

# Min-Sum Clustering (With Outliers)

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## Abstract

We give a constant factor polynomial time pseudo-approximation algorithm for min-sum clustering with or without outliers. The algorithm is allowed to exclude an arbitrarily small constant fraction of the points. For instance, we show how to compute a solution that clusters 98% of the input data points and pays no more than a constant factor times the optimal solution that clusters 99% of the input data points. More generally, we give the following bicriteria approximation: For any  $\epsilon > 0$ , for any instance with  $n$  input points and for any positive integer  $n' \leq n$ , we compute in polynomial time a clustering of at least  $(1 - \epsilon)n'$  points of cost at most a constant factor greater than the optimal cost of clustering  $n'$  points. The approximation guarantee grows with  $\frac{1}{\epsilon}$ . Our results apply to instances of points in real space endowed with squared Euclidean distance, as well as to points in a metric space, where the number of clusters, and also the dimension if relevant, is arbitrary (part of the input, not an absolute constant).

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## 1 Introduction

We consider min-sum  $k$ -clustering. This is the problem of partitioning an input dataset of  $n$  points into  $k$  clusters with the objective of minimizing the sum of intra-cluster pairwise distances. We consider primarily the prevalent setting of instances of points in  $\mathbb{R}^d$  endowed with a distance function equal to the squared Euclidean distance (henceforth referred to as the  $\ell_2^2$  case). Our results apply also to the case of instances of points endowed with an explicit metric (henceforth referred to as the metric case). Note that we consider  $k$  (and  $d$ , if relevant) to be part of the input, rather than an absolute constant. In these and similar cases we give polynomial time approximation algorithms that cluster all but a negligible constant fraction



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of outliers at a cost that is at most a constant factor larger than the optimum clustering. More specifically, for any  $\epsilon > 0$ , if the optimum we compete against is required to cluster any number  $n' \leq n$  of points, our algorithm clusters at least  $(1 - \epsilon)n'$  points and at most  $n'$  points, and pays a constant factor more than the optimum for  $n'$  points. The constant depends on  $\epsilon$ .

Clustering in general is a fundamental question in unsupervised learning. The question originated in the social sciences and now is widely applicable in data analysis and machine learning, in areas including bioinformatics, computer vision, pattern recognition, signal processing, fraud/spam/fake news filtering, and market/population segmentation. Clustering is also a list of fundamental discrete optimization problems in computational geometry that have been studied for decades by theoreticians, in particular (but not exclusively) as simple non-convex targets of machine learning. Some clustering problems, notably centroid-based criteria such as  $k$ -means, have been studied extensively. We currently have a fairly tight analysis of their complexity in the worst case (e.g. [4, 42, 1, 20]) and under a wide range of restrictive conditions: low dimension (e.g., [33, 21, 30]) fixed  $k$  (e.g. [41, 27, 17, 26]), various notions of stability (e.g. [44, 7, 40, 5, 22]), restrictive models of computation (e.g., [16, 3, 15, 14]), etc., as well as practically appealing heuristics (e.g., Lloyd's iteration, local search) and supportive theoretical justification (e.g., some of the afore-mentioned papers and also [6, 38]). Theoretical understanding of density-based clustering criteria, and in particular min-sum clustering, is far less developed. There are clearly cases in practice where, for instance, min-sum clustering coincides far better with the intuitive clustering objective than standard centroid-based criteria. A simple illustrative example is the case of separating two concentric dense rings of points in the plane. Moreover, min-sum clustering satisfies Kleinberg's consistency axiom, whereas a fairly large class of centroid-based criteria including  $k$ -means and  $k$ -median do not satisfy this axiom [39, 47]. However, the state-of-the-art for computing min-sum clustering remains inferior to alternatives. Min-sum  $k$ -clustering is NP-hard in the  $\ell_2^2$  case (e.g., using arguments from [4]), and also for the metric case (see [29]), even for  $k = 2$ . In the  $\ell_2^2$  case, it can be solved in polynomial time if both  $d$  and  $k$  are absolute constants [35]. In the metric case with arbitrary  $k$ , approximating min-sum clustering to within a factor better than 1.415 is NP-hard [31, 19]. If  $k$  is a fixed constant, the problem admits a PTAS, both in the  $\ell_2^2$  case and in the metric case [28]; see also [32, 36, 43, 45] for previous work in this vein. Hassin and Or [34] gave a 2-factor approximation algorithm for the metric penalized  $k$ -min-sum problem where  $k$  is a constant. If  $k = o(\log n / \log \log n)$ , then there is a constant factor approximation algorithm for the  $\ell_2^2$  case [23]. In the metric case, assuming that  $k = o(\log n / \log \log n)$  and the instance satisfies a certain clusterability/stability condition, a partition close to optimal can be computed in polynomial time [8, 9] (see also [46] for some applications and experimental results in this vein). We note that practical applications often require the number of clusters i.e.,  $k$  too many, so the above restrictions on  $k$  are unrealistic in those cases. In the worst case, and under no restrictions on the instance, the best known approximation guarantee known is an  $O(\log n)$  approximation algorithm [13] for the metric case. This improves upon a slightly worse and much earlier guarantee [12]. In both papers, the factor is derived from representing the input metric space approximately as a convex combination of hierarchically separated tree (HST) metrics [10, 11, 25]. This incurs logarithmic distortion, which is asymptotically tight in the worst case. In HST metrics, min-sum clustering can be approximated to within a constant factor. Thus, a fundamental challenge of the study of min-sum clustering is to eliminate the gap between the hardness of approximation lower bound of 1.415 and the approximation guarantee upper bound of  $O(\log n)$ . We show that a constant factor approximation is possible, if one is willing to regard as outliers a small fraction of the input dataset. For the  $\ell_2^2$  case, we are not aware of any previous non-trivial guarantee for  $k \gg \log n / \log \log n$ .

Our results are derived using a reduction from min-sum clustering to a centroid-based criterion with (soft) capacity constraints. This can be done exactly in the  $\ell_2^2$  case, and approximately in the metric case, though to get polynomial time algorithms we use an approximation in both cases. This reduction underlies also some of the above-mentioned previous results on min-sum clustering. The outcome of this reduction is a  $k$ -median or  $k$ -means problem with non-uniform capacities. If we are aiming for a constant factor approximation then we can afford to violate the capacities by a constant factor. There are nice results on approximating  $k$ -median with non-uniform capacities, for instance [24]. Unfortunately, these results do not seem applicable here, because their input is a metric space. The reduction, even for the metric case, does not generate a metric instance of capacitated  $k$ -median (the triangle inequality is violated unboundedly). Nevertheless, we do draw some ideas from this literature. Our min-sum clustering algorithm is based on the well-trodden path of using the primal-dual schema repeatedly to search for a good Lagrange multiplier in lagrangian relaxation of the problem (see [37] for the origin of this method). The dual program has a variable for every data point, and a constraint for every possible cluster. The dual ascent process requires detection of constraints that become tight. In our case, this is a non-trivial problem, which we solve only approximately. As usual, the dual values are used to “buy” the opening of the clusters that become tight, and we have to contend with points contributing simultaneously to multiple clusters. This is done, as usual, by creating a conflict graph among the tight clusters and choosing an independent set in this graph. However, in our case there are unusual complications. The connection cost is a distance (not a metric in the  $\ell_2^2$  case, but this is a minor concern) multiplied by the cardinality of the cluster. If there is a conflict between a large cluster and some small clusters, we have the following dilemma. If we open the large cluster, the unclustered points in the small clusters may lack dual “money” to connect to the large cluster; they can only afford the distance multiplied by the cardinality of their small cluster. If, on the other hand, we open (some or all of) the small clusters, assigning the unclustered points in the large cluster to those small clusters might inflate their cardinality by a super-constant factor, leaving all points with insufficient funds to connect to the inflated clusters.

We resolve this dilemma as follows (using in part some ideas from [18]). We open larger clusters first, so if a cluster is not opened, it is smaller than the conflicting cluster that blocked it. Unclustered points are not assigned to the blocking cluster, but rather aggregated around each blocking cluster to form their own clusters of appropriate cardinality. We use approximate cardinality, in scales which are powers of a constant  $b$ . As we require the Lagrange multiplier preserving (LMP) property, we must have sufficient “funds” to pay the opening costs in full (but can settle for paying just a fraction of the connection cost). This is possible if in a scale of, say,  $b^p$  we have, say, at least  $b^{2+p}$  unclustered points in clusters of scaled cardinality  $b^p$  (each set of roughly this size can afford to open its own cluster). If a blocking cluster is blocking fewer points in this scale, we can’t afford to cluster them and must discard them as outliers. This is the primary source of the excess outliers.

As usual, the search for a good Lagrange multiplier may end with two integer primal solutions, one with fewer than  $k$  clusters and one with more than  $k$  clusters, whose convex combination is a feasible fractional bipoint solution to the  $k$ -clustering problem. In our case, as we already may have to give up on some outliers, we can simply output either the  $< k$  solution or the  $k$  largest clusters in the  $> k$  solution. We point out that these extra outliers can be avoided by using a more sophisticated “rounding” of the bipoint solution, but given our loss in the primal-dual phase, it would not improve meaningfully our guarantees.

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The above description sums up the algorithm in the case that  $n' = n$ . Our result also extends to the case that the optimal solution is also allowed to discard some outliers (we may have to discard some more). The main additional issue in the case  $n' < n$  is that in the primal-dual phase we may open a cluster that brings the number of clustered points from below  $n'$  to above  $n'$ . In this case, some points in this last cluster need to be discarded, but then the remaining clustered points might have insufficient “funds” to open the last cluster. If we have many clusters, we can afford to eliminate the smallest cluster, declaring its points as outliers, and use the dual values of the points in that cluster to pay for opening the last one. If there is a small number of clusters, we may assume that the primal-dual phase opened less than  $k$  clusters (to ensure this property, if  $k$  is a small constant, we employ the known PTAS; thus we can assume that  $k$  is large). Our approach in this case draws from [2], where a similar issue is addressed in the case of the sum-of-radii  $k$ -clustering problem. Though the questions are quite different, we use a similar idea of computing a (slightly) non-Lagrange multiplier preserving approximation to the lagrangian relaxation. The LMP property is regularly used in the argument that the bipoint solution is both feasible and cheap; the approach we adopt requires an extra argument to bound the cost of a bipoint solution that incorporates a non-LMP solution.

The rest of the paper is organized as follows. Section 2 introduces some basic definitions and claims. Section 3 describes the algorithm. Section 4 analyzes the algorithm. For conciseness, the paper presents the  $\ell_2^2$  case. Our main result is Theorem 8. The metric case is essentially identical, and is briefly explained in Theorem 9. We note that we made no effort to optimize the constant factor guarantees, throughout the paper.

### 2 Definitions and Preliminary Claims

Consider an instance of min-sum clustering that is defined by a set of points  $X \subset \mathbb{R}^d$  and a target number of clusters  $k \in \mathbb{N}$ . Let  $n = |X|$ . The cost of a cluster  $Y \subset X$  is

$$\text{cost}(Y) = \frac{1}{2} \cdot \sum_{x,y \in Y} \|x - y\|_2^2.$$

The center of mass (or mean) of  $Y$  is  $\text{cm}(Y) = \frac{1}{|Y|} \cdot \sum_{x \in Y} x$ . The following proposition is a well-known fact (for instance, see [35]).

► **Proposition 1.** *The following assertions hold for every finite set  $Y \subset \mathbb{R}^d$ .*

1. *The center of mass  $\text{cm}(Y)$  is the unique minimizer of  $\sum_{x \in Y} \|x - y\|_2^2$  over  $y \in \mathbb{R}^d$ .*
2.  *$\text{cost}(Y) = |Y| \cdot \sum_{x \in Y} \|x - \text{cm}(Y)\|_2^2$ .*

A *min-sum  $k$ -clustering* of  $X$  is a partition of  $X$  into  $k$  disjoint subsets  $X_1, X_2, \dots, X_k$  that minimizes over all possible partitions

$$\sum_{i=1}^k \text{cost}(X_i) = \sum_{i=1}^k |X_i| \cdot \sum_{x \in X_i} \|x - \text{cm}(X_i)\|_2^2.$$

In the version allowing outliers, we are given a target  $n' \leq n$  of the number of points to cluster, and we are required that  $|\bigcup_{i=1}^k X_i| \geq n'$ . Clearly, the version without outliers is a special case of the version with outliers with  $n' = n$ . Let  $\text{opt}(X, n', k)$  denote the optimal min-sum cost of clustering  $n'$  points in  $X$  into  $k$  clusters. Formally, we can express the goal

as a problem of optimizing an exponential size integer program:

$$\begin{aligned}
& \text{minimize} && \sum_{Y \subset X} \text{cost}(Y) \cdot z_Y \\
& \text{s.t.} && \sum_{Y \ni x} z_Y + w_x \geq 1 \quad \forall x \in X \\
& && \sum_{Y \subset X} z_Y \leq k \\
& && \sum_{x \in X} w_x \leq n - n' \\
& && z_Y \in \{0, 1\} \quad \forall Y \subset X \\
& && w_x \in \{0, 1\} \quad \forall x \in X.
\end{aligned} \tag{1}$$

Fix  $b \in \mathbb{N}$ ,  $b > 1$ . For  $i \in \mathbb{N}$ , let  $\text{floor}_b(i) = b^{\lfloor \log_b i \rfloor}$ . For  $Y \subset X$ , let  $\text{ctr}(Y)$  be a reference point that we set for now as  $\text{ctr}(Y) = \text{cm}(Y)$ . Define

$$\text{cost}_b(Y) = \text{floor}_b(|Y|) \cdot \sum_{y \in Y} \|y - \text{ctr}(Y)\|_2^2.$$

In other words, (assuming  $\text{ctr}(Y) = \text{cm}(Y)$ ) we revise  $\text{cost}(Y)$  by rounding  $|Y|$  down to the nearest power of  $b$ . Thus,  $\frac{1}{b} \cdot \text{cost}(Y) < \text{cost}_b(Y) \leq \text{cost}(Y)$ . We relax the integer program (1) as follows ( $b$  to be determined later):

$$\begin{aligned}
& \text{minimize} && \sum_{Y \subset X} \text{cost}_b(Y) \cdot z_Y \\
& \text{s.t.} && \sum_{Y \ni x} z_Y + w_x \geq 1 \quad \forall x \in X \\
& && \sum_{Y \subset X} z_Y \leq k \\
& && \sum_{x \in X} w_x \leq n - n' \\
& && z_Y \geq 0 \quad \forall Y \subset X \\
& && w_x \geq 0 \quad \forall x \in X.
\end{aligned} \tag{2}$$

Then, following a well-traveled path, we lagrangify the constraint on the number of clusters to get the following lagrangian relaxation ( $\lambda$  denotes the unknown Lagrange multiplier).

$$\begin{aligned}
& \text{minimize} && \sum_{Y \subset X} \text{cost}_b(Y) \cdot z_Y + \lambda \cdot (\sum_{Y \subset X} z_Y - k) \\
& \text{s.t.} && \sum_{Y \ni x} z_Y + w_x \geq 1 \quad \forall x \in X \\
& && \sum_{x \in X} w_x \leq n - n' \\
& && z_Y \geq 0 \quad \forall Y \subset X \\
& && w_x \geq 0 \quad \forall x \in X.
\end{aligned} \tag{3}$$

For fixed  $\lambda$ , this is a linear program, and its dual is:

$$\begin{aligned}
& \text{maximize} && \sum_{x \in X} \alpha_x - \gamma \cdot (n - n') - \lambda \cdot k \\
& \text{s.t.} && \sum_{x \in Y} \alpha_x \leq \lambda + \text{cost}_b(Y) \quad \forall Y \subset X \\
& && 0 \leq \alpha_x \leq \gamma \quad \forall x \in X.
\end{aligned} \tag{4}$$

Notice that the linear program (3) can be interpreted as a relaxation of the “facility location” version of the problem, with  $\lambda$ -uniform cluster opening costs.

► **Lemma 2.** *For any  $\lambda$ , the optimal value of the linear program (4) is a lower bound on the optimal value of the integer program (1).*

**Proof.** Consider any optimal solution  $(z, w)$  to the integer program (1). Notice that we may assume that  $\sum_{Y \subset X} z_Y = k$ , otherwise we can split some clusters to get exactly  $k$  of them. Splitting clusters cannot increase the cost of the solution. This is also a feasible solution to the linear program (3). Moreover, the Lagrange term  $\lambda \cdot (\sum_{Y \subset X} z_Y - k)$  zeroes out, and  $\sum_{Y \subset X} \text{cost}_b(Y) \cdot z_Y \leq \sum_{Y \subset X} \text{cost}(Y) \cdot z_Y$ . By weak duality, the value of any feasible solution to the dual program (4) is a lower bound on the value of any feasible solution to the linear program (3). ◀

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An obvious issue with the dual program (4) is that the number of constraints is exponential in  $n$ . We want to construct a dual solution by growing the dual variables, however, it is not clear how to detect new tight dual constraints without enumerating over the  $\exp(n)$  number of constraints. We now address this issue. First consider the following fact.

► **Proposition 3.** *Let  $Y$  be a finite set of points in  $\mathbb{R}^d$ . There exists  $y \in Y$  such that  $\sum_{x \in Y} \|x - y\|_2^2 \leq 2 \cdot \sum_{x \in Y} \|x - \text{cm}(Y)\|_2^2$ . (We note that the factor of 2 can be improved to  $1 + \epsilon$ , for any  $\epsilon > 0$ , using the center of mass of  $O(1/\epsilon^2)$  points in  $Y$ , e.g. [35, 28].)*

**Proof sketch.** Notice that for every  $y \in \mathbb{R}^d$ ,

$$\sum_{x \in Y} \|x - y\|_2^2 \leq \sum_{x \in Y} \|x - \text{cm}(Y)\|_2^2 + |Y| \cdot \|y - \text{cm}(Y)\|_2^2$$

(see [44]). Thus, by picking  $y \in Y$  that minimizes  $\|y - \text{cm}(Y)\|_2^2$ , the proposition follows. ◀

An immediate consequence of Proposition 3 is that  $\mathcal{F} = X$  is a set of  $n$  points in  $\mathbb{R}^d$ , such that for every  $Y \subset X$  there exists a point  $c_Y \in \mathcal{F}$  such that

$$\sum_{x \in Y} \|x - \text{cm}(Y)\|_2^2 \leq \sum_{x \in Y} \|x - c_Y\|_2^2 \leq 2 \cdot \sum_{x \in Y} \|x - \text{cm}(Y)\|_2^2. \quad (5)$$

(We can improve the factor of 2 to any constant  $1 + \epsilon$  by increasing the size of  $\mathcal{F}$  to  $n^{O(1/\epsilon^2)}$ .) Now, given  $\mathcal{F}$ , set initially  $\text{ctr}(Y) = c_Y$  for all  $Y \subset X$ . Notice that this puts  $\text{cost}_b(Y) = \text{floor}_b(|Y|) \cdot \sum_{y \in Y} \|y - c_Y\|_2^2$ . We consider the following revised dual program.

$$\begin{aligned} & \text{maximize} && \sum_{x \in X} \alpha_x - \gamma \cdot (n - n') - \lambda \cdot k \\ & \text{s.t.} && \sum_{x \in Y} \alpha_x \leq \lambda + \text{floor}_b(|Y|) \cdot \sum_{x \in Y} \|x - y\|_2^2 \quad \forall Y \subset X, \forall y \in Y \\ & && 0 \leq \alpha_x \leq \gamma \quad \forall x \in X. \end{aligned} \quad (6)$$

► **Lemma 4.** *For any  $\lambda$ , the optimal value of the linear program (6) is at most twice the optimal value of the integer program (1).*

**Proof.** The dual of the linear program (6) is

$$\min \left\{ \sum_{Y \subset X} \sum_{y \in Y} \text{floor}_b(|Y|) \cdot \sum_{x \in Y} \|x - y\|_2^2 \cdot z_{Y,y} + \lambda \cdot \left( \sum_{Y \subset X} \sum_{y \in Y} z_{Y,y} - k \right) : \right. \\ \left. \forall x \in X, \sum_{Y \ni x} \sum_{y \in Y} z_{Y,y} + w_x \geq 1 \wedge \sum_{x \in X} w_x \leq n - n' \wedge z, w \geq 0 \right\} \quad (7)$$

Consider an optimal clustering of any  $n'$  points in  $X$  into  $k$  disjoint clusters  $Y_1, Y_2, \dots, Y_k$ . For all  $Y \subset X$ , set  $z_{Y,y}$  to be the indicator that  $Y$  is a cluster in this list and  $y = c_Y$ . Also, for all  $x \in X$  set  $w_x$  to be the indicator that  $x$  is not clustered. Clearly, this is a feasible solution to the linear program (7), so its value is an upper bound on the optimal value of the linear program (6). The Lagrange term vanishes as there are exactly  $k$  non-zero values  $Z_{Y,y}$ . Thus, the upper bound is

$$\sum_{j=1}^k \text{floor}_b(|Y_j|) \cdot \sum_{x \in Y_j} \|x - c_{Y_j}\|_2^2 \leq 2 \cdot \sum_{j=1}^k \text{floor}_b(|Y_j|) \cdot \sum_{x \in Y_j} \|x - \text{cm}(Y_j)\|_2^2 \leq 2 \cdot \sum_{j=1}^k \text{cost}(Y_j),$$

where the first inequality uses Equation (5). ◀

In the primal-dual procedure, there is an active set  $\text{active} \subset X$  of points for which it is safe to raise the dual variable  $\alpha_x$  for all  $x \in \text{active}$ . We need to detect when a new dual constraint becomes tight and requires the removal of the points that are involved from active. This can be done in polynomial time for the revised dual program (6) as follows. For every  $y \in X$  and for every  $j \in \{0, 1, 2, \dots, \log_b \text{floor}_b(n)\}$ , we check if there exists  $Y \subset X$  that satisfies (i)  $y \in Y$ ; (ii)  $Y \cap \text{active} \neq \emptyset$ ; (iii)  $\log_b \text{floor}_b(|Y|) = j$ ; (iv)  $\sum_{x \in Y} \alpha_x \geq \lambda + b^j \cdot \sum_{x \in Y} \|x - y\|_2^2$ . In order to do this, consider the set of points  $C_{y,j} = \{x \in X : \alpha_x \geq b^j \cdot \|x - y\|_2^2\}$ , and sort  $C_{y,j}$  by nonincreasing order of  $\alpha_x - b^j \cdot \|x - y\|_2^2$ .

► **Lemma 5.** *There exists a choice of  $Y, y, j$  that satisfies (i)–(iv) iff there exists a choice of  $y, j$  such that  $|C_{y,j}| \geq b^j$  and  $C_{y,j} \cap \text{active} \neq \emptyset$  and first  $\min\{|C_{y,j}|, b^{j+1} - 1\}$  points in the above order that include  $y$  and at least one point from active are a set satisfying (i)–(iv).*

**Proof.** Clearly the existence of  $y, j$  such that  $C_{y,j}$  has the listed properties implies the existence of  $Y, y, j$  that satisfy (i)–(iv). As for the other direction, consider  $Y, y, j$  that satisfy (i)–(iv). Clearly  $y \in C_{y,j}$ . Suppose that there exists a point  $x \in Y \setminus C_{y,j}$ . Then, putting  $Y' = Y \setminus \{x\}$  and  $j' = \log_b \text{floor}_b(|Y'|) \leq j$ , we have that  $Y', y, j'$  also satisfy (i)–(iv). Thus, we may assume that  $Y \subset C_{y,j}$ . Now, choice in lemma of a subset of  $C_{y,j}$  subject to conditions (i)–(iii) maximizes  $\sum_{x \in Y} (\alpha_x - b^j \cdot \|x - y\|_2^2)$ . Thus, this subset also satisfies (iv). ◀

There are  $O(n \log n)$  pairs  $y, j$ . Listing and sorting each  $C_{y,j}$  takes at most  $O(n \log n)$  operations. Listing the candidate  $Y \subset C_{y,j}$  and checking it takes  $O(|C_{y,j}|)$  operations. Thus, finding a new tight constraint can be done in polynomial time. (Trivially, we can discretize the increase of the dual variables and/or use binary search to find the increase that causes a new constraint to become tight. As we're dealing with squared Euclidean distance, if the input consists of finite precision rational numbers, then all computed values are finite precision rational numbers.)

### 3 The Algorithm

We now describe the following three-phase primal-dual algorithm (Algorithm 1: PRIMAL-DUAL, refer page 9) that can be used to solve the facility location version of min-sum clustering. In addition to the pointset  $X$ , the cluster opening cost  $\lambda$ , and the target number of points  $n'$ , the algorithm also gets a (sufficiently large, TBD) parameter  $b$  that governs the excess number of discarded outliers in its output. Throughout the algorithm, sets of points  $Y \subset X$  will maintain values  $\text{card}_b(Y)$  and  $\text{ctr}(Y)$ . Clearly, we cannot do this explicitly and efficiently for every set  $Y \subset X$ . We use Lemma 5 and its consequences to implement the operations that we need, without storing explicitly these values for more than  $n$  sets. This affects only the first phase of the algorithm. For  $x \in X$  and  $Y \subset X$ , we denote throughout the paper  $d(x, Y) = b^{\text{card}_b(Y)} \cdot \|x - \text{ctr}(Y)\|_2^2$ . This is interpreted according to the relevant values of  $\text{card}_b(Y)$  and  $\text{ctr}(Y)$ .

Phase 1 constructs a dual solution and collects candidate clusters. During phase 1, a point  $x$  is either active or inactive. Initially, for all  $x \in X$ , we set  $\alpha_x$  to 0, and we set  $x$  to be active. The set of candidate clusters preclusters is empty. We raise all active  $x$  at a uniform rate, and pause to change the status of points and clusters if one of the following events happens.

- There exists an active  $x \in X$  and a cluster  $Y \in \text{preclusters}$  such that  $\alpha_x \geq d(x, Y)$ . In this case, replace  $Y$  by  $Y \cup \{x\}$  in preclusters. The new cluster in preclusters inherits the  $\text{card}_b$  and  $\text{ctr}$  values from  $Y$ . Also set  $x$  to be inactive.

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- There exists  $Y \subset X$  that contains an active point and  $y \in Y$  such that the dual constraint associated with the pair  $Y, y$  is tight. Explicitly,

$$\sum_{x \in Y} \alpha_x \geq \lambda + \text{cost}_b(Y),$$

where we set  $\text{card}_b(Y) = \log_b \text{floor}_b(|Y|)$  and  $\text{ctr}(Y) = y$ . In this case, add an inclusion-wise minimal such  $Y$  to preclusters and set all  $x \in Y$  to be inactive (and set  $\text{card}_b(Y)$  and  $\text{ctr}(Y)$  as stated above).

The first phase ends as soon as the number of active  $x \in X$  drops to  $n - n'$  or lower. If this number drops below  $n - n'$ , we do not add the last cluster  $Y_{\text{last}}$  to preclusters, but keep it separately. Note that each new tight constraint causes at least one point  $x \in X$  to become inactive, hence the number of sets  $Y$  that require storing explicitly their parameters  $\text{card}_b(Y)$  and  $\text{ctr}(Y)$  is at most  $n' \leq n$ .

In phase 2, we trim the set of candidate clusters and assign points uniquely to the clusters in the trimmed list, as follows. Note that we need the parameters  $\text{card}_b$  and  $\text{ctr}$  only for clusters for which these values were stored explicitly in phase 1. Define a conflict graph on the clusters in preclusters. Two clusters  $Y_1, Y_2 \in \text{preclusters}$  are connected by an edge in the conflict graph iff there exists  $x \in Y_1 \cap Y_2$  such that  $\alpha_x > \max\{d(x, Y_1), d(x, Y_2)\}$ . In other words, the edge  $\{Y_1, Y_2\}$  indicates that there is  $x \in Y_1 \cap Y_2$  that contributes to the opening cost  $\lambda$  of both  $Y_1$  and  $Y_2$ . Next, take a lexicographically maximal independent set  $\mathcal{I}$  in the conflict graph, ordering preclusters by non-increasing order of  $\text{card}_b(Y)$ , breaking ties arbitrarily. We group the points clustered in preclusters into meta-clusters of the form  $(Y, Y')$ , where  $Y \in \mathcal{I}$  indicates the meta-cluster, and  $Y'$  is a set of points. (Thus, the entire meta-cluster associated with  $Y$  is  $\cup_{(Y, Y') \in \text{metaclusters}} Y'$ .) In particular, for  $Y \in \mathcal{I}$ , we put  $(Y, Y) \in \text{metaclusters}$ . Any remaining points in preclusters are added as follows. If  $Y' \notin \mathcal{I}$ , then let  $Y''$  be the set of remaining points in  $\{x \in Y' : \alpha_x = \max_{y \in Y'} \alpha_y\}$ , and let  $Y \in \mathcal{I}$  be such that  $Y$  precedes  $Y'$  in the order on preclusters and  $\{Y, Y'\}$  is an edge. Add  $(Y, Y'')$  to metaclusters, with  $\text{card}_b(Y'') = \text{card}_b(Y')$  and  $\text{ctr}(Y'') = \text{ctr}(Y)$ . Finally, if the number of assigned points to metaclusters is less than  $n'$ , then we add  $(Y_{\text{last}}, Y)$  to metaclusters, where  $Y$  is a set of previously unclustered points from  $Y_{\text{last}}$  of the cardinality needed to complete the number of clustered point to  $n'$ . (Notice that at least  $n'$  points are clustered in preclusters  $\cup \{Y_{\text{last}}\}$ , so this is possible.)

Phase 3 determines the final output clustering of the points. For every meta-cluster  $(Y, \cdot)$  and for every integer  $p \leq \text{card}_b(Y)$ , let  $n_{Y,p}$  denote the number of points  $x \in X$  such that there exists  $(Y, Y') \in \text{metaclusters}$  with  $Y' \ni x$  and  $\text{card}_b(Y') = p$ . We open clusters as follows. For  $p = \text{card}_b(Y)$ , we open  $\max\{1, \lfloor \frac{n_{Y,p-2} + n_{Y,p-1} + n_{Y,p}}{b^{2+p}} \rfloor\}$  clusters and assign all the points counted in  $n_{Y,p-2}, n_{Y,p-1}, n_{Y,p}$  to these clusters, as evenly as possible.

► **Lemma 6.** *The number of points in each such cluster is at most  $2b^{2+p}$ , and if  $Y \neq Y_{\text{last}}$  then this number is at least  $b^p$ .*

**Proof.** If we open one cluster, then clearly  $n_{Y,p-2} + n_{Y,p-1} + n_{Y,p} < 2b^{2+p}$ . If we open  $s > 1$  clusters, then we must have  $sb^{2+p} \leq n_{Y,p-2} + n_{Y,p-1} + n_{Y,p} < (s+1)b^{2+p}$ . Thus, the number of points in each cluster is between  $b^{2+p}$  and  $(1 + 1/s)b^{2+p}$ . Clearly for every set  $Y \neq Y_{\text{last}}$ ,  $(Y, Y) \in \text{metaclusters}$ , and by the definition of  $p = \text{card}_b(Y)$ , it holds that  $|Y| \geq b^p$ . ◀

For  $p < \text{card}_b(Y) - 2$ , we open  $\lfloor \frac{n_{Y,p}}{b^{2+p}} \rfloor$  clusters. If this number is at least 1, we assign all the points counted in  $n_{Y,p}$  to these clusters, as evenly as possible. If this number is 0, we discard all the points counted in  $n_{Y,p}$  as outliers.



► **Lemma 7.** *In this step, if no cluster is opened then number of points that are discarded is less than  $b^{2+p}$ , else the number of points in each cluster is at least  $b^{2+p}$  and less than  $2b^{2+p}$ .*

**Proof.** The assertion is trivial. ◀

■ **Algorithm 1** Algorithm PRIMAL-DUAL.

---

```

1: procedure PRIMALDUAL( $X, \lambda, n', b$ )
2:    $\alpha, \text{preclusters}, Y_{\text{last}} \leftarrow \text{PRIMALDUALPHASE1}(X, \lambda, n', b)$ 
3:    $\text{metaclusters} \leftarrow \text{PRIMALDUALPHASE2}(X, n', b, \alpha, \text{preclusters}, Y_{\text{last}})$ 
4:    $\text{clusters} \leftarrow \text{PRIMALDUALPHASE3}(X, b, \text{metaclusters})$ 
5:   return clusters
6: end procedure
7:
8: procedure PRIMALDUALPHASE1( $X, \lambda, n', b$ )
9:    $\text{active}, \text{preclusters} \leftarrow X, \emptyset$ 
10:   $\alpha_x \leftarrow 0$  for all  $x \in X$ 
11:  while  $|\text{active}| > n - n'$  do
12:    raise  $\alpha_x$  at a uniform rate for all  $x \in \text{active}$  ▷ stop raising when one of the following two cases happens
13:    if  $\exists x \in \text{active}$  and  $Y \in \text{preclusters}$  such that  $\alpha_x \geq d(x, Y)$  then
14:       $\text{card}_b(Y \cup \{x\}), \text{ctr}(Y \cup \{x\}) \leftarrow \text{card}_b(Y), \text{ctr}(Y)$ 
15:       $\text{preclusters}, \text{active} \leftarrow \text{preclusters} \setminus \{Y\} \cup \{Y \cup \{x\}\}, \text{active} \setminus \{x\}$ 
16:    else if  $\exists Y \subset X$  and  $y \in Y$  such that  $Y \cap \text{active} \neq \emptyset$  the dual constraint for  $Y, y$  is tight then
17:       $\text{card}_b(Y), \text{ctr}(Y) \leftarrow \log_b \text{floor}_b(|Y|), y$ 
18:      if  $|\text{active} \setminus Y| < n - n'$  then ▷ use an inclusion-wise minimal such  $Y$ 
19:        return  $\alpha, \text{preclusters}, Y$ 
20:      else
21:         $\text{preclusters}, \text{active} \leftarrow \text{preclusters} \cup \{Y\}, \text{active} \setminus Y$ 
22:      end if
23:    end if
24:  end while
25:  return  $\alpha, \text{preclusters}, \emptyset$ 
26: end procedure
27:
28: procedure PRIMALDUALPHASE2( $X, n', b, \alpha, \text{preclusters}, Y_{\text{last}}$ )
29:    $\text{active}, \text{metaclusters} \leftarrow \{x \in X : x \in Y \in \text{preclusters} \forall x \in Y_{\text{last}}\}, \emptyset$ 
30:   for  $Y \in \text{preclusters}$ , by order of nonincreasing  $\text{card}_b(Y)$  do
31:     if  $\exists (Y', Y'') \in \text{metaclusters}$  with  $x \in Y \cap Y'$  and  $\alpha_x > \max\{d(x, Y), d(x, Y')\}$  then
32:        $Y'', \text{card}_b(Y''), \text{ctr}(Y'') \leftarrow \{x \in Y \cap \text{active} : \alpha_x = \max_{y \in Y} \alpha_y\}, \text{card}_b(Y), \text{ctr}(Y')$ 
33:        $\text{metaclusters} \leftarrow \text{metaclusters} \cup \{(Y', Y'')\}$ 
34:        $\text{active} \leftarrow \text{active} \setminus Y''$ 
35:     else
36:       remove each  $x \in Y$  from any  $Y'' \ni x$  with  $(Y', Y'') \in \text{metaclusters}$  ▷  $\alpha_x \leq d(x, Y'')$ ;
37:        $\text{card}_b(Y''), \text{ctr}(Y'')$  don't change
38:        $\text{metaclusters} \leftarrow \text{metaclusters} \cup \{(Y, Y)\}$ 
39:        $\text{active} \leftarrow \text{active} \setminus Y$ 
40:     end if
41:   end for
42:    $Y, \text{card}_b(Y), \text{ctr}(Y) \leftarrow \{|\text{active}| - n + n' \text{ points in } Y_{\text{last}} \cap \text{active}\}, \text{card}_b(Y_{\text{last}}), \text{ctr}(Y_{\text{last}})$ 
43:   if  $Y \neq \emptyset$  then
44:      $\text{metaclusters} \leftarrow \text{metaclusters} \cup \{(Y_{\text{last}}, Y)\}$ 
45:   end if
46:   return metaclusters
47: end procedure
48: procedure PRIMALDUALPHASE3( $X, b, \text{metaclusters}$ )
49:    $\text{clusters} \leftarrow \emptyset$ 
50:   for  $(Y, \cdot) \in \text{metaclusters}$  do
51:      $Y_{\text{max}} \leftarrow \{x \in X : \exists Y' \ni x \text{ such that } (Y, Y') \in \text{metaclusters} \wedge \text{card}_b(Y') \geq \text{card}_b(Y) - 2\}$ 
52:      $\text{clusters} \leftarrow \text{clusters} \cup \text{PARTITION}(Y_{\text{max}}, \max\{1, \lfloor |Y_{\text{max}}|/b^{2+\text{card}_b(Y)} \rfloor\})$ 
53:     for  $p < \text{card}_b(Y) - 2$  do
54:        $Y_p \leftarrow \{x \in X : \exists Y' \ni x \text{ such that } (Y, Y') \in \text{metaclusters} \wedge \text{card}_b(Y') = p\}$ 
55:       if  $|Y_p| \geq b^{2+p}$  then
56:          $\text{clusters} \leftarrow \text{clusters} \cup \text{PARTITION}(Y_p, \lfloor |Y_p|/b^{2+p} \rfloor)$ 
57:       end if
58:     end for
59:   end for
60:   return clusters
61: end procedure
62:
63: procedure PARTITION( $S, m$ ) ▷  $m \geq 1$ 
64:   partition  $S$  as evenly as possible into  $m$  disjoint subsets  $S_1, S_2, \dots, S_m$ 
65:   return  $\{S_1, S_2, \dots, S_m\}$ 
66: end procedure

```

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## 16:10 Min-Sum Clustering (With Outliers)

We are now ready to define our min-sum  $k$ -clustering algorithm (Algorithm 2: MIN-SUM-CLUSTERING refer page 10). If  $k \leq \frac{4}{\epsilon}$ , we can run a PTAS or a constant factor approximation for fixed  $k$  (for instance [28, 23]).<sup>1</sup> Otherwise, our algorithm follows the general schema of the lagrangian relaxation method. Let  $\delta > 0$  be determined later. We run the procedure PRIMALDUAL on various values of  $\lambda$ , and if the smallest returned cluster for a particular value of  $\lambda$  which is denoted as  $Y_{\min, \lambda}$  has at most  $\frac{\epsilon}{3} \cdot n'$  points, we remove this cluster. Using binary search on the Lagrange multiplier  $\lambda$ , we find two values  $\lambda_1 < \lambda_2$ , with  $\lambda_2 - \lambda_1 < \delta$ , that satisfy the following property. The above process (running PRIMALDUAL, then removing the smallest cluster if it's sufficiently small) returns  $k_1 > k$  clusters (denoted as clusters<sub>1</sub>) for  $\lambda = \lambda_1$ , and  $k_2 \leq k$  clusters (denoted as clusters<sub>2</sub>) for  $\lambda = \lambda_2$ . If  $\frac{k-k_2}{k_1-k_2} \geq 1 - \frac{\epsilon}{4}$ , we output the  $k$  largest clusters in the solution for  $\lambda_1$  (i.e. from clusters<sub>1</sub>), and otherwise we output the solution for  $\lambda_2$  (i.e. from clusters<sub>2</sub>).

■ **Algorithm 2** Algorithm MIN-SUM-CLUSTERING.

---

```

1: procedure MINSUMCLUSTERING( $X, k, n', \epsilon$ )
2:    $\lambda_1 \leftarrow 0, \lambda_2 \leftarrow \sum_{x,y \in X} \|x - y\|_2^2$ 
3:   clusters1  $\leftarrow \{\{x\} : x \in X\},$  clusters2  $\leftarrow X$ 
4:    $b \leftarrow \frac{1+\epsilon}{\epsilon}$ 
5:    $\delta \leftarrow \frac{2}{(n+k)\lambda_2}$  ▷ we need  $\delta \leq \frac{2}{(n+k) \text{opt}(X, n', k)}$ 
6:   while  $\lambda_2 - \lambda_1 > \delta$  do
7:      $\lambda = \frac{1}{2} \cdot (\lambda_1 + \lambda_2)$ 
8:     clusters  $\leftarrow \text{PrimalDual}(X, \lambda, n', b)$ 
9:      $Y_{\min, \lambda} \leftarrow$  smallest cluster in clusters
10:     $k' \leftarrow |\text{clusters}| - 1$ 
11:    if  $|Y_{\min, \lambda}| \leq \frac{\epsilon}{3} \cdot n'$  then
12:      clusters  $\leftarrow \text{clusters} \setminus \{Y_{\min, \lambda}\}$ 
13:    end if
14:    if  $k' > k$  then
15:       $\lambda_1, \text{clusters}_1, k_1 \leftarrow \lambda, \text{clusters}, k'$ 
16:    else ▷  $k' \leq k$ 
17:       $\lambda_2, \text{clusters}_2, k_2 \leftarrow \lambda, \text{clusters}, k'$ 
18:    end if
19:  end while
20:   $\rho_1 \leftarrow \frac{k-k_2}{k_1-k_2}$  ▷  $k_1 > k \geq k_2 \geq 0$ 
21:  if  $\rho_1 \geq 1 - \frac{\epsilon}{4}$  then
22:    return  $\{k$  largest sets in clusters1 $\}$ 
23:  else
24:    return clusters2 ▷ If  $|\text{clusters}_2| < k$ , split clusters arbitrarily to get exactly  $k$ 
25:  end if
26: end procedure

```

---

<sup>1</sup> These papers consider only the case without outliers. The PTAS in [28] enumerates over cluster sizes and approximate cluster centers, then computes an optimal assignment of the data points to the approximate centers, given the corresponding cluster sizes. Clearly, the algorithm can be adapted trivially to handle the case with outliers by modifying the target sum of cluster sizes.

► **Theorem 8.** *The execution of **procedure** `MINSUMCLUSTERING`( $X, k, n', \epsilon$ ) computes a clustering of  $X' \subset X$  into  $k$  clusters such that  $|X'| \in [(1 - \epsilon)n', n']$ , and the total cost of the clustering of  $X'$  is at most  $O\left(\frac{1}{\epsilon^3}\right) \cdot \text{opt}(X, n', k)$ . The time complexity of this computation is  $\text{poly}(n, \log(1/\epsilon), \log \Delta)$ , where  $\Delta$  is ratio of largest to non-zero smallest  $\|\cdot\|_2^2$  distance in  $X$ .*

**Proof.** The performance guarantee is an immediate consequence of Corollary 11 below. The running time is a straightforward analysis of the code. ◀

► **Theorem 9.** *The same claim applies to instances of points in a metric space  $(X, \text{dist})$ , with  $\text{dist}$  replacing  $\|\cdot\|_2^2$  in the code and in the claim.*

**Proof sketch.** The  $\|\cdot\|_2^2$  distance can be replaced by any metric distance  $\text{dist}$  in all claims starting from Proposition 3. The proofs sometime require minor changes. In particular, in Lemma 13, the factor  $\frac{1}{9}$  can be improved to  $\frac{1}{3}$  on account of the triangle inequality, and this improves all the other constants that depend on it. ◀

## 4 Proofs

In this section we analyze the min-sum  $k$ -clustering algorithm. The analysis builds on the following guarantees of the primal-dual schema.

► **Theorem 10.** *For every  $\epsilon \in (0, 1]$  there exists a constant  $c = c_\epsilon$  such that the following holds. Let clusters be the output of **procedure** `PRIMALDUAL`( $X, \lambda, n', b$ ), and let  $\alpha$  be the dual solution computed during the execution of this procedure. Set  $\gamma = \max_{x \in X} \alpha_x$ . Then,*

1.  $(\alpha, \gamma)$  is a feasible solution to the dual program (6).
2.  $\sum_{Y \in \text{clusters}} |Y| \in [(1 - \frac{\epsilon}{3})n', n']$ .
3.  $c \cdot (|\text{clusters}| - 1) \cdot \lambda + \sum_{Y \in \text{clusters}} \text{cost}(Y) \leq c \cdot \sum_{Y \in \text{clusters}} \sum_{x \in Y} \alpha_x$ .

► **Corollary 11.** *Let clusters be the output of **procedure** `MINSUMCLUSTERING`. Then, the following assertions hold:*

1.  $|\text{clusters}| \leq k$ .
2.  $\sum_{Y \in \text{clusters}} |Y| \in [(1 - \epsilon)n', n']$ .
3.  $\sum_{Y \in \text{clusters}} \text{cost}(Y) \leq \frac{8(c+1)}{\epsilon} \cdot \text{opt}(X, n', k)$ .

**Proof.** The first assertion follows directly from the definition of the procedure.

For the second assertion, let  $\lambda_i, \text{clusters}_i$  (where  $i = 1, 2$ ) be the values that determine the output of the procedure. By Theorem 10,  $\sum_{Y \in \text{clusters}_i} |Y| \geq (1 - \frac{\epsilon}{3})n'$ . If  $Y_{\min, \lambda_i}$  is removed from  $\text{clusters}_i$ , then  $|Y_{\min, \lambda_i}| \leq \frac{\epsilon}{3} \cdot n'$ . Thus, if  $i = 2$  then clearly the assertion holds. If  $i = 1$ , then  $\rho_1 \geq 1 - \frac{\epsilon}{4}$ . Therefore,

$$k_1 \leq \frac{1}{\rho_1} \cdot k \leq \left(1 + \frac{\epsilon}{4 - \epsilon}\right) \cdot k \leq \left(1 + \frac{\epsilon}{3}\right) \cdot k.$$

Thus, the procedure removes from the output at most a fraction of  $\frac{\epsilon}{3}$  of the clusters in  $\text{clusters}_1$ . As the removed clusters are the smallest, they contain at most  $\frac{\epsilon}{3} \cdot n'$  points.

As for the third assertion, consider the two solutions  $\text{clusters}_1, \text{clusters}_2$  that are used to determine the procedure's output. For  $i = 1, 2$ , let  $\alpha_i, \text{preclusters}_i$  be the output of `PRIMALDUALPHASE1` during the computation of  $\text{clusters}_i$ . Put  $\gamma_i = \max_{x \in X} \alpha_{i,x}$ . Let

$$(\alpha, \gamma) = \rho_1(\alpha_1, \gamma_1) + (1 - \rho_1)(\alpha_2, \gamma_2).$$

Clearly,  $(\alpha, \gamma)$  is a feasible solution to the dual LP (6) with the constant  $\lambda = \rho_1 \lambda_1 + (1 - \rho_1) \lambda_2$ . Notice that there are exactly  $n - n'$  points that are not included in  $\text{preclusters}_i$ . Each point

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$x \in X$  which is not included in preclusters $_i$  has  $\alpha_{i,x} = \gamma_i$ . (Notice that all the points that are excluded are active. This is true even for points that are discarded from the last tight cluster that gets included in preclusters $_i$ .) So, the value of the solution  $(\alpha, \gamma)$  is

$$\begin{aligned}
2 \cdot \text{opt}(X, n', k) &\geq \sum_{x \in X} \alpha_x - (n - n')\gamma - \lambda k \\
&= \rho_1 \cdot \left( \sum_{x \in X} \alpha_{1,x} - (n - n')\gamma_1 - \lambda k_1 \right) + (1 - \rho_1) \cdot \left( \sum_{x \in X} \alpha_{2,x} - (n - n')\gamma_2 - \lambda k_2 \right) \\
&= \rho_1 \cdot \left( \sum_{Y \in \text{preclusters}_1} \sum_{x \in Y} \alpha_{1,x} - \lambda k_1 \right) + (1 - \rho_1) \cdot \left( \sum_{Y \in \text{preclusters}_2} \sum_{x \in Y} \alpha_{2,x} - \lambda k_2 \right) \\
&\geq \rho_1 \cdot \left( \sum_{Y \in \text{preclusters}_1} \sum_{x \in Y} \alpha_{1,x} - \lambda_1 k_1 \right) + (1 - \rho_1) \cdot \left( \sum_{Y \in \text{preclusters}_2} \sum_{x \in Y} \alpha_{2,x} - \lambda_2 k_2 \right) \\
&\quad - \delta \cdot (k_1 + k_2),
\end{aligned}$$

where the first inequality follows from Lemma 4, and the first equality uses the fact that  $k = \rho_1 k_1 + (1 - \rho_1)k_2$ .

For  $i = 1, 2$  consider the final value of clusters $_i$ . By definition,  $k_i$  is one less than the number of clusters returned from **procedure** PRIMALDUAL, so by Theorem 10,

$$\sum_{Y \in \text{clusters}_i} \text{cost}(Y) \leq c \cdot \left( \sum_{Y \in \text{clusters}_i} \sum_{x \in Y} \alpha_x - k_i \cdot \lambda_i \right).$$

In particular, the right-hand side is non-negative. Notice that if  $\rho_1 \geq 1 - \frac{\epsilon}{4}$ , then clearly  $\rho_1 > \frac{\epsilon}{4}$  and the cost of the output clustering is at most  $\sum_{Y \in \text{clusters}_1} \text{cost}(Y)$ . Similarly, if  $\rho_1 < 1 - \frac{\epsilon}{4}$ , then  $1 - \rho_1 > \frac{\epsilon}{4}$  and the cost of the output clustering is at most  $\sum_{Y \in \text{clusters}_2} \text{cost}(Y)$ . Either way, we get that the cost of the clustering is at most  $\frac{8c}{\epsilon} \cdot \text{opt}(X, n', k) + \frac{4\delta}{\epsilon} \cdot (k_1 + k_2) \leq \frac{8(c+1)}{\epsilon} \cdot \text{opt}(X, n', k)$ .  $\blacktriangleleft$

Next we analyze primal-dual algorithm and prove Theorem 10. The notation follows Algorithm 1.

► **Lemma 12.** *At the end of executing **procedure** PRIMALDUALPHASE1, for every  $Y \in$  preclusters and for every  $x \in Y$ , we have that  $\alpha_x \geq d(x, Y)$ .*

**Proof.** When  $Y$  is added to preclusters then there exists  $y \in Y$  and  $j = \log_b \text{floor}_b(|Y|)$  such that  $Y \subset C_{y,j}$ . We set  $\text{card}_b(Y) = j$  and  $\text{ctr}(Y) = y$ , so by the definition of  $C_{y,j}$  the lemma holds. If a point  $x$  is later added to  $Y$ , the condition for doing it is that  $\alpha_x \geq d(x, Y)$ .  $\blacktriangleleft$

► **Lemma 13.** *At the end of executing **procedure** PRIMALDUALPHASE2, the following assertions hold:*

1.  $\sum_{(Y, Y') \in \text{metaclusters}} |Y'| = n'$ .
2. For every  $(Y, Y') \in \text{metaclusters}$  and for every  $x \in Y'$ , we have that  $\alpha_x \geq \frac{1}{9} \cdot d(x, Y')$ .

**Proof.** The first assertion holds as the points that are clustered in metaclusters are all the points that are clustered in preclusters plus some of the points clustered in  $Y_{\text{last}}$ . The number of such points is at most  $n'$  without  $Y_{\text{last}}$ , and at least  $n'$  with  $Y_{\text{last}}$ . The algorithm takes from  $Y_{\text{last}}$  exactly the number of points needed to complete the number in preclusters to  $n'$ .

For the second assertion, consider  $(Y, Y') \in \text{metaclusters}$  and  $x \in Y'$ . If  $Y = Y'$ , then Lemma 12 guarantees the assertion. Otherwise, consider  $Y'' \in \text{preclusters}$  that caused  $(Y, Y')$  to be added to metaclusters. In particular,  $Y' \subset Y''$ ,  $\text{card}_b(Y') = \text{card}_b(Y'') \leq \text{card}_b(Y)$ , and

there exists  $z \in Y \cap Y''$  such that  $\alpha_z > \max\{d(z, Y), d(z, Y'')\}$ . By the choice of  $Y'$  in the algorithm,  $\alpha_x = \max_{x' \in Y''} \alpha_{x'}$ , so it must be that  $\alpha_z \leq \alpha_x$ . Notice that by Lemma 12,

$$\alpha_x \geq d(x, Y'') = b^{\text{card}_b(Y'')} \cdot \|x - \text{ctr}(Y'')\|_2^2.$$

$$\begin{aligned} \text{Also, } \alpha_z &> \max\{b^{\text{card}_b(Y)} \cdot \|z - \text{ctr}(Y)\|_2^2, b^{\text{card}_b(Y'')} \cdot \|z - \text{ctr}(Y'')\|_2^2\} \\ &\geq b^{\text{card}_b(Y')} \cdot \max\{\|z - \text{ctr}(Y)\|_2^2, \|z - \text{ctr}(Y'')\|_2^2\}. \end{aligned}$$

$$\begin{aligned} \text{Thus, } d(x, Y') &= b^{\text{card}_b(Y')} \cdot \|x - \text{ctr}(Y)\|_2^2 \\ &\leq b^{\text{card}_b(Y')} \cdot (\|x - \text{ctr}(Y'')\|_2 + \|z - \text{ctr}(Y'')\|_2 + \|z - \text{ctr}(Y)\|_2)^2 \\ &\leq 9 \cdot \alpha_x. \end{aligned} \quad \blacktriangleleft$$

Let clusters be the output of **procedure** PRIMALDUALPHASE3. Recall that every cluster  $Z \in \text{clusters}$  is derived in some iteration indexed by  $(Y, \cdot) \in \text{metaclusters}$ . It holds that either  $Z \subset Y_{\max}$  or  $Z \subset Y_p$  for some  $p < \text{card}_b(Y) - 2$ . Notice that in the latter case,  $Y \neq Y_{\text{last}}$ . We will set implicitly  $\text{card}_b(Z)$  as follows.

$$\text{card}_b(Z) = \begin{cases} \text{card}_b(Y) & Z \subset Y_{\max}, \\ p & Z \subset Y_p, p < \text{card}_b(Y) - 2. \end{cases}$$

We will also set implicitly  $\text{ctr}(Z) = \text{ctr}(Y)$ .

► **Lemma 14.** *If  $Z \subset Y_p$  for some  $p < \text{card}_b(Y) - 2$ , then  $\sum_{x \in Z} \alpha_x \geq b \cdot \lambda$ . The same is true if  $Z \subset Y_{\max}$ ,  $Y \neq Y_{\text{last}}$ , and  $|Y_{\max}| \geq b^{2+\text{card}_b(Y)}$ .*

**Proof.** Consider  $x \in Z \subset Y_p$ ,  $p < \text{card}_b(Y) - 2$ . There is a pair  $(Y, Y') \in \text{metaclusters}$  such that  $p = \text{card}_b(Y') < \text{card}_b(Y) - 2$ , and  $x \in Y'$ . Moreover, there is  $Y'' \in \text{preclusters}$  such that  $Y' \subset Y''$  and  $\text{card}_b(Y'') = p$  and  $\alpha_x = \max_{y \in Y''} \alpha_y$ . By the definition of  $\text{card}_b$ , we have that  $|Y''| < b^{1+p}$ . Therefore,  $\alpha_x > \frac{\lambda}{b^{1+p}}$ . By Lemma 7,  $|Z| \geq b^{2+p}$ , hence the conclusion.

A similar argument applies to  $Z \subset Y_{\max}$ , assuming that  $|Y_{\max}| \geq b^{2+\text{card}_b(Y)}$ . In this case, if  $Z \supset Y$  then we have  $\sum_{x \in Y} \alpha_x \geq \lambda$ . As  $|Y| < b^{1+\text{card}_b(Y)}$ ,  $Z$  also contains more than  $b^{2+\text{card}_b(Y)} - b^{1+\text{card}_b(Y)} = b^{2+\text{card}_b(Y)} \cdot (1 - \frac{1}{b})$  points from pairs  $(Y, Y') \in \text{metaclusters}$ ,  $Y' \neq Y$ . By the argument for  $Y_p$ , for each such point  $x$  we have  $\alpha_x > \frac{\lambda}{b^{1+\text{card}_b(Y')}} > \frac{\lambda}{b^{1+\text{card}_b(Y)}}$ . Overall, we get that  $\sum_{x \in Z} \alpha_x > \lambda + b^{2+\text{card}_b(Y)} \cdot (1 - \frac{1}{b}) \cdot \frac{\lambda}{b^{1+\text{card}_b(Y)}} = b \cdot \lambda$ . If  $Z$  does not contain  $Y$ , then the argument for  $Y_p$  holds. ◀

► **Lemma 15.** *For every  $Z \in \text{clusters}$ ,  $\text{cost}(Z) \leq 2b^2 \cdot \sum_{x \in Z} d(x, Z)$ .*

**Proof.** We have  $\text{cost}(Z) = |Z| \cdot \sum_{x \in Z} \|x - \text{cm}(Z)\|_2^2 \leq |Z| \cdot \sum_{x \in Z} \|x - \text{ctr}(Y)\|_2^2$ . By Lemmas 6 and 7,  $|Z| \leq 2b^2 \cdot \text{card}_b(Z)$ . ◀

**Proof of Theorem 10.** First, consider the feasibility of  $(\alpha, \gamma)$ . Clearly,  $\gamma$  is set in the theorem to satisfy the constraints that include it. Regarding the constraints that involve only  $\alpha$ , we prove that they are satisfied throughout the execution of **procedure** PRIMALDUALPHASE1. The proof is by induction on the number of inactive points. Clearly, the initial  $\alpha$  is feasible. Now, suppose that  $\alpha$  is feasible for some number of inactive points, and consider the next step when this number increases and a set  $A \subset \text{active}$  is removed from active (we will use active here to denote the set before the removal of  $A$ ). Let  $\alpha'$  denote the values of the dual variables just before  $A$  is removed from active. If there exist  $Y \subset X$  and  $y \in Y$  such that the constraint for the pair  $Y, y$  is violated, then clearly  $Y \cap \text{active} \neq \emptyset$ , otherwise the same constraint would

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have been violated by the solution  $\alpha$ , as  $\alpha$  and  $\alpha'$  differ only on active. But then there is some intermediate value  $\alpha''$  such that  $\alpha''_x = \alpha_x$  for all  $x \notin \text{active}$  and  $\alpha_x \leq \alpha''_x < \alpha'_x$  for all  $x \in \text{active}$ , which causes this constraint (or another constraint involving active points) to become tight. Therefore, at least one point would have been removed from active before we reach the values  $\alpha'$ , in contradiction with our assumptions. Next, consider number of points clustered in the output clusters of **procedure** PRIMALDUAL. Clearly, **procedure** PRIMALDUALPHASE2 clusters in metaclusters exactly  $n'$  points. Some of these points are discarded by **procedure** PRIMALDUALPHASE3. Consider some  $(Y, \cdot) \in \text{metaclusters}$ . By Lemma 7, number of points discarded from these clusters is less than

$$\sum_{p < \text{card}_b(Y) - 2} b^{2+p} = \frac{b^{\text{card}_b(Y)} - b^2}{b - 1}.$$

On the other hand, all the points in  $Y_{\max}$  are clustered in clusters, as  $Y \neq Y_{\text{last}}$  in this case. Clearly, the number of points in  $Y_{\max}$  is at least  $|Y| \geq b^{\text{card}_b(Y)}$ . Thus, less than  $\frac{1}{b-1} \cdot n' \leq \epsilon \cdot n'$  points get discarded. Finally, let's consider the cost of the clustering. Let  $Z \in \text{clusters}$  be a cluster that satisfies the conditions of Lemma 14. Then,

$$\begin{aligned} \sum_{x \in Z} \alpha_x - \lambda &> \frac{b-1}{b} \cdot \sum_{x \in Z} \alpha_x \\ &\geq \frac{b-1}{9b} \cdot \sum_{x \in Z} d(x, Z) \\ &\geq \frac{b-1}{18b^3} \cdot \text{cost}(Z), \end{aligned}$$

where the first inequality follows from Lemma 14, the second inequality follows from Lemma 13, and the third inequality follows from Lemma 15. The remaining clusters are sets  $Y_{\max}$  with  $|Y_{\max}| < b^{2+\text{card}_b(Y)}$  and a subset of  $Y_{\text{last}}$ . Consider a cluster  $Y_{\max} \in \text{clusters}$ . We have that

$$\sum_{x \in Y_{\max}} \alpha_x - \lambda = \sum_{x \in Y} \alpha_x - \lambda + \sum_{x \in Y_{\max} \setminus Y} \alpha_x \geq \sum_{x \in Y} d(x, Y) + \frac{1}{9} \cdot \sum_{x \in Y_{\max} \setminus Y} d(x, Y) \geq \frac{1}{18b^2} \cdot \text{cost}(Y_{\max}).$$

Finally, if there's a cluster  $Z \subset Y_{\text{last}}$ , then

$$\sum_{x \in Z} \alpha_x \geq \frac{1}{9} \cdot \sum_{x \in Z} d(x, Y_{\max}) \geq \frac{1}{18b^2} \cdot \text{cost}(Z).$$

Thus, we can set  $c = c_\epsilon = \frac{18b^3}{b-1} = \frac{18(1+\epsilon)^3}{\epsilon^2}$ . ◀

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