Data-Driven Clustering via Parameterized Lloyd’s Families*

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Abstract

Algorithms for clustering points in metric spaces is a long-studied area of research. Clustering has seen a multitude of work both theoretically, in understanding the approximation guarantees possible for many objective functions such as $k$-median and $k$-means clustering, and experimentally, in finding the fastest algorithms and seeding procedures for Lloyd’s algorithm. The performance of a given clustering algorithm depends on the specific application at hand, and this may not be known up front. For example, a “typical instance” may vary depending on the application, and different clustering heuristics perform differently depending on the instance.

In this paper, we define an infinite family of algorithms generalizing Lloyd’s algorithm, with one parameter controlling the initialization procedure, and another parameter controlling the local search procedure. This family of algorithms includes the celebrated $k$-means++ algorithm, as well as the classic farthest-first traversal algorithm. We design efficient learning algorithms which receive samples from an application-specific distribution over clustering instances and learn a near-optimal clustering algorithm from the class. We show the best parameters vary significantly across datasets such as MNIST, CIFAR, and mixtures of Gaussians. Our learned algorithms never perform worse than $k$-means++, and on some datasets we see significant improvements.

1 Introduction

Clustering is a fundamental problem in machine learning with applications in many areas including text analysis, transportation networks, social networks, and so on. The high-level goal of clustering is to divide a dataset into natural subgroups. For example, in text analysis we may want to divide documents based on topic, and in social networks we might want to find communities. A common approach to clustering is to set up an objective function and then approximately find the optimal solution according to the objective. There has been a wealth of both theoretical and empirical research in clustering using this approach [21, 14, 8, 7, 26, 37, 13, 2].

The most popular method in practice for clustering is local search, where we start with $k$ centers and iteratively make incremental improvements until a local optimum is reached. For example, Lloyd’s method (sometimes called $k$-means) [32] and $k$-medioids [19, 15] are two popular local search algorithms. There are multiple decisions an algorithm designer must make when using a local search algorithm. First, the algorithm designer must decide how to seed local search, e.g., how the algorithm chooses the $k$ initial centers. There is a large body of work on seeding algorithms, since the initial choice of centers can have a large effect on the quality of the outputted clustering [23, 39, 4]. The best seeding method often depends on the specific application at hand. For example, a “typical problem instance” in one setting may have significantly different properties from that in another, causing some seeding methods to perform better than others. Second, the algorithm designer must decide on an objective function for the local search phase ($k$-means, $k$-median, etc.)

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For some applications, there is an obvious choice. For instance, if the application is wifi hotspot location, then the explicit goal is to minimize the $k$-center objective function. For many other applications such as clustering communities in a social network, the goal is to find clusters which are close to an unknown target clustering, and we may use an objective function for local search in the hopes that approximately minimizing the chosen objective will produce clusterings which are close to matching the target clustering (in terms of the number of misclassified points). As before, the best objective function for local search may depend on the specific application.

In this paper, we show positive theoretical and empirical results for learning the best initialization and local search procedures over a large family of algorithms. We take a transfer learning approach where we assume there is an unknown distribution over problem instances corresponding to our application, and the goal is to use experience from the early instances to perform well on the later instances. For example, if our application is clustering facilities in a city, we would look at a sample of cities with existing optimally-placed facilities, and use this information to find the empirically best seeding/local search pair from an infinite family, and we use this pair to cluster facilities in new cities. This is similar in spirit to the learning to learn setting of [12], where the goal is to learn the best concept class from a family of concept classes, for an unknown distribution. $(\alpha, \beta)$-Lloyds++ We define an infinite family of algorithms generalizing Lloyd’s method, with two parameters $\alpha$ and $\beta$. Our algorithms have two phases, a seeding phase to find $k$ initial centers (parameterized by $\alpha$), and a local search phase which uses Lloyd’s method to converge to a local optimum (parameterized by $\beta$). In the seeding phase, each point $v$ is sampled with probability proportional to $d_{\min}(v, C)^{\alpha}$, where $C$ is the set of centers chosen so far and $d_{\min}(v, C) = \min_{c \in C} d(v, c)$. Then Lloyd’s method is used to converge to a local minima for the $\ell_\beta$ objective. By ranging $\alpha, \beta \in [0, \infty) \cup \{\infty\}$, we define our infinite family of algorithms which we call $(\alpha, \beta)$-Lloyds++. Setting $\alpha = \beta = 2$ corresponds to the $k$-means++ algorithm [7]. The seeding phase is a spectrum between random seeding ($\alpha = 0$), and farthest-first traversal [21, 16] ($\alpha = \infty$), and the Lloyd’s step is able to optimize over common objectives including $k$-median ($\beta = 1$), $k$-means ($\beta = 2$), and $k$-center ($\beta = \infty$). We design efficient learning algorithms which receive samples from an application-specific distribution over clustering instances and learn a near-optimal clustering algorithm from our family.

**Theoretical analysis** In Section 4, we prove that $O\left(\frac{1}{\epsilon^2 \min(T, k)} \log n\right)$ samples are sufficient to guarantee the empirically optimal parameters $(\hat{\alpha}, \hat{\beta})$ have expected cost at most $\epsilon$ higher than the optimal parameters $(\alpha^*, \beta^*)$ over the distribution, with high probability over the random sample, where $n$ is the size of the clustering instances and $T$ is the maximum number of Lloyd’s iterations. The key challenge is that for any clustering instance, the cost of the outputted clustering is not even a continuous function in $\alpha$ or $\beta$ since a slight tweak in the parameters may lead to a completely different run of the algorithm. We overcome this obstacle by showing a strong bound on the expected number of discontinuities of the cost function, which requires a delicate reasoning about the structure of the “decision points” in the execution of the algorithm; in other words, for a given clustering instance, we must reason about the total number of outcomes the algorithm can produce over the full range of parameters. This allows us to use Rademacher complexity, a distribution-specific technique for achieving uniform convergence.

Next, we complement our sample complexity result with a computational efficiency result. Specifically, we give a novel algorithm which efficiently finds the empirically optimal value $\hat{\alpha}$ with high probability. The high-level idea of our algorithm is to run depth-first-search over the “execution tree” of the algorithm, where a tree in a node represents a state of the algorithm, and edges represent a decision point. A key step in our algorithm is to iteratively solve for the decision points of the algorithm, which itself is nontrivial since the equations governing the decision points do not have
a closed-form solution. We show the equations have a certain structure which allows us to binary search through the range of parameters to find the decision points.

Experiments We give a thorough experimental analysis of our family of algorithms by evaluating its performance on a number of different real-world and synthetic datasets including MNIST, Cifar10, CNAE-9, and mixtures of Gaussians. In each case, we create clustering instances by choosing subsets of the labels. For example, we look at an instance of MNIST with digits \( \{0, 1, 2, 3, 4\} \), and also an instance with digits \( \{5, 6, 7, 8, 9\} \). We show the optimal parameters transfer from one instance to the other. Across each dataset, there is no single parameter setting that is nearly optimal, and for some datasets, the best algorithm from the \((\alpha, \beta)\)-Lloyd++ family performs significantly better than known algorithms such as \(k\)-means++ and farthest-first traversal.

2 Related Work

Clustering The iterative local search method for clustering, known as Lloyd’s algorithm or sometimes called \(k\)-means, is one of the most popular algorithms for \(k\)-means clustering [32], and improvements are still being found [36, 34, 17, 38, 25, 26]. The worst-case runtime of Lloyd’s method is exponential [6] even in \(R^2\) [47], however, it converges very quickly in practice [22], and the smoothed complexity is polynomial [5]. Many different initialization approaches have been proposed [23, 39, 4]. When using \(d^2\)-sampling to find the initial \(k\) centers, the algorithm is known as \(k\)-means++, and the approximation guarantee is provably \(O(\log k)\) [7]. If the data satisfies a natural stability condition, \(k\)-means++ returns a near-optimal clustering [37].

The farthest-first traversal algorithm is an iterative method to find \(k\) centers, and it was shown to give a 2-approximation algorithm for \(k\)-center [21], and an 8-approximation for hierarchical \(k\)-center [16].

Learning to Learn A recent paper shows positive results for learning linkage-based algorithms with pruning over a distribution over clustering instances [10], although there is no empirical study done. There are several related models for learning the best representation and transfer learning for clustering. Ashtiani and Ben-David show how to use a small labeled fraction of the dataset to learn a metric embedding of the entire dataset such that \(k\)-means performs well [9]. Baxter studied the task of choosing the right concept class for a distribution over an environment of supervised learning tasks [12]. Specifically, the goal is to learn the best hypothesis space from a family of hypothesis spaces. Our problem is similar in spirit to this model, where we study environments of unsupervised learning tasks instead of supervised learning tasks.

There are a few models for the question of finding the best clustering algorithm to use on a single instance, given a small amount of expert advice. Ackerman et al. (building off of the famous clustering impossibility result of [27]) study the problem of taxonomizing clustering algorithmic paradigms, by using a list of abstract properties of clustering functions [1]. In their work, the goal is for a user to choose a clustering algorithm based on the specific properties which are important for her application.

Another related area is the problem of unsupervised domain adaption. In this problem, the machine learning algorithm has access to a labeled training dataset, and an unlabeled target dataset over a different distribution. The goal is to find an accurate classifier over the target dataset, while only training on the training distribution [44, 20, 46].

There has been more research on related questions for transfer learning on unlabeled data and unsupervised tasks. Raina et al. study transfer learning using unlabeled data, to a supervised learning task [43]. Jiang and Chung, and Yang et al. study transfer learning for clustering, in
which a clustering algorithm has access to unlabeled data, and uses it to better cluster a related problem instance [48, 24]. This setting is a bit different from ours, since we assume we have access to the “target clusterings” from the training instances, but we tackle the harder question of finding the best clustering objective.

3 Preliminaries

Clustering. A clustering instance $V$ consists of a point set $V$ of size $n$, a distance metric $d$ (such as Euclidean distance in $\mathbb{R}^d$), and a desired number of clusters $1 \leq k \leq n$. A clustering $C = \{C_1, \ldots, C_k\}$ is a $k$-partitioning of $V$. Often in practice, clustering is carried out by approximately minimizing an objective function (which maps each clustering to a nonzero value). Common objective functions such as $k$-median and $k$-means come from the $\ell_p$ family, where each cluster $C_i$ is assigned a center $c_i$ and $\text{cost}(C) = \left( \sum_i \sum_{v \in C_i} d(v, c_i)^p \right)^{\frac{1}{p}}$ ($k$-median and $k$-means correspond to $p = 1$ and $p = 2$, respectively). There are two distinct goals for clustering depending on the application. For some applications such as computing road networks or wifi hotspot locations, the algorithm designer’s only goal is to find the best centers, and the actual partition $\{C_1, \ldots, C_k\}$ is not needed. For many other applications such as clustering documents by subject, clustering proteins by function, or discovering underlying communities in a social network, there exists an unknown “target” clustering $C^* = \{C_1^*, \ldots, C_k^*\}$, and the goal is to output a clustering $C$ which is close to $C^*$. Formally, we define $C$ and $C'$ to be $\epsilon$-close if there exists a permutation $\sigma$ such that $\sum_{i=1}^k |C_i \setminus C^*_{\sigma(i)}| \leq \epsilon n$. For these applications, the algorithm designer chooses an objective function while hoping that minimizing the objective function will lead to a clustering that is close to the target clustering. In this paper, we will use an abstract cost function $\text{cost}$ which can be set to an objective function or the distance to the target clustering, or any other well-defined measure of cost.

Algorithm Configuration. In this work, we assume that there exists an unknown, application-specific distribution $D$ over a set of clustering instances such that for each instance $V$, $|V| \leq n$. We suppose there is a cost function that measures the quality of a clustering of each instance. As discussed in the previous paragraph, we can set the cost function to be the expected Hamming distance of the returned clustering to the target clustering, the cost of an $\ell_p$ objective, or any other function. The learner’s goal is to find the parameters $\alpha$ and $\beta$ that approximately minimize the expected cost with respect to the distribution $D$. Our main technical results bound the intrinsic complexity of the class of $(\alpha, \beta)$-Lloyds++ clustering algorithms, which leads to generalization guarantees through standard Rademacher complexity [11, 29] and pseudo-dimension bounds [40, 41, 3]. This implies that the empirically optimal parameters are also nearly optimal in expectation.

4 $(\alpha, \beta)$-Lloyds++

In this section, we define an infinite family of algorithms generalizing Lloyd’s algorithm, with one parameter controlling the the initialization procedure, and another parameter controlling the local search procedure. Our main results bound the intrinsic complexity of this family of algorithms (Theorems 4 and 5) and lead to sample complexity results guaranteeing the empirically optimal parameters over a sample are close to the optimal parameters over the unknown distribution. We measure optimality in terms of agreement with the target clustering. We also show theoretically that no parameters are optimal over all clustering applications (Theorem 2). Finally, we give an efficient algorithm for learning the best initialization parameter (Theorem 7).
Our family of algorithms is parameterized by choices of $\alpha \in [0, \infty) \cup \{\infty\}$ and $\beta \in [1, \infty) \cup \{\infty\}$. Given a fixed choice of $(\alpha, \beta)$, a summary of the algorithm is as follows (see Algorithm 1). The algorithm has two phases. The goal of the first phase is to output $k$ initial centers. Each center is iteratively chosen by picking a point with probability proportional to the minimum distance to all centers picked so far, raised to the power of $\alpha$. The second phase is an iterative two step procedure similar to Lloyd’s method, where the first step is to create a Voronoi partitioning of the points induced by the initial set of centers, and then a new set of centers is chosen by computing the $\ell_\beta$ mean of each Voronoi tile.

Algorithm 1 $(\alpha, \beta)$-Lloyds++ Clustering

**Input:** Instance $V = (V, d, k)$, parameter $\alpha$.

**Phase 1: Choosing initial centers with $d^\alpha$-sampling**

1. Initialize $C = \emptyset$ and draw a vector $\tilde{Z} = \{z_1, \ldots, z_k\}$ from $[0, 1]^k$ uniformly at random.
2. For each $t = 1, \ldots, k$:
   (a) Partition $[0, 1]$ into $n$ intervals, where there is an interval $I_{v_i}$ for each $v_i$ with size equal to the probability of choosing $v_i$ during $d^\alpha$-sampling in round $t$ (see Figure 2).
   (b) Denote $c_t$ as the point such that $z_t \in I_{c_t}$, and add $c_t$ to $C$.

**Phase 2: Lloyd’s algorithm**

5. Set $C' = \emptyset$. Let $\{C_1, \ldots, C_k\}$ denote the voronoi tiling of $V$ induced by centers $C$.
6. Compute $\arg\min_{x \in V} \sum_{v \in C_i} d(x, v)^\beta$ for all $1 \leq i \leq k$, and add it to $C'$.
7. If $C' \neq C$, set $C = C'$ and goto 5.

**Output:** Centers $C$ and clustering induced by $C$.

Our goal is to find parameters which return clusterings close to the ground-truth in expectation. Setting $\alpha = \beta = 2$ corresponds to the $k$-means++ algorithm. The seeding phase is a spectrum between random seeding ($\alpha = 0$), and farthest-first traversal ($\alpha = \infty$), and the Lloyd’s algorithm can optimize for common clustering objectives including $k$-median ($\beta = 1$), $k$-means ($\beta = 2$), and $k$-center ($\beta = \infty$).

We start with two structural results about the family of $(\alpha, \beta)$-Lloyds++ clustering algorithms. The first shows that for sufficiently large $\alpha$, phase 1 of Algorithm 1 is equivalent to farthest-first traversal. This means that it is sufficient to consider $\alpha$ parameters in a bounded range.

Farthest-first traversal \cite{21} starts by choosing a random center, and then iteratively choosing the point farthest to all centers chosen so far, until there are $k$ centers. We assume that ties are broken uniformly at random.

**Lemma 1.** Given a clustering instance $V$ and $\delta > 0$, if $\alpha > \frac{\log(\frac{n^2}{\delta})}{\log s}$, then $d^\alpha$-sampling will give the same output as farthest-first traversal with probability $> 1 - \delta$. Here, $s$ denotes the minimum ratio $d_1/d_2$ between two distances $d_1 > d_2$ in the point set.

For some datasets, $\frac{1}{\log s}$ might be very large. In Section \cite{5}, we empirically observe that for all datasets we tried, $(\alpha, \beta)$-Lloyds++ behaves the same as farthest-first traversal for $\alpha > 20$. \footnote{In Appendix \cite{A} we show that if the dataset satisfies a stability assumption called separability \cite{28} \cite{42}, then $(\alpha, \beta)$-Lloyds++ outputs the same clustering as farthest-first traversal with high probability when $\alpha > \log n$.}
Next, to motivate learning the best parameters, we show that for any pair of parameters \((\alpha^*, \beta^*)\), there exists a clustering instance such that \((\alpha^*, \beta^*)\)-Lloyds++ outperforms all other values of \(\alpha, \beta\). This implies that \(d^\beta\)-sampling is not always the best choice of seeding for the \(l_\beta\) objective. Let \(\text{clus}_{\alpha, \beta}(V)\) denote the expected cost of the clustering outputted by \((\alpha, \beta)\)-Lloyds++, with respect to the target clustering. Formally, \(\text{clus}_{\alpha, \beta}(V) = E_{Z \sim [0, 1]^k} \left[ \text{clus}_{\alpha, \beta}(V, Z) \right]\), where \(\text{clus}_{\alpha, \beta}(V, Z)\) is the cost of the clustering outputted by \((\alpha, \beta)\)-Lloyd++ with randomness \(Z\) ∈ \([0, 1]^k\) (see line 1 of Algorithm 1).

**Theorem 2.** For \(\alpha^*, \beta^* \in [0, \infty) \cup \{\infty\}\), there exists a clustering instance \(V\) whose target clustering is the optimal \(l_{\beta^*}\) clustering, such that \(\text{clus}_{\alpha^*, \beta^*}(V) < \text{clus}_{\alpha, \beta}(V)\) for all \((\alpha, \beta) \neq (\alpha^*, \beta^*)\).

**Proof sketch.** Consider \(\alpha^*, \beta^* \in [0, \infty) \cup \{\infty\}\). The clustering instance consists of 6 clusters, \(C_1, \ldots, C_6\). The target clustering will be the optimal \(l_{\beta^*}\) objective. The proof consists of three sections. First, we construct \(C_1, \ldots, C_4\) so that \(d^{\alpha^*}\) sampling has the best chance of putting exactly one point into each optimal cluster. Then we add “local minima traps” to each cluster, so that if any cluster received two centers in the sampling phase, Lloyd’s method will not be able to move the centers to a different cluster. Finally, we construct \(C_5\) and \(C_6\) so that if seeding put one point in each cluster, then \(\beta^*\)-Lloyd’s method will outperform any other \(\beta \neq \beta^*\).

Step 1: we let \(C_1\) and \(C_2\) equal two different cliques, and we define a third clique whose points are equal to \(C_3 \cup C_4\). See Figure 1. We space these cliques arbitrarily far apart so that with high probability, the first three sampled centers will each be in a different clique. Now the idea is to define the distances and sizes of the cliques so that \(\alpha^*\) is the value of \(\alpha\) with the greatest chance of putting the last center into the third clique. If we set the distances in cliques 1, 2, 3 to 2, 1/2, and 1, and set \(|C_1| = 2^{2a^*}|C_2|\), then the probability of sampling a 4th center in the third clique for \(\alpha = \alpha^* + \delta\) is equal to

\[
\frac{|C_3 \cup C_4|}{|C_3 \cup C_4| + (2^{a^*+\delta} + 2^{a^*-\delta})|C_2|}.
\]

This is maximized when \(\delta = 0\).

Now we add local minima traps for Lloyd’s method as follows. In the first two cliques, we add three centers so that the 2-clustering cost is only slightly better than the 1-clustering cost. In the third clique, which consists of \(C_3 \cup C_4\), add centers so that the 2-clustering cost is much lower than the 1-clustering cost. We also show that since all cliques are far apart, it is not possible for a center to move between clusters during Lloyd’s method.

![Figure 1: Optimal instance for \(d^{\alpha^*}\)-sampling](image)
Finally, we add three centers $c_5, b_5, b'_5$ to the last cluster $C_5$. We set the rest of the points so that $c_5$ minimizes the $\ell_{\beta^*}$ objective, while $b_5$ and $b'_5$ favor $\beta = \beta^* \pm \epsilon$. Therefore, $(\alpha^*, \beta^*)$ performs the best out of all pairs $(\alpha, \beta)$.

Sample efficiency  Now we give sample complexity bounds for learning the best algorithm from the class of $(\alpha, \beta)$-Lloyd++ algorithms. We analyze the phases of Algorithm 1 separately. For the first phase, our main structural result is to show that for a given clustering instance and value of $\beta$, with high probability over the randomness in Algorithm 1, the number of discontinuities of the cost function $\text{clus}_{\alpha, \beta}(V, \bar{Z})$ as we vary $\alpha \in [0, \alpha_h]$ is $O(nk(\log n)\alpha_h)$. Our analysis crucially harnesses the randomness in the algorithm to achieve this bound. For instance, if we use a combinatorial approach as in prior algorithm configuration work, we would only achieve a bound of $n^O(k)$, which is the total number of sets of $k$ centers. For completeness, we give a combinatorial proof of $O(nk^{k+3})$ discontinuities in Appendix A (Theorem 10).

To show the $O(nk(\log n)\alpha_h)$ upper bound, we start by giving a few definitions of concepts used in the proof. Assume we start to run Algorithm 1 without a specific setting of $\alpha$, but rather a range $[\alpha_1, \alpha_h]$, for some instance $V$ and randomness $\bar{Z}$. In some round $t$, if Algorithm 1 would choose a center $c_t$ for every setting of $\alpha \in [\alpha_1, \alpha_h]$, then we continue normally. However, if the algorithm would choose a different center depending on the specific value of $\alpha$ used from the interval $[\alpha_1, \alpha_h]$, then we fork the algorithm, making one copy for each possible center. In particular, we partition $[\alpha_1, \alpha_h]$ into a finite number of sub-intervals such that the next center is constant on each interval. The boundaries between these intervals are “breakpoints”, since as $\alpha$ crosses those values, the next center chosen by the algorithm changes. Our goal is to bound the total number of breakpoints over all $k$ rounds in phase 1 of Algorithm 1, which bounds the number of discontinuities of the cost of the outputted clustering as a function of $\alpha$ over $[\alpha_1, \alpha_h]$.

A crucial step in the above approach is determining when to fork and where the breakpoints are located. Recall that in round $t$ of Algorithm 1, each datapoint $v_i$ has an interval in $[0, 1]$ of size $d_\alpha v_i D_n(\alpha)$, where $d_i$ is the minimum distance from $v_i$ to the current set of centers, and $D_j(\alpha) = d_1^\alpha + \cdots + d_j^\alpha$. Furthermore, the interval is located between $D_{i-1}(\alpha)$ and $D_i(\alpha)$ (see Figure 2). WLOG, we assume $d_1 \geq \cdots \geq d_n$. We prove the following nice structure about these intervals.

**Lemma 3.** If $v_(1), \ldots, v_(n)$ are sorted in decreasing distance from a set $C$ of centers, then for each $i = 1, \ldots, n$, the function $\alpha \mapsto \frac{D_i(\alpha)}{D_n(\alpha)}$ is monotone increasing.
This lemma guarantees two crucial properties. First, we know that for every (ordered) set $C$ of $t \leq k$ centers chosen by phase 1 of Algorithm 1 up to round $t$, there is a single interval (as opposed to a more complicated set) of $\alpha$-parameters that would give rise to $C$. Second, for an interval $[\alpha_{t}, \alpha_{h}]$, the set of possible next centers is exactly $v_{t(i)}, v_{t(i+1)}, \ldots, v_{t(h)}$, where $t_{i}$ and $t_{h}$ are the centers sampled when $\alpha = \alpha_{t}$ and $\alpha_{h}$, respectively (see Figure 2). Now we are ready to prove our main structural result. Formally, we define $\text{seed}_{\alpha}(\mathcal{V}, \vec{Z})$ as the outputted centers from phase 1 of Algorithm 1 on instance $\mathcal{V}$ with randomness $\vec{Z}$.

Theorem 4. Given a clustering instance $\mathcal{V}$, the expected number of discontinuities of $\text{seed}_{\alpha}(\mathcal{V}, \vec{Z})$ as a function of $\alpha$ over $[0, \alpha_{h}]$ is $O(nk(\log n)\alpha_{h})$. Here, the expectation is over the uniformly random draw of $\vec{Z} \in [0, 1]^{k}$.

Proof sketch. Consider round $t$ of a run of Algorithm 1. Suppose at the beginning of round $t$, there are $L$ possible states of the algorithm, e.g., $L$ sets of $\alpha$ such that within a set, the choice of the first $t - 1$ centers is fixed. By Lemma 3, we can write these sets as $[\alpha_{0}, \alpha_{1}], \ldots, [\alpha_{L-1}, \alpha_{L}]$, where $0 = \alpha_{0} < \cdots < \alpha_{L} = \alpha_{h}$. Given one interval, $[\alpha_{t}, \alpha_{t+1}]$, we claim the expected number of new breakpoints $\#I_{t, \ell}$ by choosing a center in round $t$ is bounded by $4n(\log n)(\alpha_{t+1} - \alpha_{t})$. Note that $\#I_{t, \ell} + 1$ is the number of possible choices for the next center in round $\ell$ using $\alpha$ in $[\alpha_{t}, \alpha_{t+1}]$.

The claim gives an upper bound on the expected number of new breakpoints, where the expectation is only over $z_{t}$ (the uniformly random draw from $[0, 1]$ used by Algorithm 1 in round $t$), and the bound holds for any given configuration of $d_{1} \geq \cdots \geq d_{n}$. Assuming the claim, we can finish off the proof by using linearity of expectation as follows. Let $\#I$ denote the total number of discontinuities of $\text{seed}_{\alpha}(\mathcal{V}, \vec{Z})$.

$$
E_{Z \in [0, 1]^{k}}[\#I] \leq E_{Z \in [0, 1]^{k}} \left[ \sum_{t=1}^{k} \sum_{\ell=1}^{L} (#I_{t, \ell}) \right] \leq \sum_{t=1}^{k} \sum_{\ell=1}^{L} E_{Z \in [0, 1]^{k}}[\#I_{t, \ell}] \leq 4nk \log n \cdot \alpha_{h}.
$$

Now we will prove the claim. Given $z_{t} \in [0, 1]$, let $x$ and $y$ denote the minimum indices s.t. $\frac{D_{t}(\alpha_{i})}{D_{n}(\alpha_{i})} > z_{t}$ and $\frac{D_{t}(\alpha_{i+1})}{D_{n}(\alpha_{i+1})} > z_{t}$, respectively. Then from Lemma 3, the number of breakpoints is exactly $x - y$ (see Figure 2). Therefore, our goal is to compute $E_{z_{t} \in [0, 1]}[x - y]$. One method is to sum up the expected number of breakpoints for each interval $I_{y}$ by bounding the maximum possible number of breakpoints given that $z_{t}$ lands in $I_{y}$. Given interval $I_{y}$, let $i$ denote the minimum index such that $\frac{D_{t}(\alpha_{i})}{D_{n}(\alpha_{i})} > \frac{D_{t}(\alpha_{i+1})}{D_{n}(\alpha_{i+1})}$. If $z_{t}$ is in $I_{y}$ and greater than $\frac{D_{t}(\alpha_{i+1})}{D_{n}(\alpha_{i+1})}$, then the number of breakpoints is $j - i$. However, if $z_{t}$ is between $\frac{D_{t}(\alpha_{i})}{D_{n}(\alpha_{i})}$ and $\frac{D_{t}(\alpha_{i+1})}{D_{n}(\alpha_{i+1})}$, then the number of breakpoints is $j - i + 1$, which is not sufficient to prove the claim. For example, as $\alpha_{t+1} - \alpha_{t}$ goes to zero, the expected number of breakpoints should tend to zero, but bounding the expected number of breakpoints by $j - i + 1$ will tend to 1.

Therefore, we give a more refined analysis by further breaking into cases based on whether $z_{t}$ is smaller or larger than $\frac{D_{t}(\alpha_{i+1})}{D_{n}(\alpha_{i+1})}$. In case 1, when $z_{t} > \frac{D_{t}(\alpha_{i+1})}{D_{n}(\alpha_{i+1})}$, the number of breakpoints is $j - i$, and we will show that $j - i \leq n(\log n)(\alpha_{t+1} - \alpha_{t})$. In case 2, when $z_{t} < \frac{D_{t}(\alpha_{i+1})}{D_{n}(\alpha_{i+1})}$, the number of breakpoints is $j - i + 1$, and we will show the probability of this case is low.

For case 2, the probability that $z_{t}$ is in between $\frac{D_{t}(\alpha_{i})}{D_{n}(\alpha_{i})}$ and $\frac{D_{t}(\alpha_{i+1})}{D_{n}(\alpha_{i+1})}$ is $\frac{D_{t}(\alpha_{i+1})}{D_{n}(\alpha_{i+1})} - \frac{D_{t}(\alpha_{i})}{D_{n}(\alpha_{i})} \leq \frac{D_{t}(\alpha_{i+1})}{D_{n}(\alpha_{i+1})} - \frac{D_{t}(\alpha_{i})}{D_{n}(\alpha_{i})}$. Therefore, we can bound this quantity by bounding the derivative $\frac{\partial}{\partial \alpha} \left( \frac{D_{t}(\alpha)}{D_{n}(\alpha)} \right)$, which we show is at most $4 \log n$ in Appendix A.
For case 1, recall that \( j - i \) represents the number of intervals between \( \frac{D_i(\alpha)}{D_n(\alpha)} \) and \( \frac{D_i(\alpha)}{D_n(\alpha)} \). Note that the smallest interval in this range is \( \frac{d_j^\ell}{D_n(\alpha)} \), and \( \frac{D_j(\alpha)}{D_n(\alpha)} - \frac{D_i(\alpha)}{D_n(\alpha)} \leq \frac{D_i(\alpha+1)}{D_n(\alpha+1)} - \frac{D_i(\alpha)}{D_n(\alpha)} \). Therefore, the expected number of breakpoints is at most \( \frac{D_n(\alpha)}{d_j^\ell} \cdot 4 \log n \).

Putting case 1 and case 2 together, we have

\[
E[\# I_{t,\ell}] \leq \sum_j P \left( \frac{D_i(\alpha_{t+1})}{D_n(\alpha_{t+1})} < z_t < \frac{D_j(\alpha_{\ell})}{D_n(\alpha_{\ell})} \right) \cdot (j - i) + \sum_j P \left( \frac{D_j(\alpha_{\ell})}{D_n(\alpha_{\ell})} < z_t < \frac{D_i(\alpha_{t+1})}{D_n(\alpha_{t+1})} \right) \cdot (j - i + 1).
\]

\[
\leq \sum_j \left( \frac{d_j^\ell}{D_n(\alpha_{t+1})} \cdot \left( \frac{D_i(\alpha_{t+1})}{D_n(\alpha_{t+1})} - \frac{D_i(\alpha_{\ell})}{D_n(\alpha_{\ell})} \right) \right) + \sum_j \left( \frac{D_j(\alpha_{\ell})}{D_n(\alpha_{\ell})} - \frac{D_j(\alpha_{\ell})}{D_n(\alpha_{\ell})} \right)
\]

\[
\leq \sum_j 4 \log n(\alpha_{t+1} - \alpha_{\ell}) + \sum_j 4 \log n(\alpha_{t+1} - \alpha_{\ell})
\]

\[
\leq 8n \log n(\alpha_{t+1} - \alpha_{\ell})
\]

This concludes the proof. \( \square \)

Now we analyze phase 2 of Algorithm 1. Since phase 2 does not have randomness, we give a combinatorial proof. We define \( \text{lloyd}_3(\mathcal{V}, C, T) \) as the cost of the outputted clustering from phase 2 of Algorithm 1 on instance \( \mathcal{V} \) with initial centers \( C \), and a maximum of \( T \) iterations.

**Theorem 5.** Given \( T \in \mathbb{N} \), a clustering instance \( \mathcal{V} \), and a fixed set \( C \) of initial centers, the number of discontinuities of \( \text{lloyd}_3(\mathcal{V}, C, T) \) as a function of \( \beta \) on instance \( \mathcal{V} \) is \( O(\min(n^{3T}, n^{k+3})) \).

**Proof sketch.** Given \( \mathcal{V} \) and a set of initial centers \( C \), we bound the number of discontinuities introduced in the Lloyd’s step of Algorithm 1. First, we give a bound of \( n^{k+3} \) which holds for any value of \( T \). Recall that Lloyd’s algorithm is a two-step procedure, and note that the Voronoi partitioning step is independent of \( \beta \). Let \( \{C_1, \ldots, C_k\} \) denote the Voronoi partition of \( \mathcal{V} \) induced by \( C \). Given one of these clusters \( C_i \), the next center is computed by \( \min_{c \in C_i} \sum_{v \in C_i} d(c, v)^\beta \). Given any \( c_1, c_2 \in C_i \), the decision for whether \( c_1 \) is a better center than \( c_2 \) is governed by \( \sum_{v \in C_i} d(c_1, v)^\beta < \sum_{v \in C_i} d(c_2, v)^\beta \). By a consequence of Rolle’s theorem, this equation has at most \( 2n + 1 \) roots. This equation depends on the set \( C \) of centers, and the two points \( c_1 \) and \( c_2 \), therefore, there are \( \binom{n}{k} \cdot \binom{n}{2} \) equations each with \( 2n + 1 \) roots. We conclude that there are \( n^{k+3} \) total intervals of \( \beta \) such that the outcome of Lloyd’s method is fixed.

Next we give a different analysis which bounds the number of discontinuities by \( n^{3T} \), where \( T \) is the maximum number of Lloyd’s iterations. By the same analysis as the previous paragraph, if we only consider one round, then the total number of equations which govern the output of a Lloyd’s iteration is \( \binom{n}{2} \), since the set of centers \( C \) is fixed. These equations have \( 2n + 1 \) roots, so the total number of intervals in one round is \( O(n^3) \). Therefore, over \( T \) rounds, the number of intervals is \( O(n^{3T}) \).

By combining Theorem 4 with Theorem 5 and using standard learning theory results, we can bound the sample complexity needed to learn near optimal parameters \( \alpha, \beta \) for an unknown

\( \square \)
distribution $\mathcal{D}$ over clustering instances. Recall that $\text{clus}_{\alpha,\beta}(\mathcal{V})$ denotes the expected cost of the clustering outputted by $(\alpha, \beta)$-Lloyd+++, with respect to the target clustering, and let $H$ denote the maximum value of $\text{clus}_{\alpha,\beta}(\mathcal{V})$.

**Theorem 6.** Given $\alpha_h$ and a sample of size $m = O\left(\left(\frac{H}{\epsilon}\right)^2 \left(\min(T, k) \log n + \log \frac{1}{\delta} + \log \alpha_h\right)\right)$ from $(\mathcal{D} \times [0,1]^k)^m$, with probability at least $1 - \delta$ over the choice of the sample, for all $\alpha \in [0, \alpha_h]$ and $\beta \in [1, \infty) \cup \{\infty\}$, 
\[
\frac{1}{m} \sum_{i=1}^{m} \text{clus}_{\alpha,\beta}(V^{(i)}, \hat{Z}^{(i)}) - \mathbb{E}_{V \sim \mathcal{D}}[\text{clus}_{\alpha,\beta}(V)] < \epsilon.
\]

**Proof.** Fix $\delta > 0$. From Theorems 4 and 5 for each $i$, the expected number of discontinuities of $\text{clus}_\alpha(V_i, Z_i)$ is at most $(8nk \log n) \min(n^k, n^{3T})$. By a Markov inequality, the number of discontinuities is $\leq \frac{1}{\delta} \cdot (16mnk \log n) \min(n^k, n^{3T})$ with probability $\geq 1 - \frac{\delta}{2m}$. Therefore, with probability $\geq 1 - \frac{\delta}{2}$, the total number of discontinuities of $\frac{1}{m} \sum_{i=1}^{m} \text{clus}_\alpha(V_i, Z_i)$ over $\alpha$ is $\leq \frac{1}{\delta} \cdot (16m^2 nk \log n) \min(n^k, n^{3T})$.

Now we apply Massart’s Lemma 35. Let $N \leq \frac{1}{\delta} \cdot (16m^2 nk \log n) \min(n^k, n^{3T})$ denote the number of $\alpha$-intervals such that $\frac{1}{m} \sum_{i=1}^{m} \text{clus}_\alpha(V_i, Z_i)$ is constant along each interval. For each interval $1 \leq i \leq N$, choose an arbitrary $\alpha_i$ in the interval, and define $a_i = [\text{clus}_{\alpha_i}(V_1, Z_1), \ldots, \text{clus}_{\alpha_N}(V_m, Z_m)]$. Then with probability $\geq 1 - \frac{\delta}{2}$,
\[
\hat{R}(A) \leq \max_i \|a_i - \bar{a}\| \cdot \sqrt{\frac{2 \log N}{m}} \leq \sqrt{\frac{2 \log (16m^2 nk \log n \min(n^k, n^{3T}))}{m}},
\]
and the proof follows from standard Rademacher complexity bounds [11].

Note that a corollary of Theorem 6 and Lemma 1 is a uniform convergence bound for all $\alpha \in [0, \infty) \cup \{\infty\}$, however, the algorithm designer may decide to set $\alpha_h < \infty$.

**Computational efficiency** In this section, we present an algorithm for tuning $\alpha$ whose running time scales with the true number of discontinuities over the sample. Combined with Theorem 4, this gives a bound on the expected running time of tuning $\alpha$.

The high-level idea of our efficient algorithm is to directly enumerate the set of centers that can possibly be output by $\theta$-sampling for a given clustering instance $\mathcal{V}$ and pre-sampled randomness $\hat{Z}$. We know from the previous section how to count the number of new breakpoints at any given state.
in the algorithm, however, efficiently solving for the exact breakpoints poses a new challenge. From the previous section, we know the breakpoints in $\alpha$ occur when $\frac{D_i(\alpha)}{D_n(\alpha)} = z_i$. This is an exponential equation with $n$ terms, and there is no closed-form solution for $\alpha$. Although an arbitrary equation of this form may have up to $n$ solutions, our key observation is that if $d_1 \geq \cdots \geq d_n$, then $\frac{D_i(\alpha)}{D_n(\alpha)}$ must be monotone decreasing (from Lemma 3), therefore, it suffices to binary search over $\alpha$ to find the solution to this equation. This motivates Algorithm 2 since we can now efficiently compute all possible outputs of Algorithm 1.

In order to analyze the runtime of Algorithm 2 we consider the execution tree of $d^\alpha$-sampling run on clustering instance $V$ with randomness $\vec{Z}$. This is a tree where each node is labeled by a state (i.e., a sequence $C$ of up to $k$ centers chosen so far by the algorithm) and the interval $A$ of $\alpha$ values that would result in the algorithm choosing this sequence of centers. The children of a node correspond to the states that are reachable in a single step (i.e., choosing the next center) for some value of $\alpha \in A$. The tree has depth $k$, and there is one leaf for each possible sequence of $k$ centers that $d^\alpha$-sampling will output when run on $V$ with randomness $\vec{Z}$. Our algorithm enumerates these leaves by performing a depth-first traversal of the tree.

**Theorem 7.** Given a clustering instance $V$ and randomness $\vec{Z}$, Algorithm 2 outputs all possible sets of centers chosen by $d^\alpha$-sampling for any $\alpha \in [0, \alpha_h]$. The expected runtime is $O(n^2 k^2 \alpha_h (\log n)^2)$.

**Proof.** The correctness of Algorithm 2 (that it outputs all possible sets of centers chosen by $d^\alpha$ sampling) follows from the fact that it outputs the centers in each leaf of the execution tree for $d^\alpha$-sampling.

Now we analyze the runtime of Algorithm 2. Let $(C, A)$ be any node in the algorithm, with centers $C$ and alpha interval $A = [\alpha_\ell, \alpha_h]$. Sorting the points in $V$ according to their distance to $C$ has complexity $O(n \log n)$. Finding the points sampled by $d^\alpha$-sampling with $\alpha$ set to $\alpha_\ell$ and $\alpha_h$ costs $O(n)$ time. Finally, computing the alpha interval $A_i$ for each child node of $(C, A)$ costs $O(n \log \frac{1}{\epsilon})$ time, since we need to perform $O(\log \frac{1}{\epsilon})$ iterations of binary search on $\alpha \mapsto \frac{D_i(\alpha)}{D_n(\alpha)}$ (where $\epsilon$ is machine precision) and each evaluation of the function costs $O(n)$ time. We charge this $O(n \log \frac{1}{\epsilon})$ time to the corresponding child node. If there are $N$ nodes in the execution tree, summing this cost over all nodes gives total running time of $O(N \cdot n \log \frac{2}{\epsilon})$. If we let $\#I$ denote the total number of $\alpha$-intervals for $V$, then each layer of the execution tree has at most $\#I$ nodes, and the depth is $k$, giving a total running time of $O(\#I \cdot kn \log \frac{2}{\epsilon})$.

From Theorem 4 we have $E[\#I] \leq 8nk \log n \cdot \alpha_h$, and we assume machine precision $\epsilon$ is a constant. Therefore, the expected runtime of Algorithm 2 is $O(n^2 k^2 \alpha_h (\log n)^2)$. This completes the proof. \hfill $\square$

In Appendix A we also show that for any bounded cost function, the expected cost of $d^\alpha$-sampling as a function of $\alpha$ is $H n^2 k \log n$-Lipschitz (recall that $H$ denotes the maximum value of $\text{clus}_{\alpha, \beta}(V)$). This implies that we can find an $\alpha$ parameter with sub-optimality at most $\epsilon$ by finding the best point from a discretization of $[0, \alpha_h]$ with step-size $s = \epsilon/(H n^2 k \log n)$. The running time of this algorithm is $O(n^2 k^2 H \log n / \epsilon)$, which is significantly slower than the efficient algorithm presented in this section. Moreover, our experiments show that the alpha intervals are not uniformly distributed. Instead, they are more fine-grained near zero. The discretization-based algorithm wastes effort exploring the fine-grained discretization of large values of $\alpha$, while our efficient algorithm does not.
5 Experiments

In this section, we empirically evaluate the effect of the $\alpha$ and $\beta$ parameters on clustering cost for real-world and synthetic clustering domains. We find that the optimal $\alpha$ and $\beta$ parameters vary significantly from domain to domain. We also find that the number of possible initial centers chosen by $d^\alpha$-sampling scales linearly with $n$ and $k$, suggesting our Theorem 4 is tight up to logarithmic factors. Finally, we show the empirical distribution of $\alpha$-interval boundaries.

**Experiment Setup.** Our experiments evaluate the $(\alpha, \beta)$-Lloyds++ family of algorithms on several distributions over clustering instances. Our clustering instance distributions are derived from classification datasets. For each dataset, we choose a subset of the class labels and construct a clustering instance consisting of points with those labels. For example, our MNIST distribution contains $\binom{10}{5} = 252$ clustering instances. In each case, the target clustering corresponds to the ground truth classification, and we measure distances between points in terms of the $\ell_2$ distance. By constructing instances corresponding to different subsets of labels, we obtain one distribution over related clustering instances for each classification dataset. We evaluate clustering performance in terms of the Hamming distance to the optimal clustering, or the total number of ‘mistakes’. Formally, the Hamming distance between the outputted clustering $\{C_1, \ldots, C_k\}$ and the optimal clustering $\{C^*_1, \ldots, C^*_k\}$ is measured by $\min_{\sigma} \sum_{i=1}^k C_i \setminus C^*_\sigma(i)$. In all cases, we limit the algorithm to performing 3 iterations of $\beta$-Lloyds. We use the following datasets:

- **MNIST:** We use the raw pixel representations of the subset of MNIST [33]. For each subset of 5 digit labels, we generate 1000 clustering instances, each consisting of 300 points.
- **CIFAR-10:** The CIFAR-10 dataset [30] is an image dataset with 10 classes. Following [31] we include 50 randomly rotated and cropped copies of each example. We extract the features from the Google Inception network [45] using layer in4d. For CIFAR-10 we set $k = 5$. For each subset of 5 image classes, we generate 1000 clustering instances, each consisting of 300 points.
- **CNAE-9:** The CNAE-9 [18] dataset consists of 1080 documents describing Brazilian companies categorized into 9 categories. Each example is represented by an 875-dimensional vector, where each entry is the frequency of a specific word. For CNAE-9 we set $k = 4$. For each subset of 4 document classes, we generate 1000 clustering instances, each consisting of 300 points.
- **Gaussian Grid:** We also use a synthetic 2-dimensional clustering instance where points are sampled from a mixture of 9 standard Gaussians arranged in a $3 \times 3$ grid with step-size 5. For the Gaussian grid we set $k = 4$. As with the other examples, we generate varied clustering instances by choosing all subsets of 4 out of the 9 Gaussians. For each subset of 4 Gaussians, we generate 1000 clustering instances, each consisting of 300 points.

**Parameter Study.** Our first experiment explores the effect of the $\alpha$ and $\beta$ parameters. For each dataset, we performed 50 trials of $(\alpha, \beta)$-Lloyds++ on instances of $n = 300$ points for all subsets of the class labels. Figure 3 shows the average error on each dataset as a function of $\alpha$ and $\beta$. The optimal parameters vary significantly across the datasets. On MNIST and the Gaussian grid, it is best to set $\alpha$ to be large, while on the remaining datasets the optimal value is low. Neither the $k$-means++ algorithm nor farthest-first traversal have good performance across all datasets. On the Gaussian grid example, $k$-means++ has loss 9% while the best parameter setting only has loss 3%. Similarly, on MNIST, $k$-means++ has loss 47%, while the best parameter setting only has loss 44%. Recovering the class labels of MNIST by clustering is a challenging setting, so an improvement of 3% is substantial.

Next, we run Algorithm 2 to tune $\alpha$, setting $\beta = 2$. For each dataset, we plot the average majority cost as a function of $\alpha$ on a training dataset consisting of 75% of the label subsets, and a testing dataset consisting of the remaining 25% of label subsets. For each instance, we repeat the experiment 500 or 1000 times and report the average majority cost. The optimal value of $\alpha$ varies
between the different datasets, showing that tuning the parameters leads to improved performance. Moreover, in each case the difference between the training and testing error plots is small, giving evidence for generalization.

Number of \(\alpha\)-Intervals. Next we evaluate the average number of \(\alpha\)-intervals for random instances sampled from each of the datasets. Averaging over \(N = 5000\) sampled clustering instances of \(n = 600\) points. On average, MNIST had 2355.4 \(\alpha\)-intervals, CIFAR-10 had 1205.7 \(\alpha\)-intervals, CNAE-9 had 2502.1 \(\alpha\)-intervals, and the gaussian grid had 1997.8 \(\alpha\)-intervals. In all cases, the number of \(\alpha\)-intervals is many orders of magnitude smaller than \(n^k > 10^{18}\). Figure 5 is a histogram showing the average distribution of the boundaries between the \(\alpha\)-intervals on the CNAE-9 instances. The boundaries are concentrated around \(\alpha = 2.5\) with density decaying rapidly as \(\alpha\) increases. This trend is persistent across all our datasets. Finally, Figure 5 shows that for all four datasets, the number of \(\alpha\)-intervals grows only linearly with \(n\).

Distribution of \(\alpha\)-decision Points. For each of our datasets we produced histograms showing the distribution of the \(\alpha\)-decision points. Figure 6 shows the distributions for MNIST, CIFAR-10, CNAE-9, and the Gaussian Grid.

6 Conclusion

We define an infinite family of algorithms generalizing Lloyd’s method, with one parameter controlling the the initialization procedure, and another parameter controlling the local search procedure. This family of algorithms includes the celebrated \(k\)-means++ algorithm, as well as the classic
farthest-first traversal algorithm. We provide a sample efficient and computationally efficient algorithm to learn a near optimal parameter over an unknown distribution of clustering instances, by developing techniques to bound the expected number of discontinuities in the cost as a function of the parameter. We give a thorough empirical analysis, showing that the value of the optimal parameters transfer to related clustering instances. We show the optimal parameters vary among different types of datasets, and the optimal parameters often significantly improves the error compared to existing algorithms such as k-means++ and farthest-first traversal.

7 Acknowledgements

This work was supported in part by NSF grants CCF-1535967, IIS-1618714, an Amazon Research Award, a Microsoft Research Faculty Fellowship, and a National Defense Science & Engineering Graduate (NDSEG) fellowship.

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Figure 6: Distribution of $\alpha$-decision points.

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A Details from Section 4

In this section, we give details and proofs from Section 4.

Lemma 1 (restated). Given a clustering instance $\mathcal{V}$ and $\delta > 0$, if $\alpha > \frac{\log(n/k)}{\log s}$, then $d^\alpha$-sampling will give the same output as farthest-first traversal with probability $> 1 - \delta$. Here, $s$ denotes the minimum ratio $d_1/d_2$ between two distances $d_1 > d_2$ in the point set.

Proof. Given such a clustering instance $\mathcal{V} = (V, d, k)$ and $\alpha$, first we note that farthest-first traversal and $d^\alpha$-sampling both start by picking a center uniformly at random from $V$. Assume both algorithms have chosen initial center $v_1$, and let $C = \{v_1\}$ denote the set of current centers. In rounds 2 to $n$, farthest-first traversal deterministically chooses the center $u$ which maximizes $d_{\text{min}}(u, C)$ (breaking ties uniformly at random). We will show that with high probability, in every round, $d^\alpha$-sampling will also choose the center maximizing $d_{\text{min}}(u, C)$ or break ties at random. In round $t$, let $d_t = \max_{u \in V} d_{\text{min}}(u, C)$ (assuming $C$ are the first $t-1$ centers chosen by farthest-first traversal). Let $d'_t$ denote the largest distance smaller than $d_t$, so by assumption, $d_t > s \cdot d'_t$. Assume there are $x$ points whose minimum distance to $C$ is $d_t$. Then the probability that $d^\alpha$-sampling will fail to choose one of these points is at most

$$\frac{(n-x)d'^\alpha_t}{(n-x)d^\alpha_t + x(sd'_t)^\alpha} \leq \frac{n-x}{n-x + x \cdot s^\alpha} \leq \frac{n}{s^\alpha}$$

Over all $k$ rounds of the algorithm, the probability that $d^\alpha$-sampling will deviate from farthest-first traversal (assuming they start with the same first choice of a center and break ties at random in the same way) is at most $\frac{nk}{s^\alpha}$, and if we set this probability smaller than $\delta$ and solve for $\alpha$, we obtain

$$\alpha > \frac{\log(n/k)}{\log s}.$$

Now we define a common stability assumption called separability [28, 42], which states that there exists a value $r$ such that all points in the same cluster have distance less than $r$ and all points in different clusters have distance greater than $r$.

Definition 8. A clustering instance satisfies $(1+c)$-separation if $(1+c) \max_{i|u,v \in C_i} d(u, v) < \min_{j \neq j'|u \in C_j, v \in C_{j'}} d(u, v)$.

Now we show that under $(1+c)$-separation, $d^\alpha$-sampling will give the same output as farthest-first traversal with high probability if $\alpha > \log n$, even for $c = 1$.

Lemma 9. Given a clustering instance $\mathcal{V}$ satisfying $(1+c)$-separation, and $0 < \delta$, then if $\alpha > \frac{1}{c} \cdot (\log n + \log \frac{1}{\delta})$, with probability $> 1 - \delta$, $d^\alpha$-sampling with Lloyd’s algorithm will output the optimal clustering.

Proof. Given $\mathcal{V}$ satisfying $(1+c)$-separation, we know there exists a value $r$ such that for all $i$, for all $u, v \in C_i$, $d(u, v) < r$, and for all $u \in C_j, v \in C_{j'} \neq j$, $d(u, v) > (1+c)r$. WLOG, let $r = 1$. Consider round $t$ of $d^\alpha$-sampling and assume that each center $v$ in the current set of centers $C$ is from a unique cluster in the optimal solution. Now we will bound the probability that the center chosen in
round $t$ is not from a unique cluster in the optimal solution. Given a point $u$ from a cluster already represented in $C$, there must exist $v \in C$ such that $d(u, v) < 1$, so $d_{\min}(u, C) < 1$. Given a point $u$ from a new cluster, it must be the case that $d_{\min}(u, C) > (1 + c)$. The total number of points in represented clusters is $< n$. Then the probability we pick a point from an already represented cluster is $\leq \frac{tn}{tn+c}$. If we set $\frac{tn}{tn+c} \leq \frac{\delta}{k}$ and solve for $\alpha$, we obtain $\alpha > \frac{\log n + \log \frac{1}{\delta}}{\log c} \leq \frac{1}{\epsilon} \left( \log n + \frac{1}{\delta} \right)$. Since this is true for an arbitrary round $t$, and there are $k$ rounds in total, we may union bound over all rounds to show the probability $d^\al$-sampling outputting one center per optimal clustering is $> 1 - \delta$. Then, using $(1 + c)$-separation, the Voronoi tiling of these centers must be the optimal clustering, so Lloyd’s algorithm converges to the optimal solution in one step.

Next, we give the formal proof of Theorem 2.

**Theorem 2 (restated).** For $\alpha^*, \beta^* \in [0, \infty) \cup \{\infty\}$, there exists a clustering instance $\mathcal{V}$ whose target clustering is the optimal $\ell_\beta$-clustering, such that $\text{clus}_{\alpha^*, \beta^*}(\mathcal{V}) < \text{clus}_{\alpha, \beta}(\mathcal{V})$ for all $(\alpha, \beta) \neq (\alpha^*, \beta^*)$.

**Proof.** Consider $\alpha^*, \beta^* \in [0, \infty) \cup \{\infty\}$. The clustering instance consists of 6 clusters, $C_1, \ldots, C_6$. The target clustering will be the optimal $\ell_{\beta^*}$-objective. The basic idea of the proof is as follows.

First, we show that for all $\beta$ and $\alpha \neq \alpha^*$, $\text{clus}_{\alpha^*, \beta^*}(\mathcal{V}) < \text{clus}_{\alpha, \beta}(\mathcal{V})$. We use clusters $C_1, \ldots, C_4$ to accomplish this. We set up the distances so that $d^\al$ sampling is more likely to sample one point per cluster than any other value of $\alpha$. If the sampling does not sample one point per cluster, then it will fall into a high-error local minima trap that $\beta$-Lloyd’s method cannot escape, for any value of $\beta$. Therefore, $d^\al$ sampling is more effective than any other value of $\alpha$.

Next, we use clusters $C_5$ and $C_6$ to show that if we start with one center in $C_5$ and one in $C_6$, then $\beta^*$-Lloyd’s method will strictly outperform any other value of $\beta$. We accomplish this by adding three choices of centers for $C_5$. Running $\beta^*$-Lloyd’s method will return the correct center, but any other value of $\beta$ will return suboptimal centers which incur error on $C_5$ and $C_6$. Also, we show that Lloyd’s method returns the same centers on $C_1, \ldots, C_4$, independent of $\beta$.

For the first part of the proof, we define three cliques (see Figure 1). The first two cliques are $C_1$ and $C_2$, and the third clique is $C_3 \cup C_4$. $C_1$ contains $w_1$ points at distance $x > 1$, and $C_2$ contains $w_2$ points at distance $\frac{1}{2}$. We set $w_1 = x^{2\alpha^*}w_2$. The last clique contains $w$ points at distance 1. Since the cliques are very far apart, the first three sampled centers will each be in a different clique, with high probability (for $\alpha > .1$). The probability of sampling a 4th center $x_4$ in the third clique, for $\alpha = \alpha^* + \delta$ is equal to

$$\frac{w}{w + (x^{\alpha^*+\delta} + x^{\alpha^*-\delta})w_2}.$$ 

Since $x^{\alpha^*+\delta} + x^{\alpha^*-\delta}$ is minimized when $\delta = 0$, this probability is maximized when $\alpha = \alpha^*$. Now we show that the error will be much larger when $x_4$ is not in the third clique. We add center $c_1$ which is distance $x - \epsilon$ to all points in $C_1$. We also add centers $b_1$ and $b_1'$ which are distance $x - 2\epsilon$ to $B_1$ and $B_1'$ such that $B_1$ and $B_1'$ form a partition of $C_1$. Similarly, we add centers $c_2, b_2$, and $b_2'$ at distance $\frac{x}{2} - \epsilon$ to $C_2$, $B_2$, and $B_2'$, respectively, such that $B_2$ and $B_2'$ form a partition of $C_2$. Finally, we add $c_3$ and $c_4$ which are distance $.5$ to $C_3$ and $C_4$, respectively, and we add $b_3$ which is distance $1 - \epsilon$ to $C_3 \cup C_4$. Then the optimal centers for any $\beta$ must be $c_1, c_2, c_3, c_4$, and this will be the solution of $\beta$-Lloyd’s method, as long as the sampling procedure returned one point in the first two cliques, and two points in the third clique. If the sampling procedure returns two points in the first clique or second clique, then $\beta$-Lloyd’s method will return $b_1, b_1', c_2, b_3$ or $c_1, b_2, b_2', b_3$, respectively. This will incur error $w/2 + w_1/2$ or $w/2 + w_2/2$, since we set the target clustering to be the optimal $\ell_{\beta^*}$ objective which is equal to $\{C_1, C_2, C_3, C_4\}$. Note that we have
set up the distances so that Lloyd’s method is independent of \( \beta \). Therefore, the expected error is equal to

\[
\frac{w}{w + (x^{2\alpha+\delta} + x^{\alpha-\delta})w_2} \cdot (w/2 + \min(w_1,w_2)/2).
\]

This finishes off the first part of the proof. Next, we construct \( C_5 \) and \( C_6 \) so that \( \beta^* \)-Lloyd’s method will return the best solution, assuming the sampling returned one point in \( C_5 \) and \( C_6 \). Later we will show how adding these clusters does not affect the previous part of the proof. We again define three cliques. The first clique is size \( \frac{2}{3}w_5 \) and distance \( .1 \), the second clique is size \( \frac{1}{3}w_5 \) and distance \( .1 \), and the third clique is size \( w_6 \) and distance \( .1 \). The first two cliques are \( C_5 \), and the second clique is \( C_6 \). The distance between the first two cliques is \( .2 \), and the distance between the first two and the third clique is 1000. Now imagine the first two cliques are parallel to each other, and there is a perpendicular bisector which contains possible centers for \( C_5 \). i.e., we will consider possible centers \( c \) for \( C_5 \) where the \( \ell_\beta \) cost of \( c \) is \( \frac{2}{3}w_5 \cdot z^\beta + \frac{1}{3}w_5(2 - z)^\beta \) for some \( 0 \leq z \leq 2 \). For \( \beta \in (0,\infty) \), the \( \beta \) which minimizes the expression must be in \([0,2]\). We set \( c_5 \) corresponding to the \( z \) which minimizes the expression for \( \beta^* \), call it \( z^* \). Therefore, \( \beta^* \)-Lloyd’s method will output \( c_5 \). We also set centers \( b_5 \) and \( b_5' \) corresponding to \( z^* - \epsilon \) and \( z^* + \epsilon \). Therefore, any value of \( \beta \) slightly above or below \( \beta^* \) will return a different center. We add a center \( C_5 \) at distance \( .1 - \epsilon \) to the third clique. This is the only point we add, so it will always be chosen by \( \beta \)-Lloyd’s method for all \( \beta \). Finally, we add two points \( p_1 \) and \( p_2 \) in between the second and third cliques. We set the distances as follows. \( d(c_5,p_1) = d(c_6,p_2) = 500 - \epsilon \), \( d(c_5,p_2) = d(c_6,p_1) = 500 \), \( d(b_5,p_1) = 500 + \epsilon \), and \( d(b_5',p_2) = 500 - 2\epsilon \). Since the weight of these two points are very small compared to the cliques, these points will have no effect on the prior sampling and Lloyd’s method analyses. The optimal clustering for the \( \ell_\beta \) objective is to add \( p_1 \) to \( C_5 \) and \( p_2 \) to \( C_6 \). However, running \( \beta \)-Lloyd’s method for \( \beta \) smaller or larger than \( \beta^* \) will return center \( b_5 \) or \( b_5' \) and incur error \( 1 \) by mislabeling \( p_1 \) or \( p_2 \).

Since all cliques from both parts of the proof are 1000 apart, with high probability, the first 5 sampled points will be in cliques \( C_1, C_2, C_3 \cup C_4, C_5 \), and \( C_6 \). Since the cliques from the second part of the proof are distance \( .2 \), while in the first part they were \( > \frac{1}{2} \) apart, we can set the variables \( x, w_1, w_2, w, w_5, w_6 \) so that with high probability, the sixth sampled point will not be in \( C_5 \) or \( C_6 \). Therefore, the constructions in the second part do not affect the first part. This concludes the proof. 

Now we upper bound the number of discontinuities of \( \text{seed}_n(\mathcal{V}, \vec{Z}) \). Recall that \( \text{seed}_n(\mathcal{V}, \vec{Z}) \) denotes the outputted centers from phase 1 of Algorithm 1 on instance \( \mathcal{V} \) with randomness \( \vec{Z} \). For the first phase, our main structural result is to show that for a given clustering instance and value of \( \beta \), with high probability over the randomness in Algorithm 1, the number of discontinuities of the cost function \( \text{clus}_{\alpha,\beta}(\mathcal{V}, \vec{Z}) \) as we vary \( \alpha \in [0, \alpha_h] \) is \( O(nk(\log n)\alpha_h) \). Our analysis crucially harnesses the randomness in the algorithm to achieve this bound. In contrast, a combinatorial approach would only achieve a bound of \( n^{O(k)} \), which is the total number of sets of \( k \) centers. For completeness, we start with a combinatorial proof of \( O(n^{k+3}) \) discontinuities. Although Theorem 10 is exponential as opposed to Theorem 4, it holds with probability 1 and has no dependence on \( \alpha_h \).

**Theorem 10.** Given a clustering instance \( \mathcal{V} \) and vector \( \vec{Z} \in [0,1]^k \), the number of discontinuities of \( \text{seed}_n(\mathcal{V}, \vec{Z}) \) as a function of \( \alpha \) over \([0,\infty) \cup \{\infty\} \) is \( O\left(\min\left(n^{k+3}, n^22^n\right)\right) \).

**Proof.** Given a clustering instance \( \mathcal{V} \) and a vector \( \vec{Z} \), consider round \( t \) of the \( d^n \) seeding algorithm. At this point, there are \( \binom{n}{t-1} \) choices for the set of current centers \( C \). Recall that the decision for the next center depends on \( z_t \in [0,1] \). We denote the points \( V = \{v_1, \ldots, v_n\} \) and WLOG assume
the algorithm orders the intervals \(I_{v_1}, I_{v_2}, \ldots, I_{v_n}\). Given a point \(v_i \in V\), it will be chosen as the next center if and only if \(z_t\) lands in its interval, formally,

\[
\frac{\sum_{j=1}^{i-1} d_{\min}(v_j, C)^\alpha}{\sum_{j=1}^{n} d_{\min}(v_j, C)^\alpha} < z_t < \frac{\sum_{j=1}^{i} d_{\min}(v_j, C)^\alpha}{\sum_{j=1}^{n} d_{\min}(v_j, C)^\alpha}
\]

By a consequence of Rolle’s theorem, these two equations have at most \(n + 1\) roots each. Therefore, in the \(n + 2\) intervals of \(\alpha\) between each root, the decision whether or not to choose \(v_i\) as a center in round \(t\) is fixed. Note that the center set \(C\), the point \(v_i\), and the number \(z_t\) fixed the coefficients of the equation. Since in round \(t\), there are \(\binom{n}{t}\) choices of centers, then there are \(\sum_{t=1}^{k} \binom{n}{t} \cdot n \cdot 2\) total equations which determine the outcome of the algorithm. Each equation has at most \(n + 1\) roots, so it follows there are \(1 + \sum_{t=1}^{k} \binom{n}{t} \cdot n \cdot 2(n + 1) = O(n^3 \cdot n^k)\) total intervals of \(\alpha\) along \([0, \infty) \cup \{\infty\}\) such that within each interval, the entire outcome of the algorithm, \text{seed}(V, \vec{Z})\), is fixed. Note that we used \(k \cdot n^k\) to bound the total number of choices for the set of current centers. We can also bound this quantity by \(2^n\), since each point is either a center or not a center. This results in a final bound of \(O(\min (n^{k+3}, n^2 2^n))\).

\[\square\]

**Lemma 3 (restated).** If \(v(1), \ldots, v(n)\) are sorted in decreasing distance from a set \(C\) of centers, then for each \(i = 1, \ldots, n\), the function \(\alpha \mapsto \frac{D_i(\alpha)}{D_n(\alpha)}\) is monotone increasing.

**Proof.** Recall that \(D_i(\alpha) = \sum_{j=1}^{i} d_{\min}(v(j), C)^\alpha\), where \(v(1), \ldots, v(n)\) are the points sorted in decreasing order of distance to the set of centers \(C\).

We prove that for each \(i\), the function \(\alpha \mapsto D_i(\alpha)/D_n(\alpha)\) is monotone increasing. Given \(\alpha_1 < \alpha_2\), we must show that for each \(i\),

\[
\frac{D_i(\alpha_1)}{D_n(\alpha_1)} \leq \frac{D_i(\alpha_2)}{D_n(\alpha_2)}.
\]

This is equivalent to showing

\[
D_i(\alpha_2)D_n(\alpha_1) \leq D_i(\alpha_1)D_n(\alpha_2).
\]

Using the shorthand notation \(d_j = d(v_j, C)\), we have

\[
D_i(\alpha_2)D_n(\alpha_1) = \left(\sum_{j=1}^{i} d_j^{\alpha_1}\right) z \left(\sum_{j=1}^{n} d_j^{\alpha_2}\right)
= \left(\sum_{j=1}^{i} d_j^{\alpha_1}\right) \left(\sum_{j=1}^{i} d_j^{\alpha_2}\right) + \left(\sum_{j=1}^{i} d_j^{\alpha_1}\right) \left(\sum_{j=i+1}^{n} d_j^{\alpha_2}\right)
\]

\[
\leq \left(\sum_{j=1}^{i} d_j^{\alpha_1}\right) \left(\sum_{j=1}^{i} d_j^{\alpha_2}\right) + \sum_{j=1}^{i} \sum_{k=i+1}^{n} d_j^{\alpha_1} d_k^{\alpha_1}
\]

\[
\leq \left(\sum_{j=1}^{i} d_j^{\alpha_1}\right) \left(\sum_{j=1}^{i} d_j^{\alpha_2}\right) + \sum_{j=1}^{i} \sum_{k=i+1}^{n} d_j^{\alpha_2} d_k^{\alpha_1} \left(\frac{d_j}{d_k}\right)^{\alpha_1 - \alpha_2}
\]

\[
\leq \left(\sum_{j=1}^{i} d_j^{\alpha_1}\right) \left(\sum_{j=1}^{i} d_j^{\alpha_2}\right) + \sum_{j=1}^{i} \sum_{k=i+1}^{n} d_j^{\alpha_2} d_k^{\alpha_1}.
\]
\[
\left( \sum_{j=1}^{i} d_{ij}^{\alpha_{2}} \right) \left( \sum_{j=1}^{n} d_{ij}^{\alpha_{1}} \right) = D_{i}(\alpha_{1}) D_{n}(\alpha_{1}),
\]
as required.

Now to work up to the proof of Theorem 4, we bound the derivative of \( \frac{D_{i}(\alpha)}{D_{n}(\alpha)} \).

**Lemma 11.** Given \( d_{1} \geq \cdots \geq d_{n} \), and \( i = 1, \ldots, n \), for \( \alpha \in [0, \alpha_{h}] \), \( \left| \frac{\partial}{\partial \alpha} \left( \frac{D_{i}(\alpha)}{D_{n}(\alpha)} \right) \right| \leq 4 \log n \).

**Proof.**
\[
\frac{\partial}{\partial \alpha} \left( \frac{D_{i}(\alpha)}{D_{n}(\alpha)} \right) \leq \frac{(D_{i}(\alpha)'(D_{n}(\alpha)) - (D_{n}(\alpha))'(D_{i}(\alpha)))}{(D_{n}(\alpha))^{2}}
\]
\[
\leq \frac{\left( \sum_{x=1}^{i} d_{y}^{\alpha} \log(d_{x}^{\alpha}) \right) \left( \sum_{y=1}^{n} d_{x}^{\alpha} \right) - \left( \sum_{x=1}^{i} d_{y}^{\alpha} \right) \left( \sum_{y=1}^{n} d_{x}^{\alpha} \log(d_{y}^{\alpha}) \right)}{\left( \sum_{x=1}^{i} \sum_{y=1}^{n} d_{y}^{\alpha} d_{x}^{\alpha} \right)}
\]
\[
\leq 2 \cdot \frac{\sum_{x=1}^{i} \sum_{y=i+1}^{n} d_{y}^{\alpha} \log(d_{x}^{\alpha}) - \log(d_{y}^{\alpha})}{\sum_{x=1}^{i} \sum_{y=1}^{n} d_{y}^{\alpha}}
\]
\[
\leq 2 \cdot \frac{\sum_{x=1}^{i} \left( d_{y}^{\alpha} \right) \left( \sum_{y=i+1}^{n} d_{y}^{\alpha} \log(d_{x}^{\alpha}) \right)}{\sum_{x=1}^{i} d_{y}^{\alpha} \left( \sum_{y=1}^{n} d_{y}^{\alpha} \right)}
\]

Now we will show that \( \sum_{y=i+1}^{n} d_{y}^{\alpha} \log \left( \frac{d_{y}^{\alpha}}{d_{y}^{\alpha}} \right) \leq 2 \log n \sum_{y=1}^{n} d_{y}^{\alpha} \) by grouping each \( i + 1 \leq y \leq n \) into one of two different cases.

Case 1: \( d_{y}^{\alpha} > \frac{d_{x}^{\alpha}}{n} \). Then \( d_{y}^{\alpha} \log \left( \frac{d_{y}^{\alpha}}{d_{y}^{\alpha}} \right) \leq 2 d_{y}^{\alpha} \log n \).

Case 2: \( d_{y}^{\alpha} < \frac{d_{x}^{\alpha}}{n} \). Then \( d_{y}^{\alpha} \log \left( \frac{d_{y}^{\alpha}}{d_{y}^{\alpha}} \right) \leq d_{y}^{\alpha} \left( \frac{d_{x}^{\alpha}}{d_{y}^{\alpha}} \log \frac{d_{x}^{\alpha}}{d_{y}^{\alpha}} \right) \leq \frac{1}{n} \cdot d_{x}^{\alpha} \), where the last inequality follows because \( \frac{1}{x} \log x \leq \frac{1}{n} \) for all \( x > n^{2} \). Therefore, the sum over all \( y \) in case 2 are smaller than \( d_{x}^{\alpha} \).

So, for all \( y \) in case 1, \( d_{y}^{\alpha} \log \left( \frac{d_{y}^{\alpha}}{d_{y}^{\alpha}} \right) \leq 2 d_{y}^{\alpha} \log n \), and \( \sum_{y \text{case 2}} d_{y}^{\alpha} \log \left( \frac{d_{y}^{\alpha}}{d_{y}^{\alpha}} \right) \leq d_{x}^{\alpha} \). It follows that for all \( i \geq 1 \), \( \sum_{y=i+1}^{n} d_{y} \log \left( \frac{d_{y}}{d_{y}} \right) \leq 2 \log n \sum_{y=1}^{n} d_{y} \). Therefore, \( \frac{\partial}{\partial \alpha} \left( \frac{D_{i}(\alpha)}{D_{n}(\alpha)} \right) \leq 4 \log n \). \( \square \)

**Theorem 4 (restated).** Given a clustering instance \( \mathcal{V} \), the expected number of discontinuities of \( \text{seed}_{\alpha} (\mathcal{V}, \tilde{Z}) \) as a function of \( \alpha \) over \( [0, \alpha_{h}] \) is \( O(nk(\log n)\alpha_{h}) \). Here, the expectation is over the uniformly random draw of \( \tilde{Z} \in [0, 1]^{k} \).

**Proof.** Given \( \mathcal{V} \) and \( [0, \alpha_{h}] \), we will show that \( \mathbb{E}[\#I] \leq nk \log n \cdot \alpha_{h} \), where \( \#I \) denotes the total number of discontinuities of \( \text{seed}_{\alpha} (\mathcal{V}, \tilde{Z}) \) and the expectation is over the randomness \( Z \in [0, 1]^{k} \) of the \( d_{\alpha} \)-sampling algorithm. Consider round \( t \) of a run of the algorithm. Suppose at the beginning of round \( t \), there are \( L \) possible states of the algorithm, e.g., \( L \) sets of \( \alpha \) such that within a set, the choice of the first \( t - 1 \) centers is fixed. By Lemma 3, we can write these sets as \( [\alpha_{0}, \alpha_{1}], \ldots, [\alpha_{L-1}, \alpha_{L}] \), where \( 0 = \alpha_{0} < \cdots < \alpha_{L} = \alpha_{h} \). Given one interval, \( [\alpha_{\ell}, \alpha_{\ell+1}] \), we claim the expected number of new breakpoints \( \#I_{\ell, \ell+1} \) by choosing a center in round \( t \) is bounded by \( 4n \log n (\alpha_{\ell+1} - \alpha_{\ell}) \). Note that \( \#I_{\ell, \ell+1} + 1 \) is the number of possible choices for the next center in round \( t \) using \( \alpha \) in \( [\alpha_{\ell}, \alpha_{\ell+1}] \).
The claim gives an upper bound on the expected number of new breakpoints, where the expectation is only over \( z_t \) (the uniformly random draw from \([0, 1]\) used by Algorithm 1 in round \( t \)), and the bound holds for any given configuration of \( d_1 \geq \cdots \geq d_n \). Assuming the claim, we can finish off the proof by using linearity of expectation as follows.

\[
E_{Z \in [0, 1]^k}[\#I] \leq E_{Z \in [0, 1]^k}\left[ \sum_{t=1}^{k} \sum_{\ell=1}^{L} (\#I_{t, \ell}) \right]
\leq \sum_{t=1}^{k} \sum_{\ell=1}^{L} E_{Z \in [0, 1]^k}[\#I_{t, \ell}]
\leq \sum_{t=1}^{k} \sum_{\ell=1}^{L} 4n \log n (\alpha_{\ell+1} - \alpha_{\ell})
\leq 4nk \log n \cdot \alpha_h
\]

Now we will prove the claim. Recall that for \( \alpha \)-sampling, each point \( x \) receives an interval along \([0, 1]\) of size \( \frac{d_{j}^\alpha}{D_n(\alpha)} \), so the number of breakpoints in round \( t \) along \([\alpha_{\ell}, \alpha_{\ell+1}]\) corresponds to the number of times \( z_t \) switches intervals as we increase \( \alpha \) from \( \alpha_{\ell} \) to \( \alpha_{\ell+1} \). By Lemma 3, the endpoints of these intervals are monotone increasing, so the number of breakpoints is exactly \( x - y \), where \( x \) and \( y \) are the minimum indices s.t. \( \frac{D_j(\alpha)}{D_n(\alpha)} > z_t \) and \( \frac{D_j(\alpha_{\ell+1})}{D_n(\alpha_{\ell+1})} > z_t \), respectively. We want to compute the expected value of \( x - y \) for \( z_t \) uniform in \([0, 1]\) (here, \( x \) and \( y \) are functions of \( z_t \)).

We take the approach of analyzing each interval individually. One method for bounding \( E_{z_t \in [0, 1]}[x - y] \) is to compute the maximum possible number of breakpoints for each interval \( I_{\ell} \). Specifically, if we let \( i \) denote the minimum index such that \( \frac{D_j(\alpha_{i})}{D_n(\alpha_{i})} < \frac{D_j(\alpha_{i+1})}{D_n(\alpha_{i+1})} \), then

\[
E[\#I_{t, \ell}] \leq \sum_{j=1}^{n} P \left( \frac{D_j(\alpha_{i})}{D_n(\alpha_{i})} < z_t < \frac{D_j(\alpha_{i+1})}{D_n(\alpha_{i+1})} \right) \cdot (j - i + 1)
\leq \sum_{j=1}^{n} \frac{d_{j}^\alpha}{D_n(\alpha_{i})} \cdot (j - i + 1).
\]

In this expression, we are using the worst case number of breakpoints within each bucket, \( j - i + 1 \).

We cannot quite use this expression to obtain our bound; for example, when \( \alpha_{\ell+1} - \alpha_{\ell} \) is extremely small, \( j - i + 1 = 1 \), so this expression will give us \( E[\#I_{t, \ell}] \leq 1 \) over \([\alpha_{\ell}, \alpha_{\ell+1}]\), which is not sufficient to prove the claim. Therefore, we give a more refined analysis by further breaking into cases based on whether \( z_t \) is smaller or larger than \( \frac{D_j(\alpha_{\ell})}{D_n(\alpha_{\ell})} \). In case 1, when \( z_t > \frac{D_j(\alpha_{\ell})}{D_n(\alpha_{\ell})} \), the number of breakpoints is \( j - i \), and we will show that \( j - i \leq n(\log n)(\alpha_{\ell+1} - \alpha_{\ell}) \). In case 2, when \( z_t < \frac{D_j(\alpha_{\ell+1})}{D_n(\alpha_{\ell+1})} \), the number of breakpoints is \( j - i + 1 \), but we will show the probability of this case is low.

For case 2, the probability that \( z_t \) is in between \( \frac{D_j(\alpha_{i})}{D_n(\alpha_{i})} \) and \( \frac{D_j(\alpha_{i+1})}{D_n(\alpha_{i+1})} \) is \( \frac{D_j(\alpha_{i+1})}{D_n(\alpha_{i+1})} - \frac{D_j(\alpha_{i})}{D_n(\alpha_{i})} \leq \frac{D_j(\alpha_{i+1})}{D_n(\alpha_{i+1})} - \frac{D_j(\alpha_{i})}{D_n(\alpha_{i})} \). Therefore, we can bound this quantity by bounding the derivative \( |\frac{\partial}{\partial \alpha} \left( \frac{D_j(\alpha)}{D_n(\alpha)} \right)| \), which is at most 4 \( \log n \) by Lemma 11.

For case 1, recall that \( j - i \) represents the number of intervals between \( \frac{D_j(\alpha_{i})}{D_n(\alpha_{i})} \) and \( \frac{D_j(\alpha_{i+1})}{D_n(\alpha_{i+1})} \). Note that the smallest interval in this range is \( \frac{d_{j}^\alpha}{D_n(\alpha_{i})} \), and \( \frac{D_j(\alpha_{i})}{D_n(\alpha_{i})} - \frac{D_j(\alpha_{i+1})}{D_n(\alpha_{i+1})} \leq \frac{D_j(\alpha_{i+1})}{D_n(\alpha_{i+1})} - \frac{D_j(\alpha_{i})}{D_n(\alpha_{i})} \). Therefore,
the expected number of breakpoints is at most \( \frac{D_n(\alpha_\ell)}{\alpha_\ell} \cdot \left( \frac{D_i(\alpha_{\ell+1})}{D_n(\alpha_{\ell+1})} - \frac{D_i(\alpha_\ell)}{D_n(\alpha_\ell)} \right) \), and we can bound the second half of this fraction by again using Lemma 11.

Putting case 1 and case 2 together, we have

\[
E[\# I_{\ell, \ell}] \leq \sum_j P \left( \frac{D_i(\alpha_{\ell+1})}{D_n(\alpha_{\ell+1})} < z_\ell < \frac{D_{j+1}(\alpha_\ell)}{D_n(\alpha_\ell)} \right) \cdot (j - i) + \sum_j P \left( \frac{D_j(\alpha_\ell)}{D_n(\alpha_\ell)} < z_\ell < \frac{D_i(\alpha_{\ell+1})}{D_n(\alpha_{\ell+1})} \right) \cdot (j - i + 1)
\]

\[
\leq \sum_j \left( \frac{D_i(\alpha_{\ell+1})}{D_n(\alpha_{\ell+1})} - \frac{D_i(\alpha_\ell)}{D_n(\alpha_\ell)} \right) + \sum_j \left( \frac{D_j(\alpha_{\ell+1})}{D_n(\alpha_{\ell+1})} - \frac{D_j(\alpha_\ell)}{D_n(\alpha_\ell)} \right)
\]

\[
\leq 4 \log n(\alpha_{\ell+1} - \alpha_\ell) + \sum_j 4 \log n(\alpha_{\ell+1} - \alpha_\ell)
\]

\[
\leq 8n \log n(\alpha_{\ell+1} - \alpha_\ell)
\]

This concludes the proof. \(\square\)

In fact, we can also show that the worst-case number of discontinuities is exponential.

**Lemma 12.** Given \( n \), there exists a clustering instance \( \mathcal{V} \) of size \( n \) and a vector \( \vec{z} \) such that the number of discontinuities of \( \text{seed}_n(\mathcal{V}, \vec{z}) \) as a function of \( \alpha \) over \([0, 2]\) is \( 2^{\Omega(n)} \).

**Proof.** We construct \( \mathcal{V} = (V, d, k) \) and \( \vec{z} = \{z_1, \ldots, z_k\} \) such that \( \text{seed}_n(\mathcal{V}, \vec{z}) \) has \( 2^{k/3} \) different intervals in \( \alpha \) which give different outputs.

Here is the outline of the construction. At the start, we set \( z_1 \) so that one point, \( v \), will always be the first center chosen. Then we add points \( a_1, b_1, \ldots, a_k, b_k \) such that in round \( i \), either \( a_i \) or \( b_i \) will be chosen as centers. We carefully set the distances so that for each combination of centers, there is an \( \alpha \) interval which achieves this combination of centers. Therefore, the total number of \( \alpha \) intervals such that the output of the sampling step is fixed, is \( 2^{k-1} \). Our construction also uses points \( a'_1, b'_1, \ldots, a'_k, b'_k \) and \( v_1, \ldots, v_k \) which are never chosen as centers, but will be crucial in the analysis.

Next, we describe the distances between the points in our clustering instance. Almost all distances will be set to 100, except for a few distances: for all \( i \), \( d(a_i, a'_i) = d(b_i, b'_i) = \epsilon \), \( d(b_i, v_i) = 100 - o_i \), \( d(a_i, b_i) = 2a_i \), \( d(v, a_1) = d(v, b_1) = 99 \), and \( d(a_{i-1}, a_i) = d(a_{i-1}, b_i) = d(b_{i-1}, a_i) = d(b_{i-1}, b_i) = 100 - o_i \), for \( 0 \leq \epsilon, o_1, \ldots, o_k \leq 1 \) to be specified later. At the end, we will perturb all other distances by a slight amount \((< \epsilon)\) away from 100, to break ties.

Now we set up notation to be used in the remainder of the proof. We set \( z_i = \frac{1}{2} \) for all \( i \). For \( 1 \leq i \leq k \), given \( \vec{x} \in \{0, 1\}^{i-1} \), let \( E_{\vec{x}} \) denote the equation in round \( i \) which determines whether \( a_i \) or \( b_i \) is chosen as the next center, in the case where for all \( 1 \leq j < i \), \( a_j \in C \) if \( \vec{x}_j = 0 \), or else \( b_j \in C \) (and let \( E' \) denote the single equation in round 2). Specifically, \( E_{\vec{x}} \) is the following expression

\[
100^\alpha \left( \frac{n-(i-1)}{2} \right) \left( 100^\alpha(n-2(i-1)) + (100-o_i)^\alpha + \sum_{j=1}^{i-1} (100-\vec{x}_j o_j)^\alpha \right).
\]
Let $\alpha_x$ denote the solution to equation $E_x = \frac{1}{2}$ in $[1,3]$, if it exists. In the rest of the proof, we must show there exist parameters $\epsilon, o_0, \ldots, o_k$ which admit an ordering to the values $\alpha_x$ which ensures that each $\alpha_x$ falls in the correct range to split up each interval, thus achieving $2^{k_i}$ intervals. The ordering of the $\alpha_x$’s can be specified by two conditions: (1) $\alpha_0[0] < \alpha_0[1]$ and (2) $\alpha[i \neq 0][y] < \alpha[i \neq 1][z]$ for all $\vec{x}, \vec{y}, \vec{z} \in \bigcup_{i<k} \{0,1\}^i$ and $|\vec{y}| = |\vec{z}|$. To prove the $\alpha_x$’s follow this ordering, we use an inductive argument. We must show the following claim: there exist $0 < o_1, \ldots, o_k < 1$ such that if we solve $E_x = \frac{1}{2}$ for $\alpha_x$ for all $\vec{x} \in \bigcup_{i<k} \{0,1\}^i$, then the $\alpha$’s satisfy $\alpha_0[0] < \alpha_0[1] < \alpha[i \neq 1][z]$ and for all $i < k, \alpha[i \neq 1][y] < \alpha[i \neq 1][z]$ for $\vec{x}, \vec{y} \in \{0,1\}^i$ and $x_1 \ldots x_i < y_1 \ldots y_i$.

Given $\vec{x} \in \{0,1\}^i$, for $1 \leq i \leq k - 1$, let $p(\vec{x}), n(\vec{x}) \in \{0,1\}^i$ denote the vectors which sit on either side of $\alpha_x$ in the desired ordering, i.e., $\alpha_x$ is the only $\alpha_y$ in the range $(\alpha_{p(\vec{x})}, \alpha_{n(\vec{x})})$ such that $|\vec{y}| = i$. If $\vec{x} = [1 \ldots 1]$, then set $\alpha_{n(\vec{x})} = 3$, and if $\vec{x} = [0 \ldots 0]$, then set $\alpha_{p(\vec{x})} = 1$.

Given $1 \leq i \leq k - 2$, assume there exist $0 < o_1, \ldots, o_i < 1$ such that the statement is true. Now we will show the statement holds for $i + 1$. Given $\vec{x} \in \{0,1\}^i$, by assumption, we have that the solution to $E_x = \frac{1}{2}$ is equal to $\alpha_x$. First we consider $E_x[0] = \frac{1}{2}$. Note there are two differences in the equations $E_x$ and $E_x[0]$. First, the number of $100\alpha$ terms in the numerator decreases by 1, and the number of terms in the denominator decreases by 2. WLOG, at the end we set a constant $c = \frac{n}{k}$ large enough so that this effect on the root of the equation is negligible for all $n$. Next, the offset in the denominator changes from $(100 - o_i)\alpha$ to $(100 - o_{i+1})\alpha$. Therefore, if $0 < o_{i+1} < o_i$, then $\alpha[0] < \alpha_x$. Furthermore, there exists an upper bound $0 < z_i < o_i$ such that for all $0 < o_{i+1} < z_i$, we have $\alpha[i \neq 0] \in (\alpha_{p(\vec{x})}, \alpha_x)$. Next we consider $E_x[1] = \frac{1}{2}$. As before, the number of $100\alpha$ terms decrease, which is negligible. Note the only other change is that an $100\alpha$ term is replaced with $(100 - o_{i+1})\alpha$. Therefore, as long as $0 < o_{i+1} < o_i$, then $\alpha_x < \alpha[1]$, and similar to the previous case, there exists an upper bound $0 < z_i' < o_i$ such that for all $0 < o_{i+1} < z_i'$, we have $\alpha[1] \in (\alpha_x, \alpha(n(\vec{x})))$. We conclude that there exists $0 < o_{i+1} < \min(z_i, z_i') < o_i$ such that $\alpha_p(\vec{x}) < \alpha[0] < \alpha_x < \alpha[1] < \alpha_{n(\vec{x})}$, thus finishing the inductive proof.

Now we have shown that there are $2^{k_i}$ nonoverlapping $\alpha$ intervals, such that within each interval, $d^\alpha$-sampling chooses a unique set of centers, for $k' = k - 1$. To finish our structural claim, we will show that after $\beta$-Lloyd’s method, the cost function $\text{clus}_{\alpha, \beta}(\mathcal{V}, \vec{Z})$ alternates $2^{k_i}$ times above and below a value $r$ as $\alpha$ increases. We add two points, $a$ and $b$, so that $d(v,a) = d(v,b) = 100$, $d(a,k) = d(b,k) = 100 - \epsilon$, and the distances from all other points to $a$ and $b$ are length $100 + \epsilon$. Then we add many points in the same location as $v, a_i, \text{ and } b_i$, so that any set $c$ returned by $d^\alpha$-sampling is a local minima for $\beta$-Lloyd’s method, for all $\beta$. Furthermore, these changes do not affect the previous analysis, as long as we appropriately balance the terms in the numerator and denominator of each equation $E_x$ (and for small enough $\epsilon$). Finally, we set $v$ and $a$ to have label 1 in the target clustering, and all points are labeled 2. Therefore, as $d^\alpha$-sampling will alternate between $a_k \in C$ and $b_k \notin C$ as we increase $\alpha$, $a$ and $v$ alternate being in the same or different clusters, so the function $\text{seed}_\alpha(\mathcal{V}, \vec{Z})$ will alternate between different outputs $2^{\Omega(n)}$ times as a function of $\alpha$.

Now we give the details for Theorem 5.

**Theorem 5 (restated).** Given $T \in \mathcal{N}$, a clustering instance $\mathcal{V}$, and a fixed set $C$ of initial centers, the number of discontinuities of $\text{lloyd}_\beta(\mathcal{V}, C, T)$ as a function of $\beta$ on instance $\mathcal{V}$ is $O(\min(n^{3T}, n^{k+3}))$.

**Proof.** Given a clustering instance $\mathcal{V}$ and a vector $\vec{Z}$, we bound the number of possible intervals created by the Lloyd’s step, given a fixed set of initial centers. Define $\text{lloyd}_\beta(\mathcal{V}, C)$ as the cost of the clustering output by the $\beta$-Lloyd iteration algorithm on $\mathcal{V}$ using initial centers $C$. Note that the Voronoi partitioning step is only dependent on $C$, in particular, it is independent of $\beta$. 

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Let \( \{C_1, \ldots, C_k\} \) denote the Voronoi partition of \( V \) induced by \( C \). Given one of these clusters \( C_i \), the next center is computed by \( \min_{c \in C_i} \sum_{v \in C_i} d(c, v) \beta \). Given any \( c_1, c_2 \in C_i \), the decision for whether \( c_1 \) is a better center than \( c_2 \) is governed by \( \sum_{v \in C_i} d(c_1, v) \beta < \sum_{v \in C_i} d(c_2, v) \beta \). Again by a consequence of Rolle’s theorem, this equation has at most \( 2n + 1 \) roots. Notice that this equation depends on the set \( C \) of centers, the choice of a cluster \( C_i \), and the two points \( c_1, c_2 \in C_i \). Then there are \( \binom{n}{k} \cdot n \cdot \binom{n}{2} \) total equations which fix the outcome of the Lloyd’s method, and there are \( \binom{n}{k} \cdot n \cdot \binom{n}{2} \cdot (2n + 1) \leq n^{k+4} \) total intervals of \( \beta \) such that the outcome of Lloyd’s method is fixed.

Next we give a different analysis which bounds the number of discontinuities by \( n^{3T} \), where \( T \) is the maximum number of Lloyd’s iterations. By the same analysis as the previous paragraph, if we only consider one round, then the total number of equations which govern the output of a Lloyd’s iteration is \( \binom{n}{2} \), since the set of centers \( C \) is fixed. These equations have \( 2n + 1 \) roots, so the total number of intervals in one round is \( O(n^3) \). Therefore, over \( T \) rounds, the number of intervals is \( O(n^{3T}) \).

We show that the cost function of \( d^\alpha \)-sampling is Lipschitz. Let \( \text{seed}_\alpha(V) \) denote the output of \( d^\alpha \)-sampling run on \( V \).

**Lemma 13.** Given a clustering instance \( V \) with diameter \( D \), and \( \alpha \in [0, \infty) \cup \{\infty\} \), \( P(\text{seed}_\alpha(V) \neq \text{seed}_\alpha(V)) \leq 4nk \log n \).

**Proof.** Given a clustering instance \( V \) with diameter \( D \), and a vector \( \vec{Z} \sim [0, 1]^k \), we will show there is low probability that \( \text{seed}_\alpha(V, \vec{Z}) \) outputs a different set of centers than \( \text{seed}_\alpha(V, \vec{Z}) \), as long as \( \epsilon \) is small. Assume in round \( t \) of \( d^\alpha \)-sampling and \( d^{\alpha+\epsilon} \)-sampling, both algorithms have \( C \) as the current list of centers. Given we draw \( z_t \sim [0, 1] \), we will show there is only a small chance that the algorithms choose different centers in this round. Since the algorithms have an identical set of current centers, the distances \( d(v, C) \) are the same, but the break points of the intervals, \( \sum_{j=1}^i d(v_j, C)^\alpha \), differ slightly. If \( z_t \sim [0, 1] \) lands in the the same interval \( I_i \) and \( I'_i \) for \( d^\alpha \)-sampling and \( d^{\alpha+\epsilon} \)-sampling, respectively, then the two algorithms will choose the same point. Thus, we need to bound the size of \( \sum_{i=1}^n (I_i \setminus I'_i) \cup (I'_i \setminus I) \). Recall the endpoint of interval \( i \) is \( \frac{D_i(\alpha)}{D_n(\alpha)} \), where

\[
D_i = \sum_{j=1}^i d(v_j, C)^\alpha.
\]

Thus, we want to bound \( \left| \frac{D_i(\alpha)}{D_n(\alpha)} - \frac{D_i(\alpha+\epsilon)}{D_n(\alpha+\epsilon)} \right| \), and we can use Lemma 11 to show \( \frac{D_i(\alpha)}{D_n(\alpha)} - \frac{D_i(\alpha+\epsilon)}{D_n(\alpha+\epsilon)} \leq 4\epsilon \log n \).

Therefore, we have

\[
\sum_{i=1}^n (I_i \setminus I'_i) \cup (I'_i \setminus I_i) \\
\leq \sum_{i=1}^n \left| \frac{D_i(\alpha)}{D_n(\alpha)} - \frac{D_i(\alpha+\epsilon)}{D_n(\alpha+\epsilon)} \right| \\
\leq \sum_{i=1}^n \epsilon \cdot (4 \log n) \leq 4\epsilon n \log n.
\]

Therefore, assuming \( d^\alpha \)-sampling and \( d^{\alpha+\epsilon} \)-sampling have chosen the same centers so far, the probability that they choose different centers in round \( t \) is \( \leq 4\epsilon n \log n \). Over all rounds, the probability the outputted set of centers is not identical, is \( \leq 4\epsilon nk \log n \).