define \( \ell := \#K \). By construction, we can bound:

\[
sup_{k \geq \ell} m_{k,p}(\mu_n) = \sup_{k \geq \ell} \inf_{1 \leq \#S \leq k} \int_X \min_{x \in S} d^p(x, y) \, d\mu_n(y) \\
\leq \int_{X \setminus B_R(o)} \min_{x \in K} d^p(x, y) \, d\mu_n(y) \\
= \int_{B_R(o)} \min_{x \in K} d^p(x, y) \, d\mu_n(y) + \int_{X \setminus B_R(o)} \min_{x \in K} d^p(x, y) \, d\mu_n(y) \\
\leq \mu(B_R(o)) \frac{M}{16} + \int_{X \setminus B_R(o)} d^p(o, y) \, d\mu_n(y).
\]

Thus, taking \( n \to \infty \) and applying (3.6) yields

\[
\limsup_{n \to \infty} \sup_{k \geq \ell} m_{k,p}(\mu_n) \leq \frac{M}{8}.
\]

Now simply apply the triangle inequality to get

\[
\limsup_{n \to \infty} \sup_{k \geq \ell} \Delta^2 m_{k,p}(\mu_n) \leq \frac{M}{2}.
\]

This means that, for sufficiently large \( n \in \mathbb{N} \), the maximum of \( \{\Delta^2 m_{k,p}(\mu_n) : k \in \mathbb{N}\} \) is not achieved on \( \{\ell, \ell + 1, \ldots\} \).

Finally, set

\( \varepsilon := \min\{|\Delta^2 m_{k,p}(\mu) - \Delta^2 m_{k',p}(\mu)| : k, k' \leq \ell, k \neq k'\} > 0 \).

By Lemma 3.10, there is sufficiently large \( n \in \mathbb{N} \) such that we have \( |m_{k,p}(\mu_n) - m_{k,p}(\mu)| < \frac{\varepsilon}{2} \) for all \( k \leq \ell \). Combining this with the above shows that, for sufficiently large \( n \in \mathbb{N} \), we have

\[
\arg\max\{\Delta^2 m_{k,p}(\mu_n) : k \in \mathbb{N}\} = \arg\max\{\Delta^2 m_{k,p}(\mu) : k \in \mathbb{N}\} = \{k_*\},
\]

hence \( k_{E,p}^{\text{arb}}(\mu_n) = k_E(\mu) \). \( \square \)

The condition \( \#\arg\max\{\Delta^2 m_{k,p}(\mu) : k \in \mathbb{N}\} = 1 \) should be interpreted as saying that the distribution \( \mu \) has a uniquely-defined number of clusters, in the sense of the elbow method. Thus, the preceding result says that, if \( \mu_n \to \mu \) in \( \tau_w^p \) and \( \mu \) has a uniquely-defined number of clusters, then the same is true for \( \mu_n \) for sufficiently large \( n \in \mathbb{N} \).

4. Probabilistic Results

We now show how the considerations of the previous section can be used to prove a number of limit theorems for clustering algorithms of interest in statistical applications. More precisely, Subsection 4.1 addresses the main question of strong consistency under IID samples. We then consider two secondary questions. That
is, in Subsection 4.2 we address the question of large deviations estimates for \((k, p)\)-means under IID data, and, in Subsection 4.3 we address the question of strong consistency for \((k, p)\)-medoids under data coming from a MC.

For this section, we let \((X, d)\) be a metric space and \(1 \leq p < \infty\). An underlying probability space will be denoted \((\Omega, \mathcal{F}, \mathbb{P})\) and will be assumed to be complete.

**Remark 4.1.** One may be concerned about the measurability of the “events” appearing throughout this section. As the proofs all demonstrate, these events are supersets of bona fide events whose \(\mathbb{P}\)-probabilities are equal to one, hence they are at least measurable with respect to the \(\mathbb{P}\)-completion of \(\mathcal{F}\). For this reason we will not address further questions of measurability in this paper; the interested reader should see [11, Section 3] for a resolution of similar measurability concerns in the context of Fréchet means, which is equivalent to fixing \(k = 1\) in the current work.

### 4.1. Strong Consistency for IID data.

Suppose that \(Y_1, Y_2, \ldots\) is an IID sequence of random variables with common distribution \(\mu \in \mathcal{P}_p(X)\), and define the empirical measures via \(\bar{\mu}_n := \frac{1}{n} \sum_{i=1}^n \delta_{Y_i}\) for all \(n \in \mathbb{N}\). First, we have the following fundamental strong consistency results, which follow easily from our preparations.

**Proof of Theorem 1.1.** By [11, Proposition 4.1], we have \(\bar{\mu}_n \to \mu\) in \(\tau_p^\infty\) almost surely. Thus, the result follows from Proposition 3.3. \(\square\)

**Proof of Theorem 1.2.** As above, we have by [11, Proposition 4.1] that \(\bar{\mu}_n \to \mu\) in \(\tau_p^\infty\) almost surely, so we conclude by Proposition 3.13. \(\square\)

Next, we show that these results, in particular Theorem 1.2, have immediate consequences for more concrete statistical settings of interest. Indeed, let us assume the setting of the enumerated points of the introduction, where \(X = \mathbb{R}^m\) for \(m \in \mathbb{N}\) with the metric induced by its usual \(\ell_2\) norm, \(\| \cdot \|\). Suppose that \(\mu \in \mathcal{P}_p(\mathbb{R}^m)\) has \#supp(\(\mu\)) = \(\infty\) and \(\int_{\mathbb{R}^m} \| y \|^p \, d\mu(y) < \infty\). Then by taking \(R_n = R = \mathbb{R}^d\) and \(k_n = k\) for all \(n \in \mathbb{N}\), we have

\[
\max_{S_n \in C_{k,p}^\infty(\bar{\mu}_n)} \min_{S \in C_{k,p}(\mu)} \| H(S_n, S) \| \to 0
\]

almost surely, which establishes (i). Alternatively, we can take \(R = \text{supp}(\mu)\), as well as \(R_n = \text{supp}(\bar{\mu}_n)\) and \(k_n = k\) for all \(n \in \mathbb{N}\). By [11, Proposition 4.2] we have \(\text{Lt}_{n \in \mathbb{N}} \text{supp}(\bar{\mu}_n) = \text{supp}(\mu)\) almost surely, and this implies

\[
\max_{S_n \in C_{k,p}^\infty(\bar{\mu}_n)} \min_{S \in C_{k,p}(\mu)} \| H(S_n, S) \| \to 0
\]

almost surely, whence (ii). Finally, we consider \(R_n = \mathbb{R}^m\) and \(k_n = k_{p}^{\text{elb}}(\bar{\mu}_n)\) for all \(n \in \mathbb{N}\), as well as \(R = \mathbb{R}^m\) and \(k = k_{p}^{\text{elb}}(\mu)\). If \(\# \arg\max\{\Delta^2 m_{k,p}(\mu) : k \in \mathbb{N}\} = 1\), then by Lemma 3.14 we have \(k_{p}^{\text{elb}}(\bar{\mu}_n) \neq k_{p}^{\text{elb}}(\mu)\) finitely often almost surely, hence

\[
\max_{S_n \in C_{p}^{\text{med}}(\bar{\mu}_n)} \min_{S \in C_{p}^{\text{med}}(\mu)} \| H(S_n, S) \| \to 0
\]

almost surely.

Lastly, let us address a computational application of these results. Indeed, we return to the general setting, and we suppose \(\text{supp}(\mu) = X\) and \(k \in \mathbb{N}\). Then we have \(C_{k,p}^{\text{med}}(\mu) = C_{k,p}(\mu)\), hence

\[
\max_{S_n \in C_{k,p}^{\text{med}}(\bar{\mu}_n)} \min_{S \in C_{k,p}(\mu)} \| H(S_n, S) \| \to 0
\]
almost surely. Roughly speaking, this means that each set of empirical \((k,p)\)-medoids cluster centers must be close to some set of population \((k,p)\)-means cluster centers, at least asymptotically. To see that this is interesting, recall on the one hand that there is no known algorithm to exactly compute the empirical \((k,p)\)-means cluster centers of \(n\) data points, and observe on the other hand that the empirical \((k,p)\)-medoids cluster centers of \(n\) data points can be computed exactly in \(O(Dkn^{k+1})\) time, where \(D\) is the time of computing the distance between any two points. Thus, it is interesting to notice that the empirical \((k,p)\)-medoids problem can be consistently used as a surrogate for the harder \((k,p)\)-means problem. Although the cost of exactly computing \((k,p)\)-medoids is certainly prohibitively large, we believe that it would be interesting to try to develop efficient randomized algorithms for this task, in the same spirit as [3].

4.2. Large Deviations for IID data. As in the previous subsection, suppose that \(Y_1, Y_2, \ldots\) is an IID sequence of random variables with common distribution \(\mu\), and define the empirical measures via \(\bar{\mu}_n := \frac{1}{n} \sum_{i=1}^n \delta_{Y_i}\) for all \(n \in \mathbb{N}\). We have already established the almost sure convergence

\[
\max_{S_n \in C_{k,p}(\bar{\mu}_n)} \min_{S \in C_{k,p}(\mu)} d_H(S_n, S) \to 0,
\]

and this of course implies the convergence in probability

\[
\mathbb{P} \left( \max_{S_n \in C_{k,p}(\bar{\mu}_n)} \min_{S \in C_{k,p}(\mu)} d_H(S_n, S) \geq \varepsilon \right) \to 0,
\]

for all \(\varepsilon > 0\). Presently, we address the question of determining the rate at which these probabilities decay to zero. This is the domain of large deviations theory, the basics of which can be found in [10].

To perform this analysis, let us, for a probability measure \(\nu \in \mathcal{P}(X)\), write \(\nu \ll \mu\) to mean that \(\nu\) is absolutely continuous with respect to \(\mu\); if \(\nu \ll \mu\), write \(d\nu/d\mu\) for the Radon-Nikodym derivative of \(\nu\) with respect to \(\mu\). Then define the map \(H(\cdot|\mu) : \mathcal{P}(X) \to [0, \infty]\) via

\[
H(\nu|\mu) = \begin{cases} 
\int_X \frac{d\nu}{d\mu} \log \left( \frac{d\nu}{d\mu} \right) d\mu, & \text{if } \nu \ll \mu, \\
\infty, & \text{if } \nu \not\ll \mu,
\end{cases}
\]

for \(\nu \in \mathcal{P}(X)\). We call \(H(\nu|\mu)\) the relative entropy of \(\nu\) from \(\mu\) or KL divergence from \(\mu\) to \(\nu\).

The key to proving our large deviations upper bound is applying a type of contraction to an existing large deviations principle for the empirical measures \(\{\bar{\mu}_n\}_{n \in \mathbb{N}}\) in the space \(\mathcal{P}_p(X), \tau^p_w\).

Along the way we will need the following technical result, which states that any point \(\mu \in \mathcal{P}_p(X)\) with finite exponential moments in some neighborhood of zero has the property that the topology \(\tau^p_w\) is locally determined by the function \(H(\cdot|\mu) : \mathcal{P}_p(X) \to [0, \infty]\). This result can be seen as a non-quantitative, but much more general, version of Talagrand’s classical inequality [27] and of its many extensions [21, 6].

**Lemma 4.2.** If \(\{\mu_n\}_{n \in \mathbb{N}}\) and \(\mu\) in \(\mathcal{P}(X)\) are such that we have \(H(\mu_n|\mu) \to 0\) and \(\int_X \exp(\alpha d\mu) d\mu(y) < \infty\) for some \(x \in X\) and \(\alpha > 0\), then \(\mu_n \to \mu\) in \(\tau^p_w\).
Proof. First, note by Pinsker’s inequality [29, Lemma 2.5] that
\[
\sup_{A \in \mathcal{B}(X)} |\mu_n(A) - \mu(A)| := \|\mu_n - \mu\| \leq \sqrt{\frac{1}{2}H(\mu_n|\mu)} \to 0.
\]
In particular, we have \(\mu_n \to \mu\) in \(\tau_w\). Moreover, by the Portmanteau lemma, since \(\mathcal{d}^p(x, \cdot) : X \to \mathbb{R}\) is non-negative and continuous, we have
\[
\int_X \mathcal{d}^p(x, y) \, d\mu(y) \leq \liminf_{n \to \infty} \int_X \mathcal{d}^p(x, y) \, d\mu_n(y).
\]
Next recall that the Donsker-Varadhan variational principle [10, Lemma 6.2.13] states that we have
\[
H(\mu_n|\mu) = \sup_{\phi \in \mathcal{b}(X)} \left( \int \phi \, d\mu_n - \log \left( \int_X \exp(\phi) \, d\mu(y) \right) \right),
\]
where \(\mathcal{b}(X)\) represents the space of all bounded measurable functions from \(X\) to \(\mathbb{R}\). Now fix \(\beta \in (0, \alpha)\). For \(R > 0\) arbitrary, set \(\phi_R : X \to \mathbb{R}\) via \(\phi_R(y) := \beta \mathcal{d}^p(x, y)\mathcal{b}_R(y)\) for \(y \in X\), and note that \(\phi_R \in \mathcal{b}(X)\). Moreover, we have \(\phi_R(y) \uparrow \beta \mathcal{d}^p(x, y)\) as \(R \to \infty\) for all \(y \in X\). By applying (4.2) for each \(R > 0\) we have
\[
H(\mu_n|\mu) \geq \int \phi_R \, d\mu_n - \log \left( \int_X \exp(\phi_R) \, d\mu(y) \right),
\]
so taking \(R \to \infty\) and applying monotone convergence gives
\[
H(\mu_n|\mu) \geq \int \beta \mathcal{d}^p(x, y) \, d\mu_n - \log \left( \int_X \exp(\beta \mathcal{d}^p(x, y)) \, d\mu(y) \right).
\]
Now send \(n \to \infty\) and rearrange to get
\[
\limsup_{n \to \infty} \int_X \mathcal{d}^p(x, y) \, d\mu_n \leq \frac{1}{\beta} \log \left( \int_X \exp(\beta \mathcal{d}^p(x, y)) \, d\mu(y) \right).
\]
Finally, send \(\beta \to 0\) and use dominated convergence to conclude
\[
\limsup_{n \to \infty} \int_X \mathcal{d}^p(x, y) \, d\mu_n \leq \int_X \mathcal{d}^p(x, y) \, d\mu(y).
\]
Combining (4.3) and (4.1) yields
\[
\int_X \mathcal{d}^p(x, y) \, d\mu_n \to \int_X \mathcal{d}^p(x, y) \, d\mu(y),
\]
hence we have shown \(\mu_n \to \mu\) in \(\tau_w^p\). \(\square\)

Proof of Theorem 1.3. Consider the set
\[
A := \{\nu \in \mathcal{P}_p(X) : d_H(C_{k,p}(\nu), C_{k,p}(\mu)) \geq \varepsilon\},
\]
and let us show that \(A\) is \(\tau_w^p\)-closed. Indeed, suppose \(\{\nu_n\}_{n \in \mathbb{N}} \in A\) and \(\nu \in \mathcal{P}_p(X)\) have \(\nu_n \to \nu\) in \(\tau_w^p\). Then apply the non-symmetric triangle inequality (2.3) to get:
\[
d_H(C_{k,p}(\nu_n), C_{k,p}(\nu)) + d_H(C_{k,p}(\nu), C_{k,p}(\mu)) \geq d_H(C_{k,p}(\nu_n), C_{k,p}(\mu)) \geq \varepsilon.
\]
Now use Proposition 3.13 with \(k_n = k\) and \(R_n = X\) for all \(n \in \mathbb{N}\), which guarantees that we have \(d_H(C_{k,p}(\nu_n), C_{k,p}(\nu)) \to 0\), hence \(d_H(C_{k,p}(\nu_n), C_{k,p}(\mu)) \geq \varepsilon\) by the above. In particular, \(\nu \in A\), thus \(A\) is \(\tau_w^p\)-closed.

Next, note that a Heine-Borel metric space is necessarily a Polish space. Thus \(\mu\) is a Borel probability measure on a Polish metric space with all exponential moments finite, so we conclude via [33, Theorem 1.1] that \(\{\bar{\mu}_n\}_{n \in \mathbb{N}}\) satisfy a large deviations
Finally, assume towards a contradiction that \( c_{k,p}(\mu, \varepsilon) = 0 \), so that there exist \( \{\nu_n\}_{n \in \mathbb{N}} \) in \( A \) with \( H(\nu_n|\mu) \to 0 \). Then Lemma \ref{lemma:limit_sup} implies \( \nu_n \to \mu \) in \( \tau^\mu \), so Proposition \ref{prop:lim_sup} implies \( \tilde{d}_H(C_{k,p}(\nu_n), C_{k,p}(\mu)) \to 0 \). This is impossible since \( \nu_n \in A \) for all \( n \in \mathbb{N} \), hence we must have \( c_{k,p}(\mu, \varepsilon) > 0 \).

Now, we make some remarks on possible limitations and extensions of this result. First of all, the constant \( c_{k,p}(\mu, \varepsilon) \) appearing as the exponential rate of decay has an exact characterization as

\[
(4.4) \quad c_{k,p}(\mu, \varepsilon) := \inf\{H(\nu|\mu) : \nu \in \mathcal{P}_p(X), \tilde{d}_H(C_{k,p}(\nu), C_{k,p}(\mu)) \geq \varepsilon\}.
\]

From this form we have shown \( c_{k,p}(\mu, \varepsilon) > 0 \) for all \( \varepsilon > 0 \), but it appears difficult to say much else. We believe it would be interesting to try to find some simple geometries \((X,d)\) and simple distributions \( \mu \in \mathcal{P}(X) \) for which \( c_{k,p}(\mu, \varepsilon) \) can be exactly or approximately computed. For example, if \( \mu \) is compactly-supported, then do we have \( \limsup_{\varepsilon \to 0} \varepsilon^{-2} c_{k,p}(\mu, \varepsilon) < \infty \), which can be interpreted as a sort of asymptotically sub-Gaussian concentration?

Second, we remark that, while asymptotic tail bounds like in Theorem \ref{thm:main} are interesting, a more useful kind of result would be a finite-sample tail bound on the same error probabilities. We see at least two possible avenues for accomplishing this. One is to apply some general-purpose method like \cite[Exercise 4.5.5]{10}. Another is to try to identify the exact “modulus of continuity” of \( C_{k,p} \) at a particular point and then to apply finite-sample tail bounds for empirical measures in Wasserstein distances, like those found in \cite{8}. In either case, the details appear difficult but possible to carry out.

Finally, we address the \( L^p \)-exponential moment assumption. Of course, it holds for all \( p \geq 1 \) as long as \( \mu \) has compact support. Moreover, as we show below, for \( X = \mathbb{R}^m \) and \( p = 1 \), the assumption holds if and only if the moment generating function of \( \mu \) is finite everywhere. However, for \( p = 2 \), the condition is too strict to even cover the case where \( \mu \) is a standard Gaussian distribution. For these reasons, we conjecture that the condition is not necessary for the conclusion to hold. For example, if \( R_n = R \) is compact for all \( n \in \mathbb{N} \), then the conclusion should hold even if \( X \) is non-compact and \( \mu \) is heavy-tailed.

**Lemma 4.3.** If \( \mu \in \mathcal{P}(\mathbb{R}^m) \) has \( \int_{\mathbb{R}^m} \exp(\langle \lambda, y \rangle) \, d\mu(y) < \infty \) for all \( \lambda \in \mathbb{R}^m \), then we have \( \int_{\mathbb{R}^m} \exp(\alpha \|x - y\|) \, d\mu(y) < \infty \) for all \( x \in \mathbb{R}^m \) and \( \alpha > 0 \).

**Proof.** Let \( N \) be a \( \frac{1}{2} \)-net of the unit ball \( B := \{\lambda \in \mathbb{R}^m : \|\lambda\| \leq 1\} \). Then for any \( \alpha > 0 \) and \( y \in \mathbb{R}^m \), use the standard duality of the \( L^2 \) inner product and
Cauchy-Schwarz to get:
\[
\exp(2\alpha\|y\|) = \max_{\lambda \in B} \exp(2\alpha\langle \lambda, y \rangle)
\]
\[
= \max_{\lambda \in B} \min_{\lambda' \in N} \exp(2\alpha\langle \lambda', y \rangle) \exp(2\alpha\langle \lambda - \lambda', y \rangle)
\]
\[
\leq \exp(\alpha\|y\|) \max_{\lambda' \in N} \exp(2\alpha\langle \lambda', y \rangle).
\]
Rearranging this yields
\[
\exp(\alpha\|y\|) \leq \max_{\lambda \in N} \exp(2\alpha\langle \lambda, y \rangle) \leq \sum_{\lambda \in N} \exp(2\alpha\langle \lambda, y \rangle).
\]
Thus, by integrating the above, we have, for any \(x \in \mathbb{R}^m\) and \(\alpha > 0\):
\[
\int_{\mathbb{R}^m} \exp(\alpha\|x - y\|) \, d\mu(y) \leq \exp(\alpha\|x\|) \int_{\mathbb{R}^m} \exp(\alpha\|y\|) \, d\mu(y)
\]
\[
\leq \exp(\alpha\|x\|) \int_{\mathbb{R}^m} \sum_{\lambda \in N} \exp(2\alpha\langle \lambda, y \rangle) \, d\mu(y)
\]
\[
\leq \exp(\alpha\|x\|) \sum_{\lambda \in N} \int_{\mathbb{R}^m} \exp(2\alpha\langle \lambda, y \rangle) \, d\mu(y).
\]
Since the right side is finite by assumption, this proves the claim. \(\square\)

4.3. Strong Consistency for MC data. Suppose that \((X, d)\) is a finite metric space and that \(P\) is a transition matrix on \(X\). Suppose further that \(X\) can be written as a disjoint union into non-empty sets \(X = X_0 \sqcup X_1\) such that \(X_0\) is an inessential class with respect to \(P\), and that \(P\) is irreducible and aperiodic on \(X_1\). Now suppose that \(Y_1, Y_2, \ldots\) is a Markov chain in \(X\) with transition matrix \(P\) satisfying \(Y_1 \in X_0\) almost surely. It follows from the classical ergodic theorem for Markov chains that there is a unique \(\nu \in \mathcal{P}(X_1)\) such that the empirical distributions \(\bar{\nu}_n := \frac{1}{n} \sum_{i=1}^n \delta_{Y_i}\) for \(n \in \mathbb{N}\) have \(\bar{\nu}_n \to \nu\) in \(\tau_w\) almost surely. Moreover, since \((X, d)\) is compact, we have \(\mathcal{P}(X) = \mathcal{P}_p(X)\) and \(\tau_w = \tau_w^p\) for all \(p \geq 1\).

From this discussion and Theorem 1.2 it follows that for \(k \leq \#\text{supp}(\nu)\) and \(p \geq 1\) we have
\[
\max_{S_n \in C_{k,p}(\bar{\nu})} \min_{S \in C_{k,p}(\nu)} d_H(S_n, S) \to 0
\]
after almost surely. In words, \((k, p)\)-medoids for data coming from this MC is strongly consistent. However, we have the following which shows that the story is more complicated for \((k, p)\)-medoids.

**Example 4.4.** Consider \(X = \{-1, 0, 1\}\) with the metric inherited from the real line. Then let \(Y_1, Y_2, \ldots\) be a MC with \(Y_1 = 0\) and with the transition matrix
\[
P = \begin{pmatrix}
\frac{1}{2} & 0 & \frac{1}{2} \\
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\
\frac{1}{2} & 0 & \frac{1}{2}
\end{pmatrix}.
\]
In words, this MC stays at state 0 for a geometric amount of time, then subsequently visits \(\{-1, 1\}\) independently and uniformly at random. This fits into the setting above with \(X_0 = \{0\}\) and \(X_1 = \{-1, 1\}\). Of course, we also have \(\nu = \frac{1}{2} \delta_{-1} + \frac{1}{2} \delta_1\).

Now write \(I := \max\{i \in \mathbb{N} : Y_i = 0\}\) for the number of data equal to 0 and \(Z_n := \sum_{i=1}^n Y_i\) for the cumulative sum of the data. Observe in particular that
$I < \infty$ almost surely and that we have

$$\tilde{\nu}_n = \frac{n - Z_n - I}{2n} \delta_{-1} + \frac{I}{n} \delta_0 + \frac{n + Z_n - I}{2n} \delta_1$$

for $n > I$. Moreover, $(Z_n)_{n \geq I}$ is a simple symmetric random walk. Next notice that on $\{n > I, Z_n = 0\}$ we have

$$\int_X d^p(\pm 1, y) d\bar{\nu}_n(y) = \frac{I}{n} + \left(1 - \frac{I}{n}\right) 2^{p-1} > 1 - \frac{I}{n}$$

$$= \int_X d^p(0, y) d\bar{\nu}_n(y),$$

hence $C_{1,p}^{med}(\tilde{\nu}_n) = \{\{0\}\}$. Likewise, $C_{1,p}^{med}(\nu) = \{-1, \{1\}\}$. In particular, we have shown

$$\max_{S_n \in C_{1,p}^{med}(\tilde{\nu}_n)} \min_{S \in C_{1,p}^{med}(\nu)} d_H(S_n, S) = 1$$

on $\{n > I, Z_n = 0\}$. Finally, notice that we have $\mathbb{P}(n > I, Z_n = 0 \text{ for infinitely many } n \in \mathbb{N}) = 1$ by the recurrence of the random walk, hence

$$\mathbb{P} \left( \max_{S_n \in C_{1,p}^{med}(\tilde{\nu}_n)} \min_{S \in C_{1,p}^{med}(\nu)} d_H(S_n, S) \to 0 \right) = 0.$$ 

In words, $(k, p)$-medoids for data coming from this MC is strongly inconsistent.

We now introduce a method to repair this apparent deficiency. The difficulty in the preceding example is that the adaptively-chosen domain of the cluster centers includes some states not included in the support of the stationary distribution, so, to get around this, we allow our clustering procedure to “forget” some initial segment of states. This is equivalent to giving the MC a suitable “burn-in” period during which the support becomes sufficiently mixed.

Indeed, let $f = \{f_n\}_{n \in \mathbb{N}}$ be any integer sequence with $0 \leq f_n \leq n$ for all $n \in \mathbb{N}$. Then define

$$\tilde{\nu}_n^f := \frac{1}{n - f_n} \sum_{i = f_n + 1}^n \delta_{Y_i}$$

for $n \in \mathbb{N}$; that is, $\{\tilde{\nu}_n^f\}_{n \in \mathbb{N}}$ are the empirical measures of only the most recent data points, where we forget initial segments of sizes determined by $f$.

If the decomposition $X = X_0 \sqcup X_1$ is known, then one can define the stopping time $\tau := \min\{i \in \mathbb{N} : Y_i \in X_1\}$ and it is immediate from Theorem 1.2 that $f_n := \min\{n, \tau\}$ satisfies

$$\max_{S_n \in C_{1,p}^{med}(\tilde{\nu}_n^f)} \min_{S \in C_{1,p}^{med}(\nu)} d_H(S_n, S) \to 0$$

almost surely. However, in practice, $X = X_0 \sqcup X_1$ is not always known. To get around this, we have the following asymptotic approach:

**Lemma 4.5.** If $f_n/n \to 0$ and $f_n \to \infty$, then

(i) $\tilde{\nu}_n^f \to \nu$ in $\tau_w$ almost surely, and

(ii) $\mathbb{L}_{n \in \mathbb{N}} \supp(\tilde{\nu}_n^f) = \supp(\nu)$ almost surely.
Proof. For (i), note that $X$ being finite means that convergence in $\tau_w$ is equivalent to convergence in the total variation norm, $\| \cdot \|_{TV}$. To use this, write

$$\bar{\nu}_n^f = \frac{n}{n-f_n} \cdot \frac{1}{n} \sum_{i=1}^n \delta_{Y_i} - \frac{1}{n-f_n} \sum_{i=1}^f \delta_{Y_i},$$

hence

$$\| \bar{\nu}_n^f - \bar{\nu}_n \|_{TV} \leq \left| \frac{n}{n-f_n} - 1 \right| \frac{1}{n} \sum_{i=1}^n \| \delta_{Y_i} \|_{TV} + \frac{1}{n-f_n} \sum_{i=1}^f \| \delta_{Y_i} \|_{TV}$$

$$\leq \left| \frac{n}{n-f_n} - 1 \right| + \frac{f_n}{n-f_n}.$$ 

Now note that $f_n/n \to 0$ implies that the right side goes to zero, hence $\| \bar{\nu}_n^f - \bar{\nu}_n \|_{TV} \to 0$. Since $\| \bar{\nu}_n - \nu \|_{TV} \to 0$ almost surely by the classical ergodic theorem, we conclude $\| \bar{\nu}_n^f - \nu \|_{TV} \to 0$ whence (i). For (ii), note by (i) and [11, Lemma 2.10] that we have $\supp(\nu) \subseteq \overline{L_{\nu}} \supp(\bar{\nu}_n^f)$ almost surely. For the converse, suppose that $x \in L_{\nu} \supp(\bar{\nu}_n^f)$. Since $X$ is discrete, this means that there is a subsequence $(n_j)_{j \in \mathbb{N}}$ with $x \in \supp(\bar{\nu}_{n_j}^f)$ for all $j \in \mathbb{N}$. Consequently, there is some sequence $(\ell_j)_{j \in \mathbb{N}}$ (not necessarily non-decreasing) with $f_{n_j} + 1 \leq \ell_j \leq n_j$ and $Y_{\ell_j} = x$ for all $j \in \mathbb{N}$. Since $f_n \to \infty$, this means $Y_1, Y_2, \ldots$ visits $x$ infinitely often. But $X_0$ is inessential with respect to $P$, so we must have $x \notin X_0$. This implies $x \in X_1$ hence $x \in \supp(\nu)$ since $X_1$ is irreducible and aperiodic with respect to $P$. We have shown $L_{\nu} \supp(\bar{\nu}_n^f) \subseteq \supp(\nu)$ almost surely, so combining with the first part gives (ii).

This, in particular, gives the following strong consistency.

**Theorem 4.6.** If $f_n/n \to 0$ and $f_n \to \infty$, then we have

$$\max_{S_n \in C_{k,p}(\bar{\nu}_{\ell})} \min_{S \in C_{k,p}(\nu)} d_H(S_n, S) \to 0$$

almost surely.

**Proof.** Immediate by Theorem 1.2 and Lemma 4.5. $\square$

To be concrete in the setting above, one can take $f_n := \lfloor \log n \rfloor$ for $n \in \mathbb{N}$.

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