

Near-Optimal Explainable k -Means for All Dimensions

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Abstract

Many clustering algorithms are guided by certain cost functions such as the widely-used k -means cost. These algorithms divide data points into clusters with often complicated boundaries, creating difficulties in explaining the clustering decision. In a recent work, Dasgupta, Frost, Moshkovitz, and Rashtchian (ICML 2020) introduced explainable clustering, where the cluster boundaries are axis-parallel hyperplanes and the clustering is obtained by applying a decision tree to the data. The central question here is: how much does the explainability constraint increase the value of the cost function?

Given d -dimensional data points, we show an efficient algorithm that finds an explainable clustering whose k -means cost is at most $k^{1-2/d} \text{poly}(d \log k)$ times the minimum cost achievable by a clustering without the explainability constraint, assuming $k, d \geq 2$. Taking the minimum of this bound and the $k \text{polylog}(k)$ bound in independent work by Makarychev-Shan (ICML 2021), Gamlath-Jia-Polak-Svensson (2021), or Esfandiari-Mirrokhani-Narayanan (2021), we get an improved bound of $k^{1-2/d} \text{polylog}(k)$, which we show is optimal for every choice of $k, d \geq 2$ up to a poly-logarithmic factor in k . For $d = 2$ in particular, we show an $O(\log k \log \log k)$ bound, improving near-exponentially over the previous best bound of $O(k \log k)$ by Laber and Murtinho (ICML 2021).

1 Introduction

As a result of the rapid deployment of data analysis and machine learning techniques, many important decision rules that impact our lives are learned from data by algorithms, rather than designed explicitly by people. For unlabeled data, clustering algorithms are a useful tool for learning such rules, and a necessary step towards making the learned rules trustworthy is to make them easily understood by people. Many clustering algorithms are designed to optimize a cost function such as the widely-used k -means cost. While being a convenient and effective way for designing and analyzing clustering algorithms, optimizing a simple cost function can produce clusterings that are not easily understood by people, causing interpretability issues when applied in practice [51, 11].

We study a notion of explainable clustering introduced recently by Dasgupta, Frost, Moshkovitz, and Rashtchian [45] that aims to improve clustering interpretability. Here, a clustering is considered explainable if the clusters are obtained by applying a decision tree with k leaves to the data. Specifically, every non-leaf node of the decision tree corresponds to an axis-parallel hyperplane that divides the current set of data points into two subsets, which are passed to the two children of the node respectively. Every leaf of the decision tree thus corresponds to all the data points contained in a (possibly unbounded) rectangular box with axis-parallel faces, and these data points are required to be placed in the same cluster.

To understand the increase in the clustering cost caused by the explainability constraint, [45] studied the *competitive ratio* of an explainable clustering, which is defined to be the ratio between its cost and the minimum cost achievable by a clustering using k clusters without the explainability constraint. For the k -medians and k -means cost, [45] showed efficient algorithms computing explainable clusterings with competitive ratios $O(k)$ and $O(k^2)$ respectively. (In their work, distances are measured using the ℓ_1 -norm for k -medians, whereas the ℓ_2 -norm is used for k -means.)

The competitive ratio bounds in [45] have been improved significantly by several independent papers [43, 25, 21]. For explainable k -medians, [43] and [21] achieved the current best competitive ratio $O(\log k \log \log k)$. For explainable k -means, the current best competitive ratio is $O(k \log k)$ by [21]. These competitive ratio bounds are known to be near-optimal, with the current best lower bound being $\Omega(\log k)$ for k -medians [45, 21] and $\Omega(k)$ for k -means [25, 21].

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The lower bounds above were proved only when the dimension of the data points is $d = \Omega(\log k)$. This leaves open the question of achieving better competitive ratios for dimensions $d = o(\log k)$. Before our work, Laber and Murtinho [37] gave algorithms with better competitive ratios in lower dimensions, but their bounds for k -medians and k -means were sub-optimal and subsumed by [21]. For k -medians, [21] showed an $O(d(\log d)^2)$ competitive ratio in d dimensions, which improves over the $O(\log k \log \log k)$ bound when $d \leq O(\log k / \log \log k)$. For the popular k -means objective, no competitive ratio better than $O(k \log k)$ was known prior to our work even for $d = 2$.

In this work, we show that significantly better competitive ratios than $O(k \log k)$ can be achieved for k -means when the dimension $d = O(\log k / \log \log k)$. We give a competitive ratio bound that depends on both d and k , which we show is near-optimal for all choices of $d, k \geq 2$.

Our results. Our main result is an efficient algorithm that takes a set of d dimensional points and computes an explainable clustering with competitive ratio at most $k^{1-2/d} \text{poly}(d \log k)$ for the k -means cost (Theorem 4.1). Compared to the previous best bound of $O(k \log k)$, our bound has a better dependence on k for every fixed dimension d . The dependence on d can be improved by taking the minimum of our bound and $O(k \log k)$. Specifically, if we run the algorithm in any of the independent work [43, 25, 21] instead when $d = \Omega(\log k)$, we get an improved bound of $k^{1-2/d} \text{polylog}(k)$ for all $k, d \geq 2$ (Corollary 4.1). We show this is near-optimal for all $k, d \geq 2$ by constructing a set of d dimensional points for which the competitive ratio is at least $k^{1-2/d} / \text{polylog}(k)$ for the k -means cost (Theorem 5.1).

In the special case of $d = 2$, we show an efficient algorithm computing explainable clusterings with competitive ratio $O(\log k \log \log k)$ (Theorem 3.1). This is a near-exponential improvement compared to the previous best bound of $O(k \log k)$ obtained first by [37].

Technical overview. As previous work [45, 37] and independent work [43, 25, 21], we design a post-processing algorithm that takes an arbitrary clustering \mathcal{C} with k clusters, and computes an explainable clustering with k -means cost at most $k^{1-2/d} \text{poly}(d \log k)$ times the cost of \mathcal{C} using the same cluster centroids in \mathcal{C} . Our competitive ratio bound is then achieved by running the post-processing algorithm on a clustering \mathcal{C} computed by a constant-factor approximation algorithm for k -means [33, 2, 28].

We build the decision tree recursively starting from the root. That is, the first step of the algorithm is to find the hyperplane corresponding to the root of the decision tree, and then solve the two induced subproblems recursively. If a point x and its assigned centroid in \mathcal{C} lie on different sides of the hyperplane, we need to re-assign a new centroid to x that lies on the same side of the hyperplane with x . Every such re-assignment incurs some cost. In a similar spirit to [37], we make sure that the re-assignment cost caused by the hyperplane is small, and that the two subproblems have similar “sizes” in order to minimize the depth of the decision tree. When the two goals are in conflict, it is important to make a balanced tradeoff: [37] applies binary search with non-uniform probing cost due to [15], whereas we take a more flexible approach originating in an argument of Seymour [53].

In previous analysis [45, 37], the re-assignment cost of every point is bounded above by the diameter of the current subproblem. While this “diameter upper bound” can be a good estimate when the dimension $d = \Omega(\log k)$, we need a more careful bound to get a near optimal competitive ratio for smaller dimensions. To this end, we form a *forbidden region* when selecting every hyperplane to prevent re-assigning a point if the re-assignment cost is too large compared to the current cost. We use a volume argument to bound the size of the forbidden region, so that we have enough non-forbidden space to apply Seymour’s argument. The strength of the volume argument increases significantly as the dimension d decreases, resulting in our significantly improved bound in lower dimensions.

The “diameter upper bound” used in previous works allows them to completely ignore a point once it is re-assigned, because the cost of any further re-assignment can be covered by the current diameter. In our analysis, however, we need to deal with situations where a point is re-assigned multiple times. We give every point a *type* during the algorithm based on its “re-assignment history”, and carefully control the cost at every re-assignment by designing the forbidden region based on the types of individual points. In addition, we show that “essentially” no point can be re-assigned too many times. Roughly speaking, for $d = 2$, we show that a point can be re-assigned at most twice before either a) the point has a large distance to its current centroid so that we can afford to use the diameter upper bound, or b) both the point and its current centroid are close to a corner of the current rectangle so that we can avoid re-assigning them further. For the more general case $d > 2$, it is possible that none of the above scenarios happen for some “bad” points, but we make sure that the “bad” points are assigned to only a small number of centroids, in which case we can also avoid re-assigning them further.

Related work. Decision trees are a classic method for classifying labeled data [30]. Due to its intrinsic interpretability, people also applied decision trees and related algorithms to clustering unlabeled data: [19, 14, 7, 39, 56, 22, 16, 27, 10, 11]. We use the framework of [45], who gave the first competitive ratio analysis for explainable clustering using decision trees. [24] relaxed the framework of [45] by allowing more leaves in the decision tree than the number of clusters, so that a cluster can correspond to multiple leaves.

In clustering tasks, the dimension of the input points plays an important role. Many influential results were obtained while studying clustering in different dimensions. While hardness results have been proved for approximately optimizing the k -medians and the k -means cost within a small constant factor [31, 5, 12], polynomial-time approximation schemes (PTAS) have been found for both k -medians and k -means in fixed dimensions [4, 36, 23, 18, 17]. A random projection to $O(\log k)$ dimensions approximately preserves the k -medians and the k -means cost of all k -clusterings of a given set of points with high probability [8, 42].

Interpretability and explainability are important aspects of making machine learning reliable, and they have received growing research attention (see [44, 46] for an overview). Compared to clustering and unsupervised learning in general, more work on interpretability considered supervised learning [48, 40, 1, 49, 38, 50, 47, 3, 20, 54, 26]. Besides decision trees, neural nets have been used to improve clustering explainability [34], whereas an interpretability score was formulated by [51], who studied the tradeoff between the interpretability score and the clustering cost. Fairness is another important consideration towards making clustering more trustworthy. There is a large body of recent work on fair clustering [6, 9, 29, 35, 52, 41, 32, 13, 55].

Independent work. Soon after we made this paper public on arXiv, three related and independent papers [25, 21, 43] appeared on arXiv, and later [43] also appeared in the proceedings of ICML 2021. As we mentioned earlier, all three papers achieved similar competitive ratios for explainable k -medians with the ℓ_1 -norm and explainable k -means with the ℓ_2 -norm that are near-optimal when the dimension $d = \Omega(\log k)$. In addition, [25] considered general ℓ_p -norms and achieved competitive ratio $O(k^{p-1}(\log k)^2)$ when the distances are raised to the p -th power with a near-matching lower bound, [21] achieved a dimension-dependent competitive ratio $O(d(\log d)^2)$ for k -medians with the ℓ_1 -norm in d dimensions, and [43] achieved a competitive ratio $O((\log k)^{3/2})$ for k -medians with the ℓ_2 -norm.

Paper organization. We formally define explainable clustering and introduce relevant notation in Section 2. We prove our $O(\log k \log \log k)$ competitive ratio upper bound for $d = 2$ in Section 3, and our $k^{1-2/d} \text{poly}(d \log k)$ upper bound for $d > 2$ in Section 4. The lower bound $k^{1-2/d}/\text{polylog}(k)$ is shown in Section 5. Some helper claims and lemmas used in our analysis are stated and proved in Appendix A.

2 Preliminaries

We use $x(j)$ to denote the j -th coordinate of a point x in the d -dimensional space \mathbb{R}^d , where j is chosen from $[d]$, namely, $\{1, \dots, d\}$. We use $\|x\|_2 = (\sum_{j=1}^d x(j)^2)^{1/2}$ and $\|x\|_\infty = \max_{j \in [d]} |x(j)|$ to denote the ℓ_2 -norm and the ℓ_∞ -norm of a point $x \in \mathbb{R}^d$, respectively.

Every pair $(j, \theta) \in [d] \times \mathbb{R}$ defines an axis-parallel hyperplane that partitions \mathbb{R}^d into two subsets: $B_{\leq}(j, \theta) := \{x \in \mathbb{R}^d : x(j) \leq \theta\}$ and $B_{>}(j, \theta) := \{x \in \mathbb{R}^d : x(j) > \theta\}$. We say two points $x, x' \in \mathbb{R}^d$ lie on the same side of the hyperplane (j, θ) if $x, x' \in B_{\leq}(j, \theta)$ or $x, x' \in B_{>}(j, \theta)$; otherwise we say the two points lie on different sides of the hyperplane, or equivalently, they are separated by the hyperplane.

We consider decision trees as rooted directed trees. Nodes in the tree with no child are called *leaves*, and we require that every non-leaf node has exactly 2 children—a left child and a right child. Every non-leaf node corresponds to an axis-parallel hyperplane $(j, \theta) \in [d] \times \mathbb{R}$. This naturally makes every node in the tree define a subset of \mathbb{R}^d with axis-parallel boundaries: the root defines the entire space \mathbb{R}^d ; if a non-leaf node corresponding to hyperplane (j, θ) defines the region B , its left child defines the region $B \cap B_{\leq}(j, \theta)$, and its right child defines the region $B \cap B_{>}(j, \theta)$. Clearly, the regions defined by the leaves of a decision tree form a partition of \mathbb{R}^d .

For positive integers d and k , a k -clustering \mathcal{C} for a set of points $x_1, \dots, x_n \in \mathbb{R}^d$ consists of k centroids $y_1, \dots, y_k \in \mathbb{R}^d$ and an assignment mapping $\xi : [n] \rightarrow [k]$. The k -means cost of the clustering \mathcal{C} is given by $\text{cost}(\mathcal{C}) = \sum_{i=1}^n \|x_i - y_{\xi(i)}\|_2^2$. We say the clustering \mathcal{C} is k -explainable with respect to a decision tree T if T has at most k leaves and $\xi(i) = \xi(i')$ holds for all points $x_i, x_{i'}$ in the region defined by the same leaf of T .

For a subset $W \subseteq \mathbb{R}^d$, we use $|W|$ to denote its Lebesgue measure. We only care about the Lebesgue measure of bounded subsets that can be represented as a union of finitely many rectangles (or intervals when $d = 1$). For those subsets W , the Lebesgue measure $|W|$ always exists.

We use \log to denote the base- e logarithm, and \log_2 to denote the base-2 logarithm.

3 Explainable k -means in the plane

We focus on the simpler case $d = 2$ in this section and give an efficient algorithm for finding a k -explainable clustering with competitive ratio $O(\log k \log \log k)$. Before we describe our algorithm, we remark that there exists a poly-time algorithm that computes a k -explainable clustering with *minimum* k -means cost given a set of n input points in $d = 2$ dimensions. In fact, for general $d \geq 2$ and $n \geq 2$, there exists such an algorithm with running time $n^{O(d)}$ via dynamic programming: if $k \geq n$, it is trivial to achieve zero cost; if $k < n$, the algorithm solves all subproblems each consisting of a box $(\alpha(1), \beta(1)] \times (\alpha(2), \beta(2)] \times \cdots \times (\alpha(d), \beta(d)] \subseteq \mathbb{R}^d$ and a positive integer $k' \leq k$, where the goal is to find a k' -explainable clustering with minimum cost for the input points inside the box. Although there are infinitely many such boxes, at most $n^{O(d)}$ among them define distinct subsets of input points, so essentially there are at most $kn^{O(d)} = n^{O(d)}$ different subproblems. Also, every subproblem with $k' = 1$ can be solved directly in $O(nd)$ time, and every subproblem with $k' > 1$ can be solved in $O(k'nd) = (nd)^{O(1)}$ time using solutions to subproblems with smaller k' .

While the above algorithm guarantees to find a k -explainable clustering with minimum cost and thus minimum competitive ratio, it does not give us a concrete bound on the competitive ratio. We develop a different algorithm that post-processes an arbitrary k -clustering \mathcal{C} into a k -explainable clustering, and we show that the k -means cost of the explainable clustering is at most $O(\log k \log \log k)$ times the cost of \mathcal{C} assuming $d = 2$. Choosing \mathcal{C} as the output of a constant-factor approximation algorithm for k -means ensures that the explainable clustering has competitive ratio $O(\log k \log \log k)$.

THEOREM 3.1. *Assume $k \geq 2$. There exists a poly-time algorithm `post-process_2d` that takes a k -clustering \mathcal{C} of n points in 2 dimensions, and outputs a clustering \mathcal{C}' of the n points and a decision tree T with at most k leaves such that*

1. \mathcal{C}' is k -explainable with respect to T ;
2. $\text{cost}(\mathcal{C}') \leq O(\log k \log \log_2(2k)) \cdot \text{cost}(\mathcal{C})$;
3. \mathcal{C}' uses the same k centroids as \mathcal{C} does.

Consequently, there exists a poly-time algorithm that takes n points in 2 dimensions and outputs a k -explainable clustering with competitive ratio $O(\log k \log \log_2(2k))$.

In the rest of the section, we assume $d = 2$ and $k \geq 2$.

3.1 Subproblem Our algorithm `post-process_2d` works in a recursive manner, constructing the tree from root to leaf. Thus, in each stage of the algorithm, we focus on a subset of the points and the centroids. Moreover, our algorithm keeps track of some helper information for every point. This leads us to the definition of a *subproblem*.

DEFINITION 3.1. (SUBPROBLEM FOR $d = 2$) *Given points $x_1, \dots, x_n \in \mathbb{R}^d$ and centroids $y_1, \dots, y_k \in \mathbb{R}^d$, a subproblem \mathcal{P} consists of the following:*

1. A subset $X \subseteq \{x_1, \dots, x_n\}$. We focus on points $x \in X$.
2. A subset $Y \subseteq \{y_1, \dots, y_k\}$. We focus on centroids $y \in Y$.
3. An assigned centroid $\sigma_x \in Y$ for every $x \in X$.
4. A length $\ell_x \geq 0$ for every point $x \in X$. We always enforce ℓ_x to be an upper bound on $\|x - \sigma_x\|_\infty$ (see Definition 3.4 Item 1). While we define the k -means cost using the ℓ_2 -norm, in our analysis we find it more convenient to keep track of the ℓ_∞ -norm instead.
5. A type t_x for every point $x \in X$. The type t_x is either a function $t_x : [d] \rightarrow \{0, 1, 2\}$ or the irrelevant type $t_x = \perp$. This gives a partition of X into two subsets: a subset

$$R = \{x \in X : t_x \neq \perp\}$$

consisting of all relevant points, and a subset $X \setminus R$ consisting of all irrelevant points. The set R is further partitioned into R_0, R_1, \dots, R_d defined as follows:

$$R_i = \{x \in R : \|t_x\|_0 = i\}, \quad \text{for all } i \in [d],$$

where $\|t_x\|_0$ denotes the number of $j \in [d]$ with $t_x(j) \neq 0$. If $x \in R$ has $t_x(j) \neq 0$ for some $j \in [d]$, we ensure that x is close to one of the boundaries in the j -th dimension, which we formalize in Definition 3.3 and Definition 3.4 Item 4.

We fix a positive real number m as the *centroid mass* which we determine later. We can now define two quantities $M(\mathcal{P})$ and $A(\mathcal{P})$ for a subproblem \mathcal{P} with respect to the centroid mass m .

DEFINITION 3.2. Given a subproblem \mathcal{P} , we define the following quantities:

$$\begin{aligned} M(\mathcal{P}) &:= m|Y| + \sum_{x \in R_0} \ell_x^2, \\ A(\mathcal{P}) &:= f(M(\mathcal{P})) + 2^{32} \sum_{x \in R_1} \ell_x^2 + 2^9 \sum_{x \in R_2} \ell_x^2 + \sum_{x \in X \setminus R} \ell_x^2, \end{aligned}$$

where

$$f(M) := 2^{57} M(1 + \log(M/m)) \log \log_2(2k).$$

The quantity $A(\mathcal{P})$ plays an important role in our proof of Theorem 3.1. The algorithm `post-process_2d` we construct for proving Theorem 3.1 forms an initial subproblem $\tilde{\mathcal{P}}$ with $A(\tilde{\mathcal{P}}) \leq O(\log k \log \log_2(2k)) \cdot \text{cost}(\mathcal{C})$ and divides it into smaller and smaller subproblems. We compute an explainable clustering for every subproblem, and we choose \mathcal{C}' to be the explainable clustering for the initial subproblem $\tilde{\mathcal{P}}$. We show that the cost of the explainable clustering we find for every subproblem \mathcal{P} is at most $2A(\mathcal{P})$ (Lemma 3.9), which implies $\text{cost}(\mathcal{C}') \leq 2A(\tilde{\mathcal{P}}) \leq O(\log k \log \log_2(2k)) \cdot \text{cost}(\mathcal{C})$, as required by Theorem 3.1.

Our algorithm `post-process_2d` crucially uses the boundaries and the diameter of a subproblem defined as follows:

DEFINITION 3.3. (SUBPROBLEM BOUNDARY) Given a subproblem \mathcal{P} , for every $j \in [d]$, we define

$$\begin{aligned} b_1(j) &= \min_{y \in Y} y(j), \quad \text{and} \\ b_2(j) &= \max_{y \in Y} y(j) \end{aligned}$$

as the lower and upper boundaries in the j -th dimension. Define $L := \max_{j \in [d]} (b_2(j) - b_1(j))$ as the diameter of the subproblem \mathcal{P} .

To impose necessary constraints on the subproblems we deal with, we focus on *valid* subproblems defined below (see Figure 1 for an example of a valid subproblem).

DEFINITION 3.4. (VALID SUBPROBLEM) Given points $x_1, \dots, x_n \in \mathbb{R}^d$ and centroids $y_1, \dots, y_k \in \mathbb{R}^d$, a subproblem $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X})$ is valid if all of the following hold:

1. $\ell_x \geq \|x - \sigma_x\|_\infty$ for all $x \in X$.
2. $M(\mathcal{P})/m \leq 2k$.
3. For every point $x \in X \setminus R$ and every $y \in Y$, $\ell_x \geq \|x - y\|_\infty$.
4. If point $x \in R$ has $t_x(j) = 1$ for some $j \in [d]$, then $|x(j) - b_1(j)| \leq \ell_x$. Similarly, if $x \in R$ has $t_x(j) = 2$, then $|x(j) - b_2(j)| \leq \ell_x$.

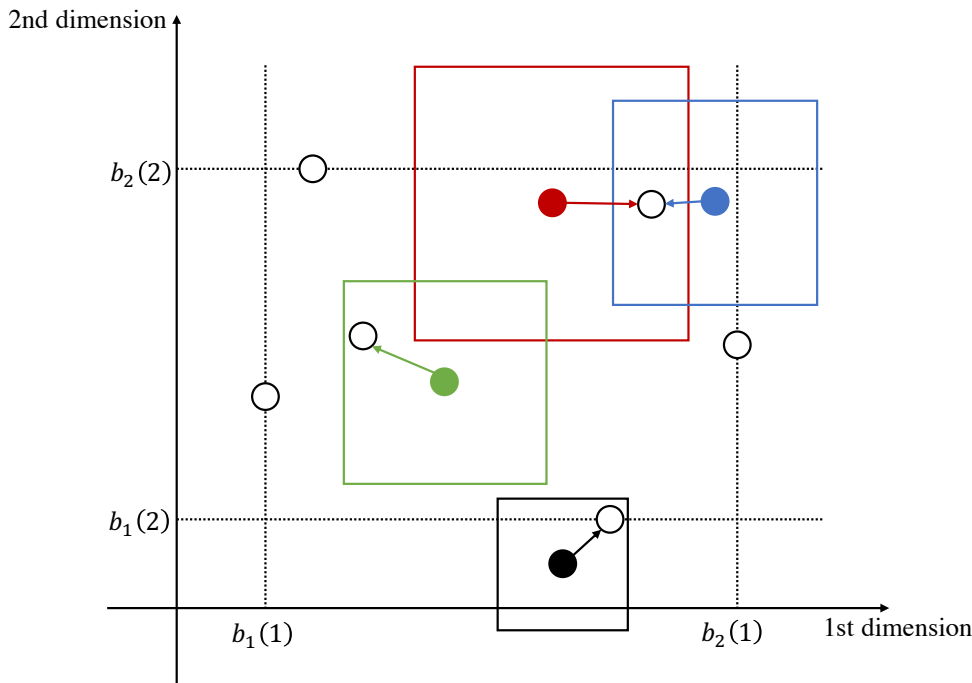


Figure 1: A valid subproblem in 2 dimensions. The hollow circles represent the centroids $y \in Y$, and the filled circles represent the relevant points $x \in R$. Irrelevant points $x \in X \setminus R$ are not shown in the figure. The four dotted lines represent the boundaries as in Definition 3.3. Every point $x \in R$ has an arrow pointing to its assigned centroid σ_x . We draw an ℓ_∞ ball (square) around every point $x \in R$ with radius ℓ_x . The square around a point x contains σ_x by Definition 3.4 Item 1. According to Definition 3.4 Item 4, the blue point can have $t_x(1) = 2$ and $t_x(2) = 2$ because the blue square intersects the upper boundaries in both dimensions. Similarly, the red point can have $t_x(2) = 2$ but must have $t_x(1) = 0$. The green point must have $t_x(1) = t_x(2) = 0$. The black point to the bottom lies below the lower boundary in the 2nd dimension, and it can have $t_x(2) = 1$.

3.2 Making a single cut We describe an efficient algorithm `single_cut_2d` that takes a valid subproblem \mathcal{P} , and produces two smaller valid subproblems \mathcal{P}_1 and \mathcal{P}_2 together with an axis-parallel hyperplane (j^*, θ) that separates them. Later in Section 3.3 we invoke this algorithm recursively to construct the algorithm `post-process_2d` required by Theorem 3.1.

Specifically, given an input subproblem $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X})$, the algorithm `single_cut_2d` computes a partition X_1, X_2 of X , a partition Y_1, Y_2 of Y , new assignments $(\sigma'_x)_{x \in X}$, new lengths $(\ell'_x)_{x \in X}$, new types $(t'_x)_{x \in X}$, and outputs two smaller subproblems

$$(3.1) \quad \begin{aligned} \mathcal{P}_1 &= (X_1, Y_1, (\sigma'_x)_{x \in X_1}, (\ell'_x)_{x \in X_1}, (t'_x)_{x \in X_1}), \\ \mathcal{P}_2 &= (X_2, Y_2, (\sigma'_x)_{x \in X_2}, (\ell'_x)_{x \in X_2}, (t'_x)_{x \in X_2}). \end{aligned}$$

The partitions (X_1, X_2) and (Y_1, Y_2) are determined by an axis-parallel hyperplane $(j^*, \theta) \in [d] \times (b_1(j^*), b_2(j^*))$:

$$(3.2) \quad \begin{aligned} X_1 &= X \cap B_{\leq}(j^*, \theta) = \{x \in X : x(j^*) \leq \theta\}, \\ X_2 &= X \cap B_{>}(j^*, \theta) = \{x \in X : x(j^*) > \theta\}, \\ Y_1 &= Y \cap B_{\leq}(j^*, \theta) = \{y \in Y : y(j^*) \leq \theta\}, \\ Y_2 &= Y \cap B_{>}(j^*, \theta) = \{y \in Y : y(j^*) > \theta\}. \end{aligned}$$

We always choose $j^* \in [d]$ so that $b_2(j^*) - b_1(j^*)$ is maximized, i.e., $b_2(j^*) - b_1(j^*) = L$. Note that by choosing $\theta \in (b_1(j^*), b_2(j^*))$, we are implicitly requiring $b_1(j^*) < b_2(j^*)$, or equivalently, $L > 0$, which we assume to be

the case. Moreover, the choice $\theta \in (b_1(j^*), b_2(j^*))$ guarantees that Y_1 and Y_2 are both non-empty, and thus they both have sizes smaller than $|Y|$, which means that the two subproblems are indeed “smaller”.

We say a point $x \in X$ is σ -separated if x and σ_x are separated by the hyperplane (j^*, θ) . In other words, σ -separated points form the subset $X_+ \subseteq X$ defined as follows:

$$(3.3) \quad X_+ := \{x \in X_1 : \sigma_x \in Y_2\} \cup \{x \in X_2 : \sigma_x \in Y_1\}.$$

Consequently, non- σ -separated points belong to one of the following two sets

$$(3.4) \quad \begin{aligned} X_{11} &:= \{x \in X_1 : \sigma_x \in Y_1\}, \quad \text{and} \\ X_{22} &:= \{x \in X_2 : \sigma_x \in Y_2\}. \end{aligned}$$

To make sure that the two subproblems $\mathcal{P}_1, \mathcal{P}_2$ are well-defined, we require that $\sigma'_x \in Y_1$ whenever $x \in X_1$ and $\sigma'_x \in Y_2$ whenever $x \in X_2$. In other words, we require that no point is σ' -separated. This implies that for every σ -separated point $x \in X$, we must ensure $\sigma'_x \neq \sigma_x$. On the other hand, our algorithm `single_cut_2d` guarantees $\sigma'_x = \sigma_x$ whenever x is not σ -separated.

Our goal is to show that the two new subproblems $\mathcal{P}_1, \mathcal{P}_2$ created by the `single_cut_2d` algorithm satisfy the following lemmas, which are crucial in our analysis to obtain Theorem 3.1. We always assume that the input subproblem \mathcal{P} is valid throughout Section 3.2 even when we do not explicitly state so.

LEMMA 3.1. *The two new subproblems $\mathcal{P}_1, \mathcal{P}_2$ output by `single_cut_2d` are both valid.*

LEMMA 3.2. *The two new subproblems $\mathcal{P}_1, \mathcal{P}_2$ output by `single_cut_2d` satisfy $A(\mathcal{P}_1) + A(\mathcal{P}_2) \leq A(\mathcal{P})$.*

We prove the above lemmas after describing the `single_cut_2d` algorithm step by step in the following subsections.

3.2.1 Preprocessing For every $x \in R$ with $\ell_x \geq L/16$, we have

$$(3.5) \quad \|x - y\|_\infty \leq \|x - \sigma_x\|_\infty + \|\sigma_x - y\|_\infty \leq \ell_x + L \leq 17\ell_x, \quad \text{for all } y \in Y.$$

For every such point x , we replace the current value of ℓ_x by $17\ell_x$, and set $t_x = \perp$ (thus removing x from R). The new subproblem is still valid (Definition 3.4 Item 3 follows from (3.5)), and all points $x \in R$ in the new subproblem satisfies $\ell_x \leq L/16$. Moreover, it is clear that the value of $A(\mathcal{P})$ does not increase (note that $17^2 < 2^9$). For the rest of Section 3.2, we use $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X})$ to denote the subproblem after the preprocessing step.

3.2.2 Forbidding We specify a subset F of the interval $(b_1(j^*), b_2(j^*))$ as the forbidden region. By making the algorithm `single_cut_2d` choose θ outside of the forbidden region, we can guarantee some desired properties for σ -separated points (see Lemma 3.4).

For every point $x \in X$, define $Y(x) \subseteq Y$ as the following set of centroids:

$$(3.6) \quad Y(x) := \begin{cases} \{y \in Y : y(j^*) \geq \min\{x(j^*), b_2(j^*)\}\}, & \text{if } x(j^*) \geq \sigma_x(j^*); \\ \{y \in Y : y(j^*) \leq \max\{x(j^*), b_1(j^*)\}\}, & \text{if } x(j^*) < \sigma_x(j^*). \end{cases}$$

If x is σ -separated, it is clear that every centroid in $Y(x)$ must lie on the same side of the hyperplane (j^*, θ) with x , in which case choosing σ'_x from $Y(x)$ prevents x from being σ' -separated. Define η_x as the centroid in $Y(x)$ with the smallest ℓ_∞ distance to σ_x , and define q_x to be the corresponding ℓ_∞ distance:

$$(3.7) \quad \begin{aligned} \eta_x &= \operatorname{argmin}_{y \in Y(x)} \|\sigma_x - y\|_\infty, \\ q_x &= \|\sigma_x - \eta_x\|_\infty. \end{aligned}$$

Now we focus on points x in the subset $T \subseteq S \subseteq R_0 \cup R_1$ defined as follows:

$$(3.8) \quad \begin{aligned} S &= \{x \in R_0 \cup R_1 : t_x(j^*) = 0, x(j^*) \neq \sigma_x(j^*)\}. \\ T &= \left\{x \in S : \frac{q_x}{L} > 2^{11} \left(\frac{\ell_x}{L}\right)^{1/(d-\|t_x\|_0)}\right\}. \end{aligned}$$

For every point $x \in X$, we define an interval W_x as follows:

$$(3.9) \quad W_x = \begin{cases} [\sigma_x(j^*), x(j^*)) \cap (b_1(j^*), b_2(j^*)), & \text{if } x(j^*) \geq \sigma_x(j^*); \\ [x(j^*), \sigma_x(j^*)) \cap (b_1(j^*), b_2(j^*)), & \text{if } x(j^*) < \sigma_x(j^*). \end{cases}$$

We define the forbidden region F as

$$F = (b_1(j^*), b_1(j^*) + L/8] \cup [b_2(j^*) - L/8, b_2(j^*)) \cup \bigcup_{x \in T} W_x.$$

It is clear that F can be represented as a union of finitely many *disjoint* intervals, and the representation can be computed in poly-time. We define F as above because choosing θ outside F guarantees that all relevant points that can possibly be σ -separated must have good properties summarized in Lemma 3.3 and Lemma 3.4 below, including having a relatively small value of q_x . Since the algorithm needs to choose $\theta \in (b_1(j^*), b_2(j^*))$ outside the forbidden region, it is necessary to show that the forbidden region does not cover the entire interval $(b_1(j^*), b_2(j^*))$. Lemma 3.5 below makes a stronger guarantee.

LEMMA 3.3. *If we choose $\theta \in (b_1(j^*), b_2(j^*)) \setminus F$, then every $x \in R$ with $t_x(j^*) = 1$ belongs to X_{11} , and similarly every $x \in R$ with $t_x(j^*) = 2$ belongs to X_{22} . Consequently, every $x \in R \cap X_+$ satisfies $t_x(j^*) = 0$.*

Proof. Consider a point $x \in R$ with $t_x(j^*) = 1$. By Definition 3.4 Item 4, we know $|x(j^*) - b_1(j^*)| \leq \ell_x \leq L/16$, where the last inequality is guaranteed by the preprocessing step. By Definition 3.4 Item 1 and the triangle inequality, $|\sigma_x(j^*) - b_1(j^*)| \leq \|x - \sigma_x\|_\infty + |x(j^*) - b_1(j^*)| \leq \ell_x + \ell_x \leq L/8$. Therefore,

$$\max\{x(j^*), \sigma_x(j^*)\} \leq b_1(j^*) + L/8 < \theta,$$

where the last inequality is because $(b_1(j^*), b_1(j^*) + L/8] \subseteq F$ and $\theta \in (b_1(j^*), b_2(j^*)) \setminus F$. This implies $x \in X_{11}$. Similarly, every $x \in R$ with $t_x(j^*) = 2$ belongs to X_{22} . Since X_+ is disjoint from $X_{11} \cup X_{22}$, points $x \in R \cap X_+$ cannot have $t_x(j^*) \in \{1, 2\}$, and thus $t_x(j^*) = 0$. \square

LEMMA 3.4. *If we choose $\theta \in (b_1(j^*), b_2(j^*)) \setminus F$, then every σ -separated relevant point $x \in R \cap X_+$ satisfies all of the following:*

1. $x(j^*) \neq \sigma_x(j^*)$;
2. $t_x(j^*) = 0$ (and thus $\|t_x\|_0 \leq 1$ and $x \in R_0 \cup R_1$);
3. $\frac{q_x}{L} \leq 2^{11}(\frac{\ell_x}{L})^{1/(d-\|t_x\|_0)}$.

Proof. Item 1 is obvious, since a point x cannot be σ -separated unless $x(j^*) \neq \sigma_x(j^*)$. Item 2 follows directly from Lemma 3.3.

Assume for the sake of contradiction that Item 3 is not satisfied by $x \in R \cap X_+$. We already know that Item 1 and Item 2 are both satisfied, so $x \in S$, and therefore $x \in T$. This implies $W_x \subseteq F$ by the definition of F . However, the fact that $x \in X_+$ implies $\theta \in W_x$, and thus $\theta \in F$, a contradiction. \square

LEMMA 3.5. *The forbidden region F has length (i.e. Lebesgue measure) at most $L/2$.*

Lemma 3.5 is a direct consequence of the following lemma:

LEMMA 3.6. $|\bigcup_{x \in T} W_x| \leq L/4$.

Proof. While we are dealing with $d = 2$ specifically, we prove the lemma using a more general language so that the proof can be reused in Section 4 where we deal with $d > 2$.

By Claim A.3, we can find $U \subseteq T$ such that the intervals $(W_x)_{x \in U}$ are disjoint, and $|\bigcup_{x \in T} W_x| \leq 3|\bigcup_{x \in U} W_x|$. It remains to prove that $|\bigcup_{x \in U} W_x| \leq L/12$. Define $U_> = \{x \in U : x(j^*) > \sigma_x(j^*)\}$.

We prove $|\bigcup_{x \in U_>} W_x| \leq L/24$ via a volume argument. For every point $x \in U_>$, define a rectangular box $B_x \subseteq \mathbb{R}^d$ as follows:

$$B_x = \{z \in \mathbb{R}^d : \|z - \sigma_x\|_\infty < q_x/3, z(j^*) - \sigma_x(j^*) > q_x/6\}.$$

We can write B_x in a different way as the cartesian product $B_x = B_x(1) \times \cdots \times B_x(d)$, where $B_x(j) \subseteq \mathbb{R}$ is the interval $(\sigma_x(j) - q_x/3, \sigma_x(j) + q_x/3)$ if $j \neq j^*$, and $B_x(j^*) \subseteq \mathbb{R}$ is the interval $(\sigma_x(j^*) + q_x/6, \sigma_x(j^*) + q_x/3)$. Thus, the width of B_x in the j^* -th dimension is $1/4$ times the width in other dimensions.

We show that the boxes B_x are pair-wise disjoint. Assume for the sake of contradiction that a point z lies in both boxes B_x and $B_{x'}$ where x, x' are distinct points in $U_{>}$. Assume w.l.o.g. $x(j^*) \leq x'(j^*)$. Since W_x and $W_{x'}$ are disjoint, we have $\sigma_x(j^*) < x(j^*) \leq \sigma_{x'}(j^*) < x'(j^*)$. Therefore, $\sigma_{x'} \in Y(x)$, and thus

$$q_x \leq \|\sigma_x - \sigma_{x'}\|_\infty \leq \|\sigma_x - z\|_\infty + \|\sigma_{x'} - z\|_\infty < q_x/3 + q_{x'}/3.$$

This implies that $q_x < q_{x'}/2$, and thus $z(j^*) < \sigma_x(j^*) + q_x/3 < \sigma_{x'}(j^*) + q_{x'}/6 < z(j^*)$, a contradiction.

It is clear by definition that $q_x \leq L$ for all $x \in U_{>}$. Therefore, the boxes B_x are all contained in the large box

$$B := \{z \in \mathbb{R}^d : \forall j \in [d], b_1(j) - L/3 \leq z(j) \leq b_2(j) + L/3\}.$$

The large box B contains a smaller box B' defined as follows:

$$B' := \{z \in B : \forall j \in [d] \setminus \{j^*\}, b_1(j) \leq z(j) \leq b_2(j)\}.$$

For every $z \in B$, we define $\pi_z \in B'$ such that $\pi_z(j^*) = z(j^*)$ and for all $j \neq j^*$,

$$\pi_z(j) = \begin{cases} z(j), & \text{if } b_1(j) \leq z(j) \leq b_2(j), \\ b_1(j), & \text{if } z(j) < b_1(j), \\ b_2(j), & \text{if } z(j) > b_2(j). \end{cases}$$

This allows us to define another family of disjoint boxes. Specifically, define $\tilde{B}_x = \tilde{B}_x(1) \times \cdots \times \tilde{B}_x(d)$ where $\tilde{B}_x(j) \subseteq \mathbb{R}$ are defined as follows:

1. $\tilde{B}_x(j^*) = (\sigma_x(j^*) + q_x/6, \sigma_x(j^*) + q_x/3)$;
2. for all $j \neq j^*$ with $t_x(j) = 0$, $\tilde{B}_x(j) = (\sigma_x(j) - q_x/3, \sigma_x(j) + q_x/3)$;
3. for all j with $t_x(j) = 1$, $\tilde{B}_x(j) = (b_1(j) - L/3, b_1(j))$;
4. for all j with $t_x(j) = 2$, $\tilde{B}_x(j) = (b_2(j), b_2(j) + L/3)$.

It is clear that $\tilde{B}_x \subseteq B$. Moreover, for $j \in [d]$ with $t_x(j) = 1$, we have

$$(3.10) \quad 0 \leq \sigma_x(j) - b_1(j) \leq |b_1(j) - x(j)| + \|x - \sigma_x\|_\infty \leq 2\ell_x < q_x/3,$$

where the last inequality is by $x \in U_{>} \subseteq T$ and thus $q_x > 2^{11}\ell_x$. Inequality (3.10) implies $b_1(j) \in B_x(j)$ whenever $t_x(j) = 1$. Similarly, we have $b_2(j) \in B_x(j)$ whenever $t_x(j) = 2$. Therefore, any $z \in \tilde{B}_x$ satisfies $\pi_z \in B_x$ because $z(j) \in \tilde{B}_x(j)$ implies $\pi_z(j) \in B_x(j)$ for all $j \in [d]$. It is then easy to show that \tilde{B}_x are disjoint: if $z \in \tilde{B}_x \cap \tilde{B}_{x'}$, then $\pi_z \in B_x \cap B_{x'}$, a contradiction. Figure 2 shows an example of the boxes B_x and \tilde{B}_x contained in B .

The volume of \tilde{B}_x can be lower bounded as follows:

$$|\tilde{B}_x| = \prod_{j=1}^d |\tilde{B}_x(j)| = (1/4)(2q_x/3)^{d-\|t_x\|_0} (L/3)^{\|t_x\|_0} \geq (5L/3)^d (24\ell_x/L),$$

where the last inequality is by the fact that $\frac{q_x}{L} > 2^{11}(\frac{\ell_x}{L})^{1/(d-\|t_x\|_0)}$, $d \geq 2$, and $\|t_x\|_0 \leq 1$. Summing up, we have

$$\sum_{x \in U_{>}} (5L/3)^d (24\ell_x/L) \leq \sum_{x \in U_{>}} |\tilde{B}_x| \leq |B| \leq (5L/3)^d.$$

Therefore,

$$\sum_{x \in U_{>}} |W_x| \leq \sum_{x \in U_{>}} \ell_x \leq L/24.$$

A similar argument proves $\bigcup_{x \in U \setminus U_{>}} |W_x| \leq L/24$, which implies $|\bigcup_{x \in U} W_x| \leq L/12$ and completes the proof of the lemma. \square

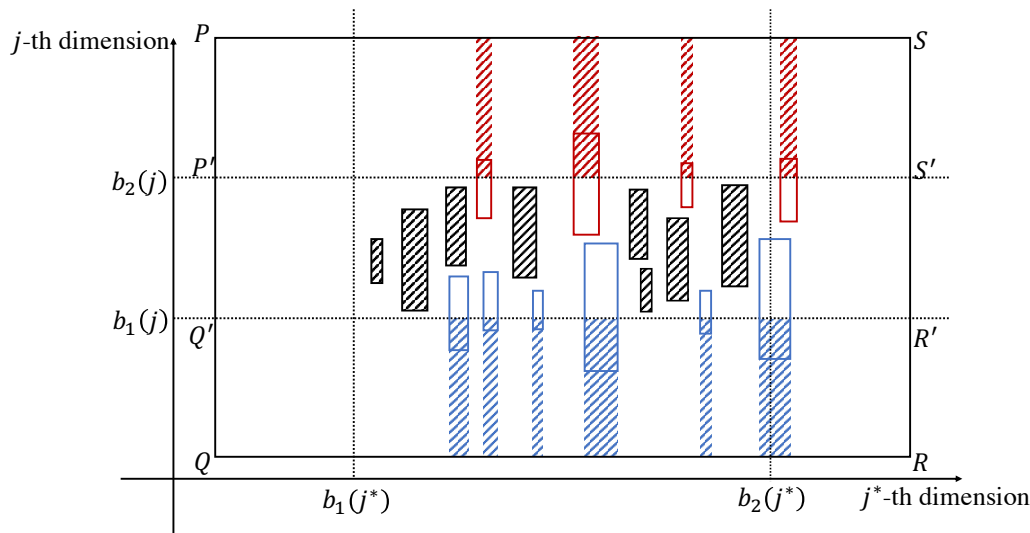


Figure 2: For every $x \in U_{>}$, the box B_x is represented by a square with solid boundary, and \tilde{B}_x is represented by a shaded square. The rectangle $PQRS$ represents the box B , and the rectangle $P'Q'R'S'$ represents the smaller box B' . If $t_x(j) = 1$, the corresponding B_x (blue) intersects the lower boundary in the j -th dimension (the dotted horizontal line at $b_1(j)$). If $t_x(j) = 2$, the corresponding B_x (red) intersects the upper boundary in the j -th dimension (the dotted horizontal line at $b_2(j)$).

3.2.3 Cutting Our algorithm `single_cut_2d` chooses $\theta \in (b_1(j^*), b_2(j^*)) \setminus F$ using a method by Seymour [53] based on Lemma 3.7 below. Recall that any choice of θ defines a partition X_1, X_2 of X and a partition Y_1, Y_2 of Y as specified in (3.2). It also defines X_+, X_{11}, X_{22} as specified in (3.3) and (3.4). We further define

$$\begin{aligned} M_1^* &= m|Y_1| + \sum_{x \in R_0 \cap X_{11}} \ell_x^2, \\ M_2^* &= m|Y_2| + \sum_{x \in R_0 \cap X_{22}} \ell_x^2, \\ M^* &= \min\{M(\mathcal{P})/2, M(\mathcal{P}) - M_1^*, M(\mathcal{P}) - M_2^*\}. \end{aligned}$$

LEMMA 3.7. *There exists $\theta \in (b_1(j^*), b_2(j^*)) \setminus F$ satisfying*

$$(3.11) \quad \sum_{x \in R_0 \cap X_+} \ell_x L \leq 8M^* \log(M(\mathcal{P})/M^*) \log \log_2(M(\mathcal{P})/m).$$

Moreover, θ can be computed in poly-time.

Proof. The fact that θ can be computed in poly-time follows immediately from its existence, because there are at most $|X| + |Y|$ choices of $\theta \in (b_1(j^*), b_2(j^*)) \setminus F$ that lead to distinct partitions (X_1, X_2) and (Y_1, Y_2) . It only takes poly-time to check (3.11) for each of the choices using the representation of F as a union of disjoint intervals. Below we prove the existence of θ .

Define $M = M(\mathcal{P})$. For every point $x \in R_0$, define a function $g_x : (b_1(j^*), b_2(j^*)) \rightarrow [0, +\infty)$ such that $g_x(\theta) = \ell_x^2/|W_x|$ if $\theta \in W_x$, and $g_x(\theta) = 0$ otherwise. Define $h(\theta)$ as the number of centroids $y \in Y$ with $y(j^*) < \theta$. Define

$$G(\theta) = mh(\theta) + \sum_{x \in R_0} \int_{b_1(j^*)}^{\theta} g_x(\theta') d\theta'.$$

It is clear that G is non-decreasing, and bounded between m and $M - m$ for all $\theta \in (b_1(j^*), b_2(j^*))$. Moreover, for every choice of θ , we have $M_1^* \leq G(\theta)$ and $M_2^* \leq M - G(\theta)$. Define $I_1 = (\{x(j^*) : x \in X\} \cup \{y(j^*) : y \in Y\}) \cap (b_1(\ell^*), b_2(\ell^*))$. G is differentiable on $(b_1(\ell^*), b_2(\ell^*)) \setminus I_1$, where $G'(\theta) = \sum_{x \in R_0} g(\theta)$.

By Lemma 3.5, the total length of the non-forbidden region is at least $L/2$. Therefore, we can find real numbers $\alpha_1, \dots, \alpha_u$ and β_1, \dots, β_u such that

1. $b_1(j^*) \leq \alpha_1 < \beta_1 \leq \alpha_2 < \beta_2 \leq \dots \leq \alpha_u < \beta_u \leq b_2(j^*)$;
2. every (α_i, β_i) is disjoint from the forbidden region F ;
3. $\sum_{i=1}^u (\beta_i - \alpha_i) = L/2$.

Define $z_i := \sum_{i'=1}^i (\beta_{i'} - \alpha_{i'})$. We define a bijection γ from $\bigcup_{i=1}^u (z_{i-1}, z_i)$ to $\bigcup_{i=1}^u (\alpha_i, \beta_i)$ as follows: for all $z \in (z_{i-1}, z_i)$, define $\gamma(z) = \alpha_i + (z - z_{i-1})$. It is clear that γ is non-decreasing and has derivative $\gamma'(z) = 1$ for all $z \in \bigcup_{i=1}^u (z_{i-1}, z_i)$.

Define $I = \{z_1, \dots, z_{m-1}\} \cup \{\gamma^{-1}(\theta) : \theta \in I_1 \cap \bigcup_{i=1}^u (\alpha_i, \beta_i)\}$. I is a finite subset of $(0, L/2)$. Define $V : (0, L/2) \setminus I \rightarrow [m, M - m]$ by $V(z) = G(\gamma(z))$. Then V is a non-decreasing function on $(0, L/2) \setminus I$ with derivative $V'(z) = G'(\gamma(z))$. By Lemma A.2, we can find $z \in (0, L/2) \setminus I$ such that

$$V'(z) \leq (4/L)M' \log(M/M') \log \log_2(M/m),$$

where $M' := \min\{V(z), M - V(z)\}$. Choose $\theta = \gamma(z)$. We have $M' \leq V(z) = G(\theta) \leq M - M_2^*$ and $M' \leq M - V(z) = M - G(\theta) \leq M - M_1^*$. Therefore, $M' \leq M^*$. By Claim A.2, we have

$$G'(\theta) = V'(z) \leq (8/L)M^* \log(M/M^*) \log \log_2(M/m).$$

The lemma is proved by noting that

$$G'(\theta) = \sum_{x \in R_0} g_x(\theta) \geq \sum_{x \in R_0 \cap X_+} g_x(\theta) \geq \sum_{x \in R_0 \cap X_+} \ell_x,$$

where the last inequality is by the easy fact that $\theta \in W_x$ whenever $x \in X_+$ and that $\ell_x^2/|W_x| \geq \ell_x$. \square

3.2.4 Updating Having computed the hyperplane (j^*, θ) , we get the partitions (X_1, X_2) and (Y_1, Y_2) by (3.2). We now specify the new assignments σ'_x , new lengths ℓ'_x , new types t'_x . The two new subproblems $\mathcal{P}_1, \mathcal{P}_2$ can then be formed by (3.1).

For every non- σ -separated point $x \in X \setminus X_+$ we define $\sigma'_x = \sigma_x$, $\ell'_x = \ell_x$, and $t'_x = t_x$. For every σ -separated irrelevant point $x \in X_+ \setminus R$, we define $\ell'_x = \ell_x$, $t'_x = t_x (= \perp)$, and define σ'_x to be an arbitrary centroid in Y that lies on the same side of the hyperplane (j^*, θ) with x . Such a centroid exists because Y_1, Y_2 are both non-empty since we choose θ from $(b_1(j^*), b_2(j^*))$.

It remains to consider relevant points that are σ -separated, i.e. points $x \in R \cap X_+$. These points satisfy the properties in Lemma 3.4. For these points, we define

$$(3.12) \quad \ell'_x = \ell_x + 2^{11} L (\ell_x / L)^{1/(d - \|t_x\|_0)}$$

and $\sigma'_x = \eta_x$. We define t'_x to be equal to t_x , except that we change $t'_x(j^*)$ to either 1 or 2 from the original value $t_x(j^*) = 0$ (Lemma 3.4 Item 2). Specifically, define $t'_x(j^*) = 1$ if $x \in X_2$, and $t'_x(j^*) = 2$ if $x \in X_1$.

This completes our definition of σ'_x, ℓ'_x and t'_x . The algorithm `single_cut_2d` returns the two subproblem $\mathcal{P}_1, \mathcal{P}_2$ formed by (3.1) together with the hyperplane (j^*, θ) . Before we prove Lemma 3.1 and Lemma 3.2, we first prove Lemma 3.8 below. Define $R' = \{x \in X : t'_x \neq \perp\}$. For $i = \{0, 1, 2\}$, define $R'_i = \{x \in R' : \|t'_x\|_0 = i\}$. It is clear from our update rules that $t'_x = \perp$ if and only if $t_x = \perp$, so $R' = R$.

LEMMA 3.8. *We have the following equalities and inequalities:*

$$(3.13) \quad M(\mathcal{P}_1) = M_1^*, \quad \text{and} \quad M(\mathcal{P}_2) = M_2^*;$$

$$(3.14) \quad \min\{M_1^*, M_2^*\} \leq M^*, \quad \text{and} \quad \max\{M_1^*, M_2^*\} \leq M(\mathcal{P}) - M^*.$$

Proof. According to our update rule, no point $x \in X_+$ has $\|t'_x\|_0 = 0$ because either $x \in X_+ \setminus R$ and $t'_x = \perp$, or $x \in R \cap X_+$ and $\|t'_x\|_0 \geq 1$. Therefore, a point $x \in X_1 \cap R'_0$ if and only if $x \in X_1 \setminus X_+ = X_{11}$, $t_x \neq \perp$, and $\|t_x\|_0 = 0$, or equivalently, $x \in R_0 \cap X_{11}$. This implies

$$M(\mathcal{P}_1) = m|Y_1| + \sum_{x \in X_1 \cap R'_0} (\ell'_x)^2 = m|Y_1| + \sum_{x \in R_0 \cap X_{11}} (\ell'_x)^2 = m|Y_1| + \sum_{x \in R_0 \cap X_{11}} \ell_x^2 = M_1^*.$$

Similarly, $M(\mathcal{P}_2) = M_2^*$. This completes the proof of (3.13).

To prove (3.14), we assume w.l.o.g. that $M_1^* \leq M_2^*$. It is clear from definition that $M_1^* + M_2^* \leq M(\mathcal{P})$. Therefore, $M_1^* \leq \min\{M(\mathcal{P})/2, M(\mathcal{P}) - M_1^*, M(\mathcal{P}) - M_2^*\} = M^*$. The definition of M^* directly implies $M_2^* \leq M(\mathcal{P}) - M^*$. \square

We conclude Section 3.2 by proving Lemma 3.1 and Lemma 3.2. We first prove Lemma 3.1

Proof. Let $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X})$ denote the valid subproblem *after* the preprocessing step.

We check every item in Definition 3.4. Item 3 follows immediately from the validity of \mathcal{P} and the fact that $\sigma'_x = \sigma_x$ whenever $x \in X \setminus R' = X \setminus R$.

Now we prove Item 1. All non- σ -separated points $x \in X \setminus X_+$ have $\sigma'_x = \sigma_x$, and $\ell'_x = \ell_x$, so they satisfy $\ell'_x = \ell_x \geq \|x - \sigma_x\|_\infty = \|x - \sigma'_x\|_\infty$. By Item 3, all points in $X \setminus R = X \setminus R'$ also satisfy $\ell'_x \geq \|x - \sigma'_x\|_\infty$. It remains to check Item 1 for σ -separated relevant points $x \in R \cap X_+$. By Lemma 3.4, these points satisfy

$$\ell'_x = \ell_x + 2^{11}L(\ell_x/L)^{1/(d-\|t_x\|_0)} \geq \ell_x + q_x \geq \|x - \sigma_x\|_\infty + \|\sigma_x - \eta_x\|_\infty \geq \|x - \eta_x\|_\infty = \|x - \sigma'_x\|_\infty.$$

We now move on to Item 2. It suffices to prove that $\max\{M(\mathcal{P}_1), M(\mathcal{P}_2)\} \leq M(\mathcal{P})$, which follows directly from Lemma 3.8.

Now we prove Item 4. We prove it for \mathcal{P}_1 , and omit the similar proof for \mathcal{P}_2 . Define $b'_1(j), b'_2(j)$ similarly as $b_1(j), b_2(j)$ are defined in Definition 3.3 except that we replace Y by Y_1 .

Suppose $x \in X_1 \cap R'$ has $t'_x(j) \neq 0$. If $j = j^*$ and $t'_x(j) = 2$, then by Lemma 3.3 it must be the case that $x \in R \cap X_+$. We have $\sigma'_x(j) \leq b'_2(j) \leq \sigma_x(j)$, so

$$|x(j) - b'_2(j)| \leq \max\{|x(j) - \sigma'_x(j)|, |x(j) - \sigma_x(j)|\} \leq \max\{\ell'_x, \ell_x\} = \ell'_x.$$

If $j \neq j^*$ or $t'_x(j) \neq 2$, we have $t'_x(j) = t_x(j)$. Define $i = t'_x(j) = t_x(j)$. If $i = 1$, we have $b_i(j) \leq b'_i(j) \leq \sigma'_x(j)$; if $i = 2$, we have $b_i(j) \geq b'_i(j) \geq \sigma'_x(j)$. In both cases,

$$|x(j) - b'_i(j)| \leq \max\{|x(j) - \sigma'_x(j)|, |x(j) - b_i(j)|\} \leq \max\{\ell'_x, \ell_x\} = \ell'_x.$$

\square

Now we prove Lemma 3.2.

Proof. Since the preprocessing step preserves the validity of \mathcal{P} and does not increase $A(\mathcal{P})$, we assume w.l.o.g. that $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X})$ is the subproblem *after* the preprocessing step. Define $M = M(\mathcal{P})$. We have

$$(3.15) \quad A(\mathcal{P}_1) + A(\mathcal{P}_2) = f(M(\mathcal{P}_1)) + f(M(\mathcal{P}_2)) + 2^{32} \sum_{x \in R'_1} (\ell'_x)^2 + 2^9 \sum_{x \in R'_2} (\ell'_x)^2 + \sum_{x \in X \setminus R} (\ell'_x)^2.$$

Moreover,

$$\begin{aligned} \sum_{x \in R'_1} (\ell'_x)^2 &= \sum_{x \in R_1 \cap R'_1} (\ell'_x)^2 + \sum_{x \in R_0 \cap R'_1} (\ell'_x)^2 \\ &= \sum_{x \in R_1 \cap R'_1} (\ell'_x)^2 + \sum_{x \in R_0 \cap X_+} (\ell'_x)^2 \\ &\stackrel{\text{(by (3.12))}}{=} \sum_{x \in R_1 \cap R'_1} \ell_x^2 + \sum_{x \in R_0 \cap X_+} (\ell_x + 2^{11}L(\ell_x/L)^{1/2})^2 \\ &\leq \sum_{x \in R_1 \cap R'_1} \ell_x^2 + 2^{23} \sum_{x \in R_0 \cap X_+} \ell_x L \\ &\stackrel{(3.16)}{\leq} \sum_{i \in R_1 \cap R'_1} \ell_x^2 + 2^{25} M^* \log(M/M^*) \log \log_2(2k), \end{aligned}$$

where the last inequality is by Lemma 3.7 and Definition 3.4 Item 2. Similarly,

$$\begin{aligned}
 \sum_{x \in R'_2} (\ell'_x)^2 &= \sum_{x \in R_2} (\ell'_x)^2 + \sum_{x \in R_1 \cap R'_2} (\ell'_x)^2 \\
 &= \sum_{x \in R_2} \ell_x^2 + \sum_{x \in R_1 \cap R'_2} (\ell_x + 2^{11} \ell_x)^2 \\
 &\leq \sum_{x \in R_2} \ell_x^2 + 2^{23} \sum_{x \in R_1 \cap R'_2} \ell_x^2,
 \end{aligned}
 \tag{3.17}$$

Applying Lemma 3.8,

$$\begin{aligned}
 &f(M(\mathcal{P}_1)) + f(M(\mathcal{P}_2)) + 2^{57} M^* \log(M/M^*) \log \log_2(2k) \\
 &= f(M_1^*) + f(M_2^*) + 2^{57} M^* \log(M/M^*) \log \log_2(2k) \\
 &\leq f(M^*) + f(M - M^*) + 2^{57} M^* \log(M/M^*) \log \log_2(2k) \\
 &\leq 2^{57} \left(M^* (1 + \log(M^*/m)) \log \log_2(2k) + (M - M^*) (1 + \log(M/m)) \log \log_2(2k) \right. \\
 &\quad \left. + M^* \log(M/M^*) \log \log_2(2k) \right) \\
 &= f(M).
 \end{aligned}
 \tag{3.18}$$

Combining the inequalities as (3.16) $\times 2^{32}$ + (3.17) $\times 2^9$ + (3.18) and simplifying using (3.15), we get $A(\mathcal{P}_1) + A(\mathcal{P}_2) \leq A(\mathcal{P})$, as desired. \square

3.3 Building a decision tree We prove Theorem 3.1 by describing the algorithm `post-process_2d` that takes an arbitrary k -clustering \mathcal{C} and turns it into a k -explainable clustering with respect to a decision tree T .

As shown in Algorithm 1, our algorithm `post-process_2d` calls an algorithm `decision_tree_2d` that takes a valid subproblem $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X})$ and produces a decision tree T and an assigned centroid $\delta_x \in Y$ for every $x \in X$. Algorithm `decision_tree_2d` works recursively as follows: if the diameter L of \mathcal{P} is zero, which means that all centroids $y \in Y$ are at the same location, return $((\delta_x)_{x \in X}, T)$, where δ_x is identical for all x and equals to an arbitrary centroid $y \in Y$, and T is the tree with a single node; else, the algorithm `decision_tree_2d` calls `single_cut_2d` on \mathcal{P} , obtains a hyperplane (j^*, θ) and two subproblems $\mathcal{P}_1, \mathcal{P}_2$. The algorithm `decision_tree_2d` recursively calls itself on \mathcal{P}_1 and \mathcal{P}_2 , and obtains $((\delta_x)_{x \in X_1}, T_1)$ and $((\delta_x)_{x \in X_2}, T_2)$. The algorithm constructs a tree T with root corresponding to (j^*, θ) and its left and right sub-trees being T_1 and T_2 . The algorithm returns $((\delta_x)_{x \in X}, T)$.

LEMMA 3.9. *Assuming the input $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X})$ to `decision_tree_2d` is valid. The output $((\delta_x)_{x \in X}, T)$ of `decision_tree_2d` satisfies the following properties. The decision tree T has at most $|Y|$ leaves. For every leaf v of the decision tree T and every pair of points $x, x' \in X$ in the region defined by v , we have $\delta_x = \delta_{x'}$. Moreover, $\sum_{x \in X} \|x - \delta_x\|_\infty^2 \leq A(\mathcal{P})$.*

Proof. We prove the lemma by induction on $|Y|$. When $|Y| = 1$, we have $L = 0$ and thus `decision_tree_2d` returns without calling `single_cut_2d`. The lemma is trivial in this case. Now suppose the lemma is true when $|Y| < u$ for an integer $u > 1$, and we prove the lemma for $|Y| = u$. If $L = 0$, then again the lemma is trivial; otherwise, the algorithm `decision_tree_2d` calls `single_cut_2d`, and the lemma follows from the induction hypothesis together with Lemma 3.1 and Lemma 3.2. \square

Given a k -clustering \mathcal{C} of points x_1, \dots, x_n consisting of centroids y_1, \dots, y_k , and an assignment mapping $\xi : [n] \rightarrow [k]$, the algorithm `post-process_2d` computes an *initial subproblem* $\tilde{\mathcal{P}}$ by setting $X = \{x_1, \dots, x_n\}$, $Y = \{y_1, \dots, y_k\}$, $\sigma_{x_i} = y_{\xi(i)}$, $\ell_x = \|x - \sigma_x\|_\infty$, $t_x(j) = 0, \forall j \in [d]$. Setting the centroid mass $m = \frac{1}{k} \sum_{x \in X} \ell_x^2$, we have $\tilde{\mathcal{P}}$ is valid and $A(\tilde{\mathcal{P}}) = O(\log k \log \log_2(2k)) \cdot \text{cost}(\mathcal{C})$. Algorithm `post-process_2d` then calls `decision_tree_2d` on $\tilde{\mathcal{P}}$ and obtains $(\delta_x)_{x \in X}$ and T . Algorithm `post-process_2d` returns the decision tree T and a clustering \mathcal{C}' with centroids y_1, \dots, y_k and assignment mapping $\xi' : [n] \rightarrow [k]$ such that $y_{\xi'(i)} = \delta_{x_i}$.

Now we finish the proof of Theorem 3.1.

Algorithm 1: Algorithm `post-process_2d` via `decision_tree_2d`

Input : A k -clustering \mathcal{C} of points x_1, \dots, x_n in $d = 2$ dimensions

Output: A k -clustering \mathcal{C}' of points x_1, \dots, x_n , a decision tree T

Algorithm `post-process_2d`($x_1, \dots, x_n; \mathcal{C}$)

```

    Let  $y_1, \dots, y_k$  be the centroids of  $\mathcal{C}$ , and  $\xi : [n] \rightarrow [d]$  be the assignment mapping of  $\mathcal{C}$ ;
     $X \leftarrow \{x_1, \dots, x_n\}, Y \leftarrow \{y_1, \dots, y_k\}$ ;
     $\forall i \in [n], \forall x \in X, \forall j \in [d]$ , set  $\sigma_{x_i} \leftarrow y_{\xi(i)}, \ell_x \leftarrow \|x - \sigma_x\|_\infty, t_x(j) \leftarrow 0$ ;
     $\tilde{\mathcal{P}} \leftarrow (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X});$                                 /* Initial subproblem */
     $m \leftarrow \frac{1}{k} \sum_{x \in X} \ell_x^2;$                                                 /* Centroid mass */
     $((\delta_x)_{x \in X}, T) \leftarrow \text{decision\_tree\_2d}(\tilde{\mathcal{P}});$ 
    Let  $\xi' : [n] \rightarrow [d]$  be such that  $y_{\xi'(i)} = \delta_{x_i}$ ;
    Let  $\mathcal{C}'$  be the clustering with centroids  $y_1, \dots, y_k$  and assignment mapping  $\xi'$ ;
    return  $\mathcal{C}', T$ ;
```

Input : A valid subproblem $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X})$

Output: An assigned centroid $\delta_x \in Y$ for every point $x \in X$, a decision tree T

Algorithm `decision_tree_2d`(\mathcal{P})

```

    Let  $L$  be the diameter of  $\mathcal{P}$ ;
    if  $L = 0$  then
        Pick an arbitrary  $y \in Y$  and set  $\delta_x = y$  for all  $x \in X$ ;
        Let  $T$  be the decision tree with a single node;
    else
         $(\mathcal{P}_1, \mathcal{P}_2, j^*, \theta) \leftarrow \text{single\_cut\_2d}(\mathcal{P});$ 
         $((\delta_x)_{x \in X_1}, T_1) \leftarrow \text{decision\_tree\_2d}(\mathcal{P}_1);$ 
         $((\delta_x)_{x \in X_2}, T_2) \leftarrow \text{decision\_tree\_2d}(\mathcal{P}_2);$ 
        Define  $T$  to be the decision tree with root corresponding to hyperplane  $(j^*, \theta)$  and its left and
        right sub-trees being  $T_1$  and  $T_2$ ;
    return  $(\delta_x)_{x \in X}, T$ ;
```

Proof. Since `single_cut_2d` computes θ in polynomial time by Lemma 3.7, the entire algorithm `single_cut_2d` can be implemented in polynomial time. Consequently, `decision_tree_2d` and `post-process_2d` both run in polynomial time. Let \mathcal{C}' and T be the output of algorithm `post-process_2d`. By Lemma 3.9, we know \mathcal{C}' is k -explainable w.r.t. T , and

$$\begin{aligned} \text{cost}(\mathcal{C}') &= \sum_{i=1}^n \|x_i - y_{\xi'(i)}\|_2^2 \leq 2 \sum_{i=1}^n \|x_i - y_{\xi'(i)}\|_\infty^2 = 2 \sum_{i=1}^n \|x_i - \delta_{x_i}\|_\infty^2 \\ &\leq 2A(\tilde{\mathcal{P}}) \leq O(\log k \log \log_2(2k)) \text{cost}(\mathcal{C}). \end{aligned}$$

It is by definition that \mathcal{C}' uses the same centroids as \mathcal{C} does. Choosing \mathcal{C} as the output of a poly-time constant factor approximation algorithm for k -means, e.g. [33, 2, 28], or since $d = 2$, a PTAS for k -means [23, 18, 17], gives the competitive ratio bound $O(\log k \log \log_2(2k))$. \square

4 Explainable k -means in $d > 2$ dimensions

We now describe our algorithm for higher dimensions, i.e., $d > 2$. The algorithm also works for $d = 2$ despite giving a worse bound than Theorem 3.1. We follow the same structure as the previous section, and emphasize the differences from it. Our goal is to prove the following high-dimensional analogue of Theorem 3.1

THEOREM 4.1. *Assume $k, d \geq 2$. There exists a poly-time algorithm `post-process` that takes a k -clustering \mathcal{C} of n points in d dimensions, and outputs a clustering \mathcal{C}' of the n points and a decision tree T with at most k leaves such that*

1. \mathcal{C}' is k -explainable with respect to T ;
2. $\text{cost}(\mathcal{C}') \leq O(k^{1-2/d}(\log k)^8(\log \log_2(2k))^3 d^4) \cdot \text{cost}(\mathcal{C})$;
3. \mathcal{C}' uses the same k centroids as \mathcal{C} does.

Consequently, there exists a poly-time algorithm that takes n points in d dimensions and outputs a k -explainable clustering with competitive ratio $O(k^{1-2/d}(\log k)^8(\log \log_2(2k))^3 d^4)$.

The bound in Theorem 4.1 can be improved when combined with [43, 25, 21].

COROLLARY 4.1. (IN LIGHT OF [43, 25, 21]) Assume $k, d \geq 2$. There exists a poly-time algorithm that takes n points in d dimensions and outputs a k -explainable clustering with competitive ratio $k^{1-2/d} \text{polylog}(k)$.

Proof. Use the following algorithm: when $d \leq \log k$, invoke the algorithm in Theorem 4.1 to achieve competitive ratio

$$O(k^{1-2/d}(\log k)^8(\log \log_2(2k))^3 d^4) = k^{1-2/d} \text{polylog}(k);$$

when $d > \log k$, invoke the algorithm in [43, 25, 21] to achieve competitive ratio

$$k \text{polylog}(k) = k^{2/d} k^{1-2/d} \text{polylog}(k) = O(1) \cdot k^{1-2/d} \text{polylog}(k) = k^{1-2/d} \text{polylog}(k).$$

□

In the rest of the section, we assume $k, d \geq 2$.

4.1 Subproblem Compared to subproblems for $d = 2$ defined in Section 3.1, subproblems for $d > 2$ contain more information:

DEFINITION 4.1. (SUBPROBLEM FOR $d > 2$) Given points $x_1, \dots, x_n \in \mathbb{R}^d$ and centroids $y_1, \dots, y_k \in \mathbb{R}^d$, besides what is included in Definition 3.1, a subproblem \mathcal{P} consists of the following in addition:

1. A color $c_x \in \{-1, 0, \dots, \lfloor \log_2 k \rfloor - 1\}$ for every point $x \in X$.
2. A scale $s_x \in [1, +\infty)$ for every point $x \in X$;
3. A potential $p_x \in (0, +\infty)$ for every point $x \in X$.

We fix a positive real number m as the *centroid mass* and define two quantities $M(\mathcal{P})$ and $A(\mathcal{P})$ for a subproblem \mathcal{P} with respect to the centroid mass m . This is similar to Definition 3.2 but we take the potentials p_x into account:

DEFINITION 4.2. Given a subproblem \mathcal{P} , we define the following quantities:

$$M(\mathcal{P}) := m|Y| + \sum_{x \in R} p_x \ell_x^2 (16(\log(2k))^2 \log \log_2(2k))^{2-\|t_x\|_0},$$

$$A(\mathcal{P}) := f(M(\mathcal{P})) + \sum_{x \in X \setminus R} p_x \ell_x^2,$$

where

$$f(M) := 16M(M/m)^{1/\log(2k)}(1 + \log(M/m)) \log \log_2(2k).$$

We define subproblem boundaries in the same way as Definition 3.3. Our definition for valid subproblems includes more requirements than Definition 4.3.

DEFINITION 4.3. (VALID SUBPROBLEM) Given points $x_1, \dots, x_n \in \mathbb{R}^d$ and centroids $y_1, \dots, y_k \in \mathbb{R}^d$, a subproblem $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X}, (c_x)_{x \in X}, (s_x)_{x \in X}, (p_x)_{x \in X})$ is valid if in addition to the requirements in Definition 3.4, it satisfies all of the following:

1. For all $x \in R$, $\|t_x\|_0 \leq 2$. (Thus, $R = R_0 \cup R_1 \cup R_2$.)

2. If $x \in R_0$, then ℓ_x is either zero or a power of 2, i.e., $\ell_x = 0$ or $\ell_x = 2^a$ for an integer a .
3. If $x \in R_0$, then $s_x = k$.
4. For every relevant point $x \in R$, its color $c_x = -1$ if and only if $x \in R_0$.
5. For every color $c \in \{0, \dots, \lfloor \log_2 k \rfloor - 1\}$ and every relevant type $t : [d] \rightarrow \{0, 1, 2\}$, define $R_{c,t} = \{x \in R : c_x = c, t_x = t\}$ and $Y_{c,t} = \{\sigma_x : x \in R_{c,t}\}$. If $R_{c,t} \neq \emptyset$, there exists scale $s_{c,t} \geq 1$ and length $\ell_{c,t} \geq 0$ such that all points $x \in R_{c,t}$ have $s_x = s_{c,t}$ and $\ell_x = \ell_{c,t}$. Moreover, $|Y_{c,t}| \leq s_{c,t}$.

4.2 Making a single cut As in Section 3.2, we describe an efficient algorithm `single_cut` that takes a valid subproblem $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X}, (c_x)_{x \in X}, (s_x)_{x \in X}, (p_x)_{x \in X})$, and produces two smaller valid subproblems \mathcal{P}_1 and \mathcal{P}_2 together with an axis-parallel hyperplane (j^*, θ) that separates them. The two subproblems are defined by new assignments $(\sigma'_x)_{x \in X}$, new lengths $(\ell'_x)_{x \in X}$, new types $(t'_x)_{x \in X}$, new colors $(c'_x)_{x \in X}$, new scales $(s'_x)_{x \in X}$, and new potentials $(p'_x)_{x \in X}$ as follows

$$(4.19) \quad \begin{aligned} \mathcal{P}_1 &= (X_1, Y_1, (\sigma'_x)_{x \in X_1}, (\ell'_x)_{x \in X_1}, (t'_x)_{x \in X_1}, (c'_x)_{x \in X_1}, (s'_x)_{x \in X_1}, (p'_x)_{x \in X_1}), \\ \mathcal{P}_2 &= (X_2, Y_2, (\sigma'_x)_{x \in X_2}, (\ell'_x)_{x \in X_2}, (t'_x)_{x \in X_2}, (c'_x)_{x \in X_2}, (s'_x)_{x \in X_2}, (p'_x)_{x \in X_2}). \end{aligned}$$

Again, we choose $j^* = \operatorname{argmax}_{j \in [d]} (b_2(j) - b_1(j))$, and define $X_1, X_2, Y_1, Y_2, X_+, X_{11}, X_{22}$ as in (3.2), (3.3) and (3.4). Throughout Section 4.2, we assume that the input subproblem \mathcal{P} is valid and has diameter $L > 0$ even when we do not explicitly state so. At the end of the section, we prove the following lemmas for the algorithm `single_cut`.

LEMMA 4.1. *The two new subproblems $\mathcal{P}_1, \mathcal{P}_2$ output by `single_cut` are both valid.*

LEMMA 4.2. *The two new subproblems $\mathcal{P}_1, \mathcal{P}_2$ output by `single_cut` satisfy $A(\mathcal{P}_1) + A(\mathcal{P}_2) \leq A(\mathcal{P})$.*

We describe the algorithm `single_cut` step by step in the following subsections.

4.2.1 Preprocessing If $x \in R$ has $\ell_x \geq L/64$, we replace ℓ_x by $65\ell_x$, replace p_x by $p_x/65^2$, and set $t_x = \perp$ (thus removing x from R). Similarly to Section 3.2.1, it is clear that the new subproblem is still valid, and in the new subproblem every point $x \in R$ satisfies $\ell_x \leq L/64$. Moreover, the value of $A(\mathcal{P})$ does not increase. For the rest of Section 4.2, we use $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X}, (c_x)_{x \in X}, (s_x)_{x \in X}, (p_x)_{x \in X})$ to denote the subproblem *after* the preprocessing step.

4.2.2 Forbidding Similarly to Section 3.2.2, we specify a subset F of the interval $(b_1(j^*), b_2(j^*))$ as the forbidden region.

For all $x \in X$, we define $Y(x), \eta_x, q_x, W_x$ as in (3.6), (3.7), and (3.9). We also define S, T as in (3.8).

For a point $x \in R_0$ with $\ell_x \geq L/32k$, we change its color from $c_x = -1$ (guaranteed by Item 4 in Definition 4.3) to $c_x = \lfloor \log_2(\ell_x/(L/32k)) \rfloor$. Our preprocessing guarantees that $\ell_x \leq L/64$, so the new c_x is an integer between 0 and $\lfloor \log_2 k \rfloor - 1$. Moreover, points $x \in R_0$ have ℓ_x being a power of 2 by Item 2 in Definition 4.3. This means that if $x, x' \in R_0$ have $c_x = c_{x'} \geq 0$ after the color change, then $\ell_x = \ell_{x'}$. By Item 3 in Definition 4.3, all points $x \in R_0$ have $s_x = k$, so Item 5 in Definition 4.3 still holds with the new colors and the induced new definitions of $R_{c,t}, Y_{c,t}, s_{c,t}, \ell_{c,t}$.

For every color $c \geq 0$ and every type $t \neq \perp$, if $R_{c,t} = \emptyset$, define $H_{c,t} = \emptyset$. If $R_{c,t} \neq \emptyset$, we know $Y_{c,t} \neq \emptyset$, and we define $H_{c,t}$ as follows, where $E_{c,t}(y)$ is the interval $[y(j^*) - \ell_{c,t}, y(j^*) + \ell_{c,t}]$ for every $y \in Y_{c,t}$, and $\mathbf{1}_E(\cdot)$ denotes the indicator function of $E \subseteq \mathbb{R}$:

$$H_{c,t} = \left\{ \theta \in (b_1(j^*), b_2(j^*)) : \sum_{y \in Y_{c,t}} \mathbf{1}_{E_{c,t}(y)}(\theta) > 48 \cdot 2^{\|t\|_0} \binom{d}{\|t\|_0} s_{c,t} \ell_{c,t} (\log_2 k) / L \right\}.$$

The entire forbidden region is

$$\begin{aligned} F = & (b_1(j^*), b_1(j^*) + L/32] \cup [b_2(j^*) - L/32, b_2(j^*)) \\ & \cup \bigcup_{y \in Y} [y(j^*) - L/32k, y(j^*) + L/32k] \cap (b_1(j^*), b_2(j^*)) \\ & \cup \bigcup_{x \in T} W_x \\ & \cup \bigcup_{c \geq 0, t \neq \perp} H_{c,t}. \end{aligned}$$

Similarly to the $d = 2$ case, F can be represented as a union of finitely many *disjoint* intervals, and the representation can be computed in poly-time. The following lemma has essentially the same proof as Lemma 3.3

LEMMA 4.3. *If we choose $\theta \in (b_1(j^*), b_2(j^*)) \setminus F$, then every $x \in R$ with $t_x(j^*) = 1$ belongs to X_{11} , and similarly every $x \in R$ with $t_x(j^*) = 2$ belongs to X_{22} . Consequently, every $x \in R \cap X_+$ satisfies $t_x(j^*) = 0$.*

Similarly to Lemma 3.4 and Lemma 3.5, we prove Lemma 4.4 and Lemma 4.5 below.

LEMMA 4.4. *If we choose $\theta \in (b_1(j^*), b_2(j^*)) \setminus F$, then every σ -separated relevant point $x \in R \cap X_+$ satisfies all of the following:*

1. $x(j^*) \neq \sigma_x(j^*)$;
2. $\ell_x \geq L/64k$ (and thus $c_x \geq 0$);
3. $t_x(j^*) = 0$;
4. if $x \in R_0 \cup R_1$, then $\frac{q_x}{L} \leq 2^{11} \left(\frac{\ell_x}{L}\right)^{1/(d-\|t_x\|_0)}$.

Moreover, for every color $c \geq 0$ and every type $t \neq \perp$,

$$(4.20) \quad |\{\sigma_x : x \in R_{c,t} \cap X_+\}| \leq 48 \cdot 2^{\|t\|_0} \binom{d}{\|t\|_0} s_{c,t} \ell_{c,t} (\log_2 k) / L.$$

Proof. Item 3 follows directly from Lemma 4.3. Item 1 and Item 4 follow from the same argument in the proof of Lemma 3.4.

Assume for the sake of contradiction that Item 2 does not hold for $x \in R \cap X_+$. Then by Definition 3.4 Item 1, $|x(j^*) - \sigma_x(j^*)| \leq \|x - \sigma_x\|_\infty \leq \ell_x < L/64k$. Therefore,

$$W_x \subseteq [\sigma_x(j^*) - L/64k, \sigma_x(j^*) + L/64k] \cap (b_1(j^*), b_2(j^*)) \subseteq F.$$

However, the fact that $x \in X_+$ implies $\theta \in W_x$, and thus $\theta \in F$, a contradiction.

Assume for the sake of contradiction that (4.20) does not hold for color $c \geq 0$ and type $t \neq \perp$. For every $y \in \{\{\sigma_x : x \in R_{c,t} \cap X_+\}\} \subseteq Y_{c,t}$, we have $\theta \in E_{c,t}(y)$. Since (4.20) is violated, this means $\theta \in H_{c,t} \subseteq F$, a contradiction. \square

LEMMA 4.5. *The forbidden region F has length at most $L/2$.*

Proof. Using a similar argument to the proof of Lemma 3.6, we have $|\bigcup_{x \in T} W_x| \leq L/4$. It suffices to prove $|\bigcup_{c \geq 0, t \neq \perp} H_{c,t}| \leq L/8$.

For a uniform random $\theta \in (b_1(j^*), b_2(j^*))$, we have $\mathbb{E}[\mathbf{1}_{E_{c,t}(y)}(\theta)] \leq |E_{c,t}(y)|/L = 2\ell_{c,t}/L$. Therefore,

$$\mathbb{E}\left[\sum_{y \in Y_{c,t}} \mathbf{1}_{E_{c,t}(y)}(\theta)\right] \leq |Y_{c,t}| \cdot 2\ell_{c,t}/L \leq 2s_{c,t}\ell_{c,t}/L.$$

By Markov's inequality, $|H_{c,t}| \leq L / \left(24 \cdot 2^{\|t\|_0} \binom{d}{\|t\|_0} \log_2 k \right)$. Summing up over c, t , we have

$$\begin{aligned} \sum_{c \geq 0, t \neq \perp} |H_{c,t}| &\leq \sum_{i=0}^2 \sum_{\|t\|_0=i} \sum_{c=0}^{\lfloor \log_2 k \rfloor - 1} L / \left(24 \cdot 2^i \binom{d}{i} \log_2 k \right) \\ &\leq \sum_{i=0}^2 \sum_{\|t\|_0=i} L / \left(24 \cdot 2^i \binom{d}{i} \right) \\ &= \sum_{i=0}^2 L / 24 \\ &= L / 8. \end{aligned}$$

□

4.2.3 Cutting We choose $\theta \in (b_1(j^*), b_2(j^*))$ in a similar way as in Section 3.2.3 based on Lemma 4.6 below. For every choice of θ , define

$$\begin{aligned} M_1^* &= m|Y_1| + \sum_{x \in R \cap X_{11}} p_x \ell_x^2 (16(\log(2k))^2 \log \log_2(2k))^{2-\|t_x\|_0}, \\ M_2^* &= m|Y_2| + \sum_{x \in R \cap X_{22}} p_x \ell_x^2 (16(\log(2k))^2 \log \log_2(2k))^{2-\|t_x\|_0}, \\ M^* &= \min\{M(\mathcal{P})/2, M(\mathcal{P}) - M_1^*, M(\mathcal{P}) - M_2^*\}. \end{aligned}$$

LEMMA 4.6. *There exists $\theta \in (b_1(j^*), b_2(j^*)) \setminus F$ satisfying*

$$\sum_{x \in R \cap X_+} p_x \ell_x L (16(\log(2k))^2 \log \log_2(2k))^{2-\|t_x\|_0} \leq 8M^* \log(M(\mathcal{P})/M^*) \log \log_2(M(\mathcal{P})/m).$$

Moreover, θ can be computed in poly-time.

We omit the proof as it is essentially the same as the proof of Lemma 3.7

4.2.4 Updating Having computed the hyperplane (j^*, θ) , we get the partitions (X_1, X_2) and (Y_1, Y_2) by (3.2). We now specify the new assignment σ'_x , new lengths ℓ'_x , new types t'_x , new colors c'_x , new scales s'_x , and new potentials p'_x . The two new subproblems $\mathcal{P}_1, \mathcal{P}_2$ can then be formed by (4.19).

For every non- σ -separated point $x \in X \setminus X_+$ we define $\sigma'_x = \sigma_x$, $\ell'_x = \ell_x$, $t'_x = t_x$, $s'_x = s_x$, $p'_x = p_x$, and define $c'_x = -1$ if $x \in R_0$ and $c'_x = c_x$ otherwise. For every σ -separated irrelevant point $x \in X_+ \setminus R$, we define $\ell'_x = \ell_x$, $t'_x = t_x (= \perp)$, $s'_x = s_x$, $p'_x = p_x$, $c'_x = c_x$, and define σ'_x to be an arbitrary centroid in Y that lies on the same side of the hyperplane (j^*, θ) with x .

It remains to consider relevant points that are σ -separated, i.e. points $x \in R \cap X_+$. We define

$$(4.21) \quad s'_x = 48 \cdot 2^{\|t_x\|_0} \binom{d}{\|t_x\|_0} s_x \ell_x (\log_2 k) / L.$$

It is clear that $s'_x \geq 1$ because otherwise no point in R_{c_x, t_x} should be σ -separated by Lemma 4.4 Item 2 and (4.20). Define σ'_x to be the centroid $y \in Y$ with the minimum $\|y - \sigma_x\|_\infty$ that lies on the same side of the hyperplane (j^*, θ) with x . This ensures that points $x \in R \cap X_+ \cap X_1$ with the same σ_x have the same σ'_x , which holds similarly for points $x \in R \cap X_+ \cap X_2$. Since every centroid in $Y(x)$ is a candidate for σ'_x , we have $\|\sigma_x - \sigma'_x\|_\infty \leq q_x$. We define $c'_x = c_x$. The definition for t'_x, ℓ'_x, p'_x depends on whether $x \in R_0 \cup R_1$ or $x \in R_2$ as follows.

If $x \in (R_0 \cup R_1) \cap X_+$, define t'_x to be equal to t_x , except that we change $t'_x(j^*)$ to either 1 or 2 from the original value $t_x(j^*) = 0$ (Lemma 4.4 Item 3). Specifically, define $t'_x(j^*) = 1$ if $x \in X_2$, and $t'_x(j^*) = 2$ if $x \in X_1$. Define

$$(4.22) \quad \ell'_x = 2^{12} L (\ell_x / L)^{1/(d-\|t_x\|_0)}.$$

Define p'_x so that $p'_x(\ell'_x)^2 = p_x \ell_x L$, or equivalently,

$$(4.23) \quad p'_x = p_x(\ell_x/L)^{1-2/(d-\|t_x\|_0)}/2^{24}.$$

If $x \in R_2 \cap X_+$, define $t'_x = \perp$ and $\ell'_x = 2L$. Again, define p'_x so that $p'_x(\ell'_x)^2 = p_x \ell_x L$, or equivalently,

$$(4.24) \quad p'_x = p_x(\ell_x/L)/4.$$

This completes our definition of $\sigma'_x, \ell'_x, t'_x, c'_x, s'_x$ and p'_x . The algorithm `single_cut` outputs the two new subproblems \mathcal{P}_1 and \mathcal{P}_2 formed according to (4.19) together with the hyperplane (j^*, θ) . Before we prove Lemma 4.1 and Lemma 4.2, we need some inequalities about $M(\mathcal{P}_1), M(\mathcal{P}_2), M_1^*, M_2^*$, and M^* .

LEMMA 4.7. *We have the following inequalities:*

$$(4.25) \quad M(\mathcal{P}_1) \geq M_1^*, \quad \text{and} \quad M(\mathcal{P}_2) \geq M_2^*,$$

$$(4.26) \quad \min\{M_1^*, M_2^*\} \leq M^*, \quad \text{and} \quad \max\{M_1^*, M_2^*\} \leq M(\mathcal{P}) - M^*.$$

Moreover,

$$(4.27) \quad M(\mathcal{P}_1) + M(\mathcal{P}_2) - M_1^* - M_2^* \leq M^*/2 \log(2k).$$

Proof. Inequalities (4.26) follow from a similar argument to the proof of (3.14) in Lemma 3.8. Inequalities (4.25) are proved as follows based on our update rules:

$$\begin{aligned} M(\mathcal{P}_1) - M_1^* &= \sum_{x \in (R_0 \cup R_1) \cap X_+ \cap X_1} p'_x(\ell'_x)^2 (16 \log(2k) \log \log_2(2k))^{2-\|t'_x\|_0} \geq 0, \\ M(\mathcal{P}_2) - M_1^* &= \sum_{x \in (R_0 \cup R_1) \cap X_+ \cap X_2} p'_x(\ell'_x)^2 (16 \log(2k) \log \log_2(2k))^{2-\|t'_x\|_0} \geq 0. \end{aligned}$$

Summing up the above inequalities, we get (4.27):

$$\begin{aligned} &M(\mathcal{P}_1) + M(\mathcal{P}_2) - M_1^* - M_2^* \\ &= \sum_{x \in (R_0 \cup R_1) \cap X_+} p'_x(\ell'_x)^2 (16 \log(2k) \log \log_2(2k))^{2-\|t'_x\|_0} \\ &= \sum_{x \in (R_0 \cup R_1) \cap X_+} p_x \ell_x L (16 \log(2k) \log \log_2(2k))^{2-\|t'_x\|_0} \\ &= \sum_{x \in (R_0 \cup R_1) \cap X_+} p_x \ell_x L (16 \log(2k) \log \log_2(2k))^{2-(\|t_x\|_0+1)} \\ &\leq (16(\log(2k))^2 \log \log_2(2k))^{-1} \sum_{x \in R \cap X_+} p_x \ell_x L (16 \log(2k) \log \log_2(2k))^{2-\|t_x\|_0} \\ &\leq M^*/2 \log(2k). \end{aligned}$$

The last inequality uses Lemma 4.6, $M(\mathcal{P})/m \leq 2k$ by Definition 3.4 Item 2, and $M^* \geq \min\{M_1^*, M_2^*\} \geq m$ by (4.26). \square

We conclude Section 4.2 by proving Lemma 4.1 and Lemma 4.2. We first prove Lemma 4.1.

Proof. Let $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X}, (c_x)_{x \in X}, (s_x)_{x \in X}, (p_x)_{x \in X})$ denote the valid subproblem after the preprocessing step.

We first check every item in Definition 3.4. Item 3 follows from a similar argument to the proof of Lemma 3.1. The only difference is that we need to consider points $x \in R_2 \cap X_+$ separately. For these points, we have $t'_x = \perp$. By our preprocessing step, we have $\ell_x \leq L/64$, and thus for all $y \in Y$,

$$\ell'_x = 2L \geq L + \ell_x \geq \|\sigma_x - y\|_\infty + \|x - \sigma_x\|_\infty \geq \|x - y\|_\infty.$$

Item [1](#) also follows from a similar argument to the proof of Lemma [3.1](#), noting that for $x \in (R_0 \cup R_1) \cap X_+$, update rule [\(4.22\)](#) implies

$$\ell'_x \geq \ell_x + 2^{11} L(\ell_x/L)^{1/(d-\|t_x\|_0)} \geq \ell_x + q_x \geq \ell_x + \|\sigma_x - \sigma'_x\|_\infty \geq \|x - \sigma'_x\|_\infty.$$

Defining $M = M(\mathcal{P})$, Item [2](#) holds because of Lemma [4.7](#)

$$\max\{M(\mathcal{P}_1), M(\mathcal{P}_2)\} \leq \max\{M_1^*, M_2^*\} + M^*/2 \log(2k) \leq M - M^* + M^*/2 \log(2k) \leq M \leq 2km.$$

Definition [3.4](#) Item [4](#) follows from the same argument as the proof of Lemma [3.1](#)

We now check every item in Definition [4.3](#). Item [1](#) is clear from our update rules. Item [2](#) Item [3](#) and Item [4](#) follow from the fact that $\|t'_x\|_0 = 0$ if and only if $x \in R_0 \setminus X_+$.

We prove Definition [4.3](#) Item [5](#) for \mathcal{P}_1 , and omit the similar proof for \mathcal{P}_2 . For color $c \geq 0$ and type $t \neq \perp$, define $R'_{c,t} = \{x \in X_1 : c'_x = c, t'_x = t\}$.

If $t(j^*) \neq 2$, we know $R'_{c,t} \cap X_+ = \emptyset$, so $R'_{c,t} \subseteq R_{c,t} \setminus X_+$. Therefore, for $x \in R'_{c,t}$, we have $s'_x = s_x = s_{c,t}$, $\ell'_x = \ell_x = s_{c,t}$, $\sigma'_x = \sigma_x$. Definition [4.3](#) Item [5](#) is trivial in this case.

If $t(j^*) = 2$, by Lemma [4.3](#), we know $R'_{c,t} \subseteq (R_0 \cup R_1) \cap X_+$, and $R'_{c,t} \subseteq R_{c,\tilde{t}}$, where \tilde{t} is equal to t except that $\tilde{t}(j^*) = 0$. By the update rules [\(4.21\)](#) and [\(4.22\)](#), all points $x \in R'_{c,t}$ have

$$(4.28) \quad \ell'_x = 2^{12} L(\ell_{c,\tilde{t}}/L)^{1/(d-\|\tilde{t}\|_0)},$$

$$(4.29) \quad s'_x = 48 \cdot 2^{\|\tilde{t}\|_0} \binom{d}{\|\tilde{t}\|_0} s_{c,\tilde{t}} \ell_{c,\tilde{t}} (\log_2 k) / L.$$

Denote the right-hand-sides of [\(4.28\)](#) and [\(4.29\)](#) as $\ell'_{c,t}$ and $s'_{c,t}$, respectively. We have

$$|\{\sigma'_x : x \in R'_{c,t}\}| \leq |\{\sigma'_x : x \in R_{c,\tilde{t}} \cap X_+ \cap X_1\}| \leq |\{\sigma_x : x \in R_{c,\tilde{t}} \cap X_+ \cap X_1\}| \leq s'_{c,t},$$

where the second inequality is because points in $R \cap X_+ \cap X_1$ with the same σ_x have the same σ'_x , and the last inequality is by [\(4.20\)](#) and [\(4.29\)](#). \square

Now we prove Lemma [4.2](#)

Proof. Since the preprocessing step preserves the validity of \mathcal{P} and does not increase $A(\mathcal{P})$, we assume w.l.o.g. that $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X}, (c_x)_{x \in X}, (s_x)_{x \in X}, (p_x)_{x \in X})$ is the subproblem *after* the preprocessing step. Assume w.l.o.g. $M_1^* \leq M_2^*$. Define $M = M(\mathcal{P})$, $M_1 = M^* + M(\mathcal{P}_1) - M_1^*$, and $M_2 = (M - M^*) + M(\mathcal{P}_2) - M_2^*$. By Lemma [4.7](#),

$$(4.30) \quad M^* \leq M_1 \leq M^* + M^*/2 \log(2k) \leq 3M^*/2 \leq 3M/4,$$

$$(4.31) \quad M^* \leq M - M^* \leq M_2,$$

$$(4.32) \quad m \leq M(\mathcal{P}_1) \leq M_1, \quad \text{and}$$

$$(4.33) \quad m \leq M(\mathcal{P}_2) \leq M_2.$$

Lemma [4.7](#), [\(4.30\)](#) and [\(4.31\)](#) give us

$$(4.34) \quad M_1 + M_2 \leq M + M^*/2 \log(2k) \leq M + \min\{M_1, M_2\}/2 \log(2k).$$

Define $R' = \{x \in X : t'_x \neq \perp\}$. We have

$$\begin{aligned} \sum_{x \in X \setminus R'} p'_x (\ell'_x)^2 - \sum_{x \in X \setminus R} p_x \ell_x^2 &= \sum_{x \in R_2 \cap X_+} p'_x (\ell'_x)^2 \\ &= \sum_{x \in R_2 \cap X_+} p_x \ell_x L \\ &\leq \sum_{x \in R \cap X_+} p_x \ell_x L (16 \log(2k) \log \log_2(2k))^{2-\|t_x\|_0} \end{aligned}$$

$$\text{(by Lemma 4.6)} \quad \leq 8M^* \log(M/M^*) \log \log_2(M/m)$$

$$\text{(by (4.30) and Claim A.2)} \quad \leq 16M_1 \log(M/M_1) \log \log_2(M/m)$$

$$\text{(by Definition 3.4 Item 2)} \quad \leq 16M_1 \log(M/M_1) \log \log_2(2k).$$

Therefore,

$$\begin{aligned}
& f(M(\mathcal{P}_1)) + f(M(\mathcal{P}_2)) + \sum_{x \in X \setminus R'} p'_x(\ell'_x)^2 - \sum_{x \in X \setminus R} p_x \ell_x^2 \\
& \text{(by (4.32), (4.33))} \leq f(M_1) + f(M_2) + 16M_1 \log(M/M_1) \log \log_2(2k) \\
& \leq 16(M_1(M_1/m)^{1/\log(2k)} + M_2(M_2/m)^{1/\log(2k)})(1 + \log(M/m)) \log \log_2(2k) \\
& \text{(by (4.34) and Claim A.1)} \leq 16M(M/m)^{1/\log(2k)}(1 + \log(M/m)) \log \log_2(2k) \\
& = f(M).
\end{aligned}$$

Rearranging the inequality above,

$$A(\mathcal{P}_1) + A(\mathcal{P}_2) = f(M(\mathcal{P}_1)) + f(M(\mathcal{P}_2)) + \sum_{x \in X \setminus R'} p'_x(\ell'_x)^2 \leq f(M) + \sum_{x \in X \setminus R} p_x \ell_x^2 = A(\mathcal{P}).$$

□

4.3 Building a decision tree The algorithm `post-process` we use to prove Theorem 4.1 is similar to `post-process_2d` in Section 3.3. We first construct an algorithm `decision_tree` similar to `decision_tree_2d`, except that it takes a subproblem \mathcal{P} in $d \geq 2$ dimensions and invokes the algorithm `single_cut` we developed in Section 4.2 instead of `single_cut_2d`. The algorithm `post-process` calls `decision_tree` on an initial subproblem $\tilde{\mathcal{P}}$ with centroid mass m , which we define as follows.

Given a k -clustering \mathcal{C} of points x_1, \dots, x_n consisting of centroids y_1, \dots, y_k , and an assignment mapping $\xi : [n] \rightarrow [k]$, the algorithm `post-process` computes the initial subproblem $\tilde{\mathcal{P}}$ by setting $X = \{x_1, \dots, x_n\}$, $Y = \{y_1, \dots, y_k\}$, $\sigma_{x_i} = y_{\xi(i)}$, $t_x(j) = 0, \forall j \in [d]$, $s_x = k$, $c_x = -1$, and

$$\begin{aligned}
\ell_x &= \begin{cases} 2^{\lceil \log_2 \|x - \sigma_x\|_\infty \rceil}, & \text{if } \|x - \sigma_x\|_\infty > 0; \\ 0, & \text{if } \|x - \sigma_x\|_\infty = 0; \end{cases} \\
p_x &= 2^{54} k^{1-2/d} d^3 (48 \log_2 k)^3.
\end{aligned}
\tag{4.35}$$

Set $m = \frac{1}{k} \sum_{x \in X} p_x \ell_x^2 (16(\log(2k))^2 \log \log_2(2k))^2$ so that $M(\tilde{\mathcal{P}})/m = 2k$. It is clear that $\tilde{\mathcal{P}}$ is valid and

$$A(\tilde{\mathcal{P}}) = O(k^{1-2/d} (\log k)^8 (\log \log_2(2k))^3 d^3) \cdot \text{cost}(\mathcal{C}). \tag{4.36}$$

After obtaining the output $((\delta_x)_{x \in X}, T)$ from `decision_tree`, `post-process` returns the decision tree T and a clustering \mathcal{C}' with centroids y_1, \dots, y_k and assignment mapping $\xi' : [n] \rightarrow [k]$ such that $y_{\xi'(i)} = \delta_{x_i}$.

Before we prove Theorem 4.1, we need the following lemma showing that the potential of a point never drops below 1:

LEMMA 4.8. *In the process of running algorithm `post-process`, whenever the algorithm `decision_tree` is called, the input subproblem $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X}, (c_x)_{x \in X}, (s_x)_{x \in X}, (p_x)_{x \in X})$ to `decision_tree` is valid and satisfies $\forall x \in X, p_x \geq 1$.*

Proof. The validity of \mathcal{P} follows from an induction using the validity of $\tilde{\mathcal{P}}$ and Lemma 4.1. Below we prove $\forall x \in X, p_x \geq 1$.

Fix a point x_v for $v \in [n]$. For $i \in \{0, 1, 2\}$ consider the moments when `decision_tree` is called with a subproblem $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X}, (c_x)_{x \in X}, (s_x)_{x \in X}, (p_x)_{x \in X})$ that satisfy $x_v \in X$ and $\|t_{x_v}\|_0 = i$. These moments may not exist, or there may be multiple such moments. However, as long as there is at least one such moment, the tuple $(s_{x_v}, p_{x_v}, \ell_{x_v}, t_{x_v})$ must be identical for all such moments, because algorithm `single_cut` always keeps $(s'_x, p'_x, \ell'_x, t'_x)$ equal to (s_x, p_x, ℓ_x, t_x) except when $t'_x = \perp \neq t_x$ or $\|t'_x\|_0 = \|t_x\|_0 + 1$. We use $(s(i), p(i), \ell(i))$ to denote the identical tuple $(s_{x_v}, p_{x_v}, \ell_{x_v})$ over all such moments. The diameter L of \mathcal{P} may not be identical over all such moments, so we use $L(i)$ to denote the value of L for the *last* such moment. We define $u(i) = L(i)/\ell(i)$. Similarly, we use $(s(\perp), p(\perp))$ to denote the identical value of (s_{x_v}, p_{x_v}) whenever $t_{x_v} = \perp$.

Our goal is to show each of $p(0), p(1), p(2), p(\perp)$, whenever exists, is at least 1.

For $i \in \{0, 1, 2\}$, whenever $p(i)$ exists, by (4.23) we have

$$(4.37) \quad p(i) = p(0) / \prod_{i'=0}^{i-1} (2^{24} u(i')^{1-2/(d-i')}) \geq p(0) 2^{-24i} / \left(\prod_{i'=0}^{i-1} u(i') \right)^{1-2/d}.$$

By (4.21) we have

$$1 \leq s(i) \leq k \prod_{i'=0}^{i-1} \left(48 \cdot 2^{i'} \binom{d}{i'} (\log_2 k) / u(i') \right).$$

Therefore,

$$\prod_{i'=0}^{i-1} u(i') \leq k \prod_{i'=0}^{i-1} \left(48 \cdot 2^{i'} \binom{d}{i'} \log_2 k \right).$$

Combining this with (4.35) and (4.37),

$$(4.38) \quad \begin{aligned} p(0) &= 2^{54} k^{1-2/d} d^3 (48 \log_2 k)^3 \geq 65^2 > 1, \\ p(1) &\geq 2^{30} d^3 (48 \log_2 k)^2 \geq 65^2 > 1, \\ p(2) &\geq 2^5 d^2 (48 \log_2 k) \geq 65^2 > 1. \end{aligned}$$

Finally, we show $p(\perp) \geq 1$ whenever $p(\perp)$ exists. If the transition of t_{x_v} to \perp happens at preprocessing, it is clear that $p(\perp) \geq \min\{p(0), p(1), p(2)\} / 65^2 \geq 1$. Otherwise, by (4.23) and (4.24) we have

$$(4.39) \quad p(\perp) = p(0) / \left(4u(2) \prod_{i=0}^1 (2^{24} u(i)^{1-2/(d-i)}) \right) = p(0) 2^{-50} / (u(0)^{1-2/d} u(1)^{1-2/(d-1)} u(2)).$$

By (4.21), we have

$$1 \leq s(\perp) \leq k \prod_{i=0}^2 \left(48 \cdot 2^i \binom{d}{i} (\log_2 k) / u(i) \right).$$

Therefore,

$$(4.40) \quad u(0)u(1)u(2) \leq 4kd^3 (48 \log_2 k)^3.$$

From the update rule (4.22), we know

$$u(2) = \frac{L(2)}{\ell(2)} \leq \frac{L(1)}{\ell(2)} = u(1)^{1/(d-1)} 2^{-12} \leq u(1)^{1/(d-1)},$$

which implies

$$u(2)^{2/d} \leq u(1)^{2/(d(d-1))} = u(1)^{2/(d-1)-2/d}.$$

Therefore,

$$(4.41) \quad u(0)^{1-2/d} u(1)^{1-2/(d-1)} u(2) \leq u(0)^{1-2/d} u(1)^{1-2/d} u(2)^{1-2/d} \leq 4k^{1-2/d} d^3 (48 \log_2 k)^3,$$

where the last inequality is by (4.40). Plugging (4.38) and (4.41) into (4.39), we get $p(\perp) \geq 1$, as desired. \square

LEMMA 4.9. *In the process of running algorithm **post-process**, whenever **decision_tree** is called with input being subproblem $\mathcal{P} = (X, Y, (\sigma_x)_{x \in X}, (\ell_x)_{x \in X}, (t_x)_{x \in X}, (c_x)_{x \in X}, (s_x)_{x \in X}, (p_x)_{x \in X})$, the output $((\delta_x)_{x \in X}, T)$ of **decision_tree** satisfies the following properties. The decision tree T has at most $|Y|$ leaves. For every leaf v of the decision tree T and every pair of points $x, x' \in X$ in the region defined by v , we have $\delta_x = \delta'_x$. Moreover, $\sum_{x \in X} \|x - \delta_x\|_\infty^2 \leq A(\mathcal{P})$.*

Proof. The proof is essentially the same as the proof of Lemma 3.9. The only difference is that when $L = 0$, to prove $\sum_{x \in X} \|x - \delta_x\|_\infty^2 \leq A(\mathcal{P})$, we need $p_x \geq 1$ from Lemma 4.8. \square

Now we finish the proof of Theorem 4.1.

Proof. The proof is essentially the same as the proof of Theorem 3.1 except that we use Lemma 4.6 instead of Lemma 3.7, and Lemma 4.9 instead of Lemma 3.9. In particular, the cost of the explainable clustering \mathcal{C}' is bounded as follows:

$$\begin{aligned} \text{cost}(\mathcal{C}') &= \sum_{i=1}^n \|x_i - y_{\xi'(i)}\|_2^2 \leq d \sum_{i=1}^n \|x_i - y_{\xi'(i)}\|_\infty^2 = d \sum_{i=1}^n \|x_i - \delta_{x_i}\|_\infty^2 \leq dA(\tilde{\mathcal{P}}) \\ &\leq O(k^{1-2/d}(\log k)^8(\log \log_2(2k))^3 d^4) \text{cost}(\mathcal{C}). \end{aligned}$$

□

5 Lower Bound

We prove a lower bound of $k^{1-2/d}/\text{polylog}(k)$ on the competitive ratio for d -dimensional explainable k -means for all $k, d \geq 2$ (Theorem 5.1). Our proof is based on a construction by [37] summarized in Lemma 5.1 below. For brevity, we do not repeat its proof here. The construction allows us to show a competitive ratio lower bound depending on two other parameters p and b in Lemma 5.2. We then prove Theorem 5.1 by specifying the values of p and b .

LEMMA 5.1. ([37]) *Let b, p be positive integers satisfying $b \geq 3$. There exists b^p points in p dimensions with the following properties:*

1. *For every $j \in [p]$, the j -th coordinate of the b^p points form a permutation of $\{0, \dots, b^p - 1\}$.*
2. *The ℓ_2 distance between any two of the points is at least $b^{p-1}/2$.*

LEMMA 5.2. *Given positive integers k, d, p, b satisfying $p \leq d, b \geq 3, b^p \leq k$, there exists a set of points in d dimensions for which any k -explainable clustering has competitive ratio $\Omega(b^{p-2}/p)$ for the k -means cost.*

Proof. When $p = 1$, it is trivial to show a competitive ratio lower bound of $1 = \Omega(b^{p-2}/p)$, so we assume $p \geq 2$.

Let Z denote the set of b^p points \mathbb{R}^p from Lemma 5.1. Every point $z \in Z$ creates a point $u(z) \in \mathbb{R}^d$, where the first p coordinates of $u(z)$ are equal to the p coordinates of z , and the remaining $d - p$ coordinates of $u(z)$ are zeros. Let $Y_1 = \{u(z) : z \in Z\}$ be the resulting set of b^p points in \mathbb{R}^d . We construct a set $Y_2 \subseteq \mathbb{R}^d$ consisting of $k - b^p$ points that are sufficiently far away from each other and from the points in Y_1 .

For every $y \in Y_1$, we create a set X_y consisting of $2p$ points in \mathbb{R}^d as follows: for every $j \in [p]$, X_y contains 2 points $y_j^+, y_j^- \in \mathbb{R}^d$ by adding $2/3$ and $-2/3$ to the j -th coordinate of y . For every $y \in Y_2$, we define X_y to be the set containing only y itself.

Given the $2pb^p + (k - b^p)$ points in $\bigcup_{y \in Y_1 \cup Y_2} X_y$, there exists a k -clustering \mathcal{C} with $\text{cost}(\mathcal{C}) = O(pb^p)$ by choosing $Y_1 \cup Y_2$ to be the centroids and assigning $x \in X_y$ to centroid y for every $y \in Y_1 \cup Y_2$. On the other hand, by Lemma 5.1 Item 1, for any k -explainable clustering \mathcal{C}' , there exist two points $x \in X_y, x' \in X_{y'}$ assigned to the same centroid in \mathcal{C}' with *distinct* $y, y' \in Y_1 \cup Y_2$ (otherwise, since $|Y_1 \cup Y_2| = k$, for every $y \in Y_1$ there exists a centroid in \mathcal{C}' to which all points in X_y are assigned, and by Lemma 5.1 Item 1 and the explainability of \mathcal{C}' , all the points in $\bigcup_{y \in Y_1} X_y$ must be assigned to the same centroid in \mathcal{C}' , a contradiction). By Lemma 5.1 Item 2,

$$\|x - x'\|_2 \geq \|y - y'\|_2 - 4/3 \geq b^{p-1}/2 - 4/3 \geq \Omega(b^{p-1}).$$

Therefore, $\text{cost}(\mathcal{C}') \geq \|x - x'\|_2^2/2 \geq \Omega(b^{2p-2})$. The competitive ratio is thus lower bounded by $\Omega(b^{p-2}/p)$. □

THEOREM 5.1. *For every $k, d \geq 2$, there exists a set of points in d dimensions for which any k -explainable clustering has competitive ratio $\Omega(k^{1-2/d}(\log k)^{-5/3} \log \log(2k))$ for the k -means cost.*

Proof. We can assume $k \geq 3$ w.l.o.g. because it is trivial to show a competitive ratio lower bound of 1.

We specify the integers b and p in Lemma 5.2 to get concrete lower bounds for the competitive ratio.

When $k^{1/d} \geq 3d$, we choose $p = d$ and $b = \lfloor k^{1/p} \rfloor$. It is clear that $b \geq 3p$, so

$$b^p = (b+1)^p / (1+1/b)^p \geq k / \exp(p/b) \geq \Omega(k).$$

This implies that $b^{p-2} = b^p/b^2 \geq \Omega(k^{1-2/d})$. Lemma 5.2 gives us a competitive ratio lower bound of

$$\Omega(b^{p-2}/p) \geq \Omega(k^{1-2/d}/d) \geq \Omega(k^{1-2/d}(\log k)^{-1} \log \log k),$$

where the last inequality is by Claim A.4

When $(\log k)^{2/3}/\log \log k \leq k^{1/d} < 3d$, we choose p to be the maximum integer such that $k^{1/p} \geq 3p$, and choose $b = \lfloor k^{1/p} \rfloor$. Again we have $b \geq 3p$, so $b^p \geq \Omega(k)$. We also have $b \leq k^{1/p} \leq (k^{1/(p+1)})^{1+1/p} \leq (p+1)^{1+1/p} \leq O(p) = O(\log k/\log \log k)$, where the last inequality is by Claim A.4. This implies $b^{p-2}/p = b^p/(b^2 p) \geq \Omega(k(\log k)^{-3}(\log \log k)^3)$. The competitive ratio lower bound from Lemma 5.2 is

$$\Omega(b^{p-2}/p) \geq \Omega(k(\log k)^{-3}(\log \log k)^3) \geq \Omega(k^{1-2/d}(\log k)^{-5/3} \log \log k).$$

When $3 \leq k^{1/d} < (\log k)^{2/3}/\log \log k$, we choose $b = \lceil k^{1/d} \rceil$ and $p = \lfloor \log_b k \rfloor$. We have $b \leq 2k^{1/d}$ and thus $b^{p-2} = b^{p+1}/b^3 \geq k/b^3 \geq k^{1-3/d}/8$. The competitive ratio lower bound from Lemma 5.2 is

$$\Omega(b^{p-2}/p) \geq \Omega(k^{1-3/d}/p) \geq \Omega(k^{1-3/d}/d) \geq \Omega(k^{1-3/d}/\log k) \geq \Omega(k^{1-2/d}(\log k)^{-5/3} \log \log k).$$

When $k^{1/d} < 3$, we choose $b = 3$ and $p = \lfloor \log_3 k \rfloor$. We have $b^{p-2} = b^{p+1}/b^3 \geq k/27$. The competitive ratio lower bound from Lemma 5.2 is

$$\Omega(b^{p-2}/p) \geq \Omega(k/p) \geq \Omega(k/\log k) \geq \Omega(k^{1-2/d}(\log k)^{-1}).$$

□

A Helper lemmas and claims

CLAIM A.1. Define $\alpha(z) = z^{1+2u}$ for $u \in (0, 1/2)$. Suppose non-negative real numbers z_1, z_2, z, Δ satisfy $z_1 + z_2 \leq z + u\Delta$, and $\Delta \leq \min\{z_1, z_2\}$. Then $\alpha(z_1) + \alpha(z_2) \leq \alpha(z)$.

Proof. Assume w.l.o.g. $z_1 \leq z_2$. By the monotonicity and convexity of α , we have

$$\alpha(z_1) + \alpha(z_2) \leq \alpha(z_1) + \alpha(z + u\Delta - z_1) \leq \alpha(\Delta) + \alpha(z + u\Delta - \Delta).$$

We only need to prove that

$$(A.1) \quad \Delta^{1+2u} + (z - (1-u)\Delta)^{1+2u} \leq z^{1+2u}.$$

Note that $0 \leq \Delta \leq z/(2-u)$ because $2\Delta \leq z_1 + z_2 \leq z + u\Delta$. Since the left-hand-side is convex in Δ , we just need to check (A.1) when $\Delta = 0$ and $\Delta = z/(2-u)$. It reduces to checking $1 + 2u \geq \frac{\log 2}{\log(2-u)}$. This holds by a standard calculation using our assumption $u \in (0, 1/2)$. □

CLAIM A.2. If $0 \leq u \leq v \leq 3M/4$, then $u \log(M/u) \leq 2v \log(M/v)$.

Proof. The function $\alpha(z) = z \log(M/z)$ is non-decreasing when $z \leq M/e$, and non-increasing when $z \geq M/e$. We just need to check the claim for $u = M/e$ and $v = 3M/4$, which follows from a standard calculation. □

CLAIM A.3. Let $I_1, \dots, I_n \subseteq \mathbb{R}$ be intervals. There exists $S \subseteq [n]$ such that $I_u \cap I_v = \emptyset$ for all distinct $u, v \in S$ and

$$|\bigcup_{u \in [n]} I_u| \leq 3|\bigcup_{v \in S} I_v|.$$

This claim is a special form of the Vitali covering lemma. For completeness, we give a proof of it as follows.

Proof. Assume w.l.o.g. that $|I_1| \geq \dots \geq |I_n|$. For $u = 1, \dots, n$, construct $S_u \subseteq [u]$ inductively as follows. We set $S_1 = \{1\}$, and for every $u > 1$, we set $S_u = S_{u-1}$ if there exists $v \in S_{u-1}$ such that $I_u \cap I_v \neq \emptyset$, and set $S_u = S_{u-1} \cup \{u\}$ otherwise. Define $S = S_n$. It is clear that $I_u \cap I_v = \emptyset$ for all distinct $u, v \in S$.

For every $u \in [n] \setminus S$, there exists $\alpha(u) \in S$ such that $\alpha(u) < u$ and $I_{\alpha(u)} \cap I_u \neq \emptyset$. We define $\alpha(u) = u$ when $u \in S$. For every $v \in S$ and $u \in \alpha^{-1}(v) \setminus \{v\}$, we have $I_v \cap I_u \neq \emptyset$ and $|I_u| \leq |I_v|$. Therefore, $|\bigcup_{u \in \alpha^{-1}(v)} I_u| \leq 3|I_v|$. We have

$$|\bigcup_{u \in [n]} I_u| = |\bigcup_{v \in S} \bigcup_{u \in \alpha^{-1}(v)} I_u| \leq \sum_{v \in S} |\bigcup_{u \in \alpha^{-1}(v)} I_u| \leq \sum_{v \in S} 3|I_v| = 3|\bigcup_{v \in S} I_v|.$$

□

LEMMA A.1. ([53]) Let m, M be positive real numbers with $M \geq 2m$. Suppose $U : (0, L) \rightarrow [m, M/2]$ is a non-decreasing function, and there is a finite set $I \subseteq (0, L)$ such that U is differentiable over $(0, L) \setminus I$. Then, there exists $z \in (0, L) \setminus I$ such that $U'(z) \leq (1/L)U(z) \log \frac{M}{U(z)} \log \log_2 \frac{M}{m}$.

Proof. Consider the function $\alpha(z) := -\log \log_2 \frac{M}{U(z)}$. It is clear that $\alpha(z)$ is non-decreasing and differentiable over $(0, L) \setminus I$. The function has derivative

$$\alpha'(z) = \frac{U'(z)}{U(z) \log(M/U(z))}.$$

Suppose there does not exist such $z \in (0, L) \setminus I$ that makes the desired inequality hold. This implies that the derivative of $\alpha(z)$ exceeds $(1/L) \log \log_2 \frac{M}{m}$ whenever $z \in (0, L) \setminus I$. This contradicts with the fact that $\alpha(z)$ is bounded between $-\log \log_2(M/m)$ and 0. \square

LEMMA A.2. ([53]) Let m, M be positive real numbers with $M \geq 2m$. Suppose $V : (0, L) \rightarrow [m, M - m]$ is a non-decreasing function, and there is a finite set $I \subseteq (0, L)$ such that V is differentiable over $(0, L) \setminus I$. Then, there exists $z \in (0, L) \setminus I$ such that $V'(z) \leq (2/L)M' \log \frac{M}{M'} \log \log_2 \frac{M}{m}$, where $M' = \min\{V(z), M - V(z)\}$.

Proof. When $V(L/2) \leq M/2$, the lemma follows from Lemma A.1 by setting $U(z) = V(z/2)$. When $V(L/2) \geq M/2$, the lemma follows from Lemma A.1 by setting $U(z) = M - V(L - z/2)$. \square

CLAIM A.4. For real numbers $k \geq 3$ and $p > 0$, if $k^{1/p} \geq p$, then $p \leq 2 \log k / \log \log k$.

Proof. Assume for the sake of contradiction that $p > 2 \log k / \log \log k$, then $k^{1/p} < (\log k)^{1/2}$. Therefore,

$$p/k^{1/p} > 2(\log k)^{1/2} / \log \log k = (\log k)^{1/2} / \log((\log k)^{1/2}) \geq 1,$$

a contradiction. \square

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