DISTRIBUTED K-MEANS WITH OUTLIERS IN GENERAL METRICS

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February 21, 2022

ABSTRACT

Center-based clustering is a pivotal primitive for unsupervised learning and data analysis. A popular variant is undoubtedly the k-means problem, which, given a set $P$ of points from a metric space and a parameter $k < |P|$, requires to determine a subset $S$ of $k$ centers minimizing the sum of all squared distances of points in $P$ from their closest center. A more general formulation, introduced to deal with noisy datasets, features a further parameter $z$ and allows up to $z$ points of $P$ (outliers) to be disregarded when computing the aforementioned sum. We present a distributed coreset-based 3-round approximation algorithm for k-means with $z$ outliers for general metric spaces, using MapReduce as a computational model. Our distributed algorithm requires sublinear local memory per reducer, and yields a solution whose approximation ratio is an additive term $O(\gamma)$ away from the one achievable by the best known sequential (possibly bicriteria) algorithm, where $\gamma$ can be made arbitrarily small. An important feature of our algorithm is that it obliviously adapts to the intrinsic complexity of the dataset, captured by its doubling dimension $D$. To the best of our knowledge, no previous distributed approaches were able to attain similar quality-performance tradeoffs for general metrics.

Keywords: Clustering; k-means; Outliers; MapReduce; Coreset.

1 Introduction

Clustering is a fundamental primitive for data analysis and unsupervised learning, with applications to such diverse domains as pattern recognition, information retrieval, bioinformatics, social networks, and many more [17]. Among the many approaches to clustering, a prominent role is played by center-based clustering, which aims at partitioning a set of data items into $k$ groups, where $k$ is an input parameter, according to a notion of similarity modeled through a metric distance over the data. Different variants of center-based clustering aim at minimizing different objective functions. The k-means problem is possibly the most popular variant of center-based clustering. Given a set $P$ of points in a general metric space and a positive integer $k < |P|$, the discrete version of the problem requires to determine a subset $S \subset P$ of $k$ points, called centers, so that the sum of all squared distances of the points of $P$ from their closest center is minimized. (In Euclidean spaces, centers may be chosen also outside the set $P$, giving rise to the continuous version of k-means, admitting a wider spectrum of feasible solutions.)

Since the objective function of k-means involves squares of distances, the optimal solution is at risk of being impacted by few “distant” points, called outliers, which may severely bias the optimal center selection towards reducing such distances. In fact, the presence of outliers is inevitable in large datasets, due to the present of points which are artifacts of data collection, either representing noisy measurements or simply erroneous information. To cope with this
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limitation, k-means admits a heavily studied robust formulation that takes into account outliers [7]: when computing the objective function for a set of \( k \) centers, the \( z \) largest squared distances from the centers are not included in the sum, where \( z < |P| \) is an additional input parameter representing a tolerable level of noise. This formulation of the problem is known as \textit{k-means with \( z \) outliers}.

There is ample and well-established literature on sequential strategies for different instantiations of center-based clustering, with and without outliers. However, with the advent of big data, the high volumes that need to be processed often rule out the use of unscalable, sequential strategies. Therefore, it is of paramount importance to devise efficient clustering strategies tailored to typical distributed computational frameworks for big data processing (e.g., MapReduce [10]). The primary objective of this paper is to devise scalable, distributed strategies for discrete k-means with \( z \) outliers for general metric spaces.

1.1 Related Work

The body of literature on solving k-means without outliers sequentially is huge [3]. The best sequential algorithms to date for the discrete case on general metrics are the deterministic \((9 + \epsilon)\)-approximation algorithm of [11], or the randomized PTAS of [2] for spaces of constant doubling dimension. A simpler and faster randomized option is the k-means++ algorithm of [2], whose approximation ratio, which is \( O(\log k) \) in expectation, can be lowered to a constant by running the algorithm for \( \rho k \) centers, with \( \rho = O(1) \) [25]. For the distributed case, a 3-round MapReduce algorithm for k-means is presented in [21]. For arbitrarily small \( \gamma > 0 \), the algorithm attains an approximation ratio which is a mere \( O(\gamma) \) term away from the best sequential approximation attainable for the weighted variant of the problem.

A considerable number of sequential algorithms have also been proposed for k-means with \( z \) outliers. Here, we report only on the works most relevant to our framework, and refer to [11] for a more detailed overview of the literature. In [14], a randomized local search strategy is described, which runs in time \( O\left(|P|z + (1/\epsilon)k^2(k + z)^2 \log(|P|\Delta)\right) \), yielding a 274-approximate bicriteria solution with \( k \) centers and \( O\left((1/\epsilon)kz \log(|P|\Delta)\right) \) outliers, where \( \Delta \) is the ratio between the maximum and minimum pairwise distances. For spaces of doubling dimension \( D \), [12] devises a different (deterministic) local search strategy yielding a bicriteria solution with \( (1+\epsilon)k \) centers and \( z \) outliers achieving approximation \( 1 + O(\epsilon) \), in time \( O\left((k/\epsilon)|P|(D/\epsilon)^{2(D/\epsilon)} \log(|P|\Delta)\right) \). Finally, the LP-based approach of [19] yields the first non-bicriteria solution featuring an expected 53.002 \( (1 + \epsilon) \)-approximation in time \( |P|^{O(1/\epsilon^3)} \).

The literature on distributed approaches to k-means with outliers is more scant. The simple, sequential coreset-based strategy of [24] can be easily made into a 2-round MapReduce algorithm yielding a solution featuring a nonconstant \( O(\log(k + z)) \) approximation and local memory \( \sqrt{|P|}(k + z) \). In [13], an LP-based algorithm is developed for the coordinator model, yielding a \( O\left(1 + 1/\epsilon\right) \)-approximate bicriteria solution, with an excess factor \( 1 + \epsilon \) either in the number of outliers or in the number of centers, using \( O(Lk + z) \) communication words, where \( L \) is the number of available workers. In the coordinator model, better bounds have been obtained for the special case of Euclidean spaces in [20, 8].

1.2 Our Contribution

We present a scalable coreset-based distributed MapReduce algorithm for k-means with \( z \) outliers, targeting the solution of very large instances from general metrics. The algorithm first computes, distributedly, a coreset of suitably selected input points which act as representatives of the whole input, where each coreset point is weighted in accordance to the number of input points it represents. Then, the final solution is computed by running on the coreset an \( \alpha \)-approximate sequential algorithm for the weighted variant of the problem. Our approach is flexible, in the sense that the final solution can also be extracted through a sequential bicriteria algorithm returning a larger number \( \rho k \) of centers and/or excluding a larger number \( \tau z \) of outliers. Our distributed algorithm features an approximation ratio of \( \alpha + O(\gamma) \), where \( \gamma \) is a user-provided accuracy parameter which can be made arbitrarily small. The algorithm requires 3 rounds and a local memory at each worker of size \( \sqrt{|P|(\rho k + \tau z)c/\gamma)2D \log^2 |P|} \), where \( c \) is a constant and \( D \) is the doubling dimension of the input. For reasonable configurations of the parameters and, in particular, low doubling dimension, the local space is substantially smaller than the input size. It is important to remark that the algorithm is \textit{oblivious} to \( D \), in the sense that while the actual value of this parameter (which is hard to compute) influences the analysis, it is not needed for the algorithm to run. As a proof of concept, we describe how the sequential bicriteria algorithms by [14] and [12] can be extended to handle weighted instances, so that, when used within our MapReduce algorithm allow us to get comparable constant approximations in distributed fashion.
We remark that the main contributions of our algorithm are: (i) its simplicity, since our coreset construction does not require multiple invocations of complex, time-consuming sequential algorithms for k-means with outliers (as is the case in [13]); and (ii) its versatility, since the scheme is able to exploit any sequential algorithm for the weighted case (bicriteria or not) to be run on the scaled-down coreset with a minimal extra loss in accuracy. In fact, to the best of our knowledge, ours is the first distributed algorithm that can achieve an approximation arbitrarily close to the one of the best available sequential solution, either exact or bicriteria. Finally, we observe that our MapReduce algorithm can solve instances of the problem without outliers with similar approximation guarantees, and its memory requirements improve substantially upon those of [21].

**Organization of the paper.** Section 2 contains the main definitions and some preliminary concepts. Section 3 describes a simplified coreset construction (Subsection 3.1), the full algorithm (Subsection 3.2), and a sketch of a more space-efficient coreset construction, which yields our main result (Subsection 3.3). Finally, Section 4 discusses the extension of the algorithms in [14] and [12] to handle weighted instances. Section 5 provides some final remarks.

## 2 Preliminaries

Let $P$ be a set of points from a metric space with distance function $d(\cdot, \cdot)$. For any point $p \in P$ and subset $S \subseteq P$, define the distance between $p$ and $S$ as $d(p, S) = \min_{q \in S} d(p, q)$. Also, we let $p^S$ denote a point of $S$ closest to $p$, that is, a point such that $d(p, p^S) = d(p, S)$, with ties broken arbitrarily. The discrete \textit{k-means} problem requires that, given $P$ and an integer $k < |P|$, a set $S \subseteq P$ of $k$ centers be determined, minimizing the cost function $\text{cost}(P, S) = \sum_{p \in P} d(p, S)^2$. We focus on a robust version of discrete $k$-means, known in the literature as \textit{k-means with $z$ outliers}, where, given an additional integer parameter $z \leq |P|$, we seek a set $S \subseteq P$ of $k$ centers minimizing the cost function $\text{cost}(P \setminus \text{out}_z(P, S), S)$, where $\text{out}_z(P, S)$ denotes the set of $z$ points of $P$ farthest from $S$, with ties broken arbitrarily. We let $\text{OPT}_k(P)$ (resp., $\text{OPT}_{k,z}(P)$) denote the cost of the optimal solution of $k$-means (resp., $k$-means with $z$ outliers) on $P$.

The following two facts state technical properties that will be needed in the analysis.

**Fact 1.** For every $k, z > 0$ we have $\text{OPT}_{k+z}(P) \leq \text{OPT}_{k,z}(P)$.

**Proof.** Let $S^*$ be the optimal solution of $k$-means with $z$ outliers on $P$, that is, such that $\text{cost}(P \setminus \text{out}_z(P, S^*), S) = \text{OPT}_{k,z}(P)$, and let $\tilde{S} = S^* \cup \text{out}_z(P, S^*)$. Since $|\tilde{S}| \leq k + z$, we have that $\text{OPT}_{k+z}(P) \leq \text{cost}(P, \tilde{S}) \leq \text{cost}(P \setminus \text{out}_z(P, S^*), S) = \text{OPT}_{k,z}(P)$.

**Fact 2.** For any $p, q, t \in P$, $S \subseteq P$, and $c > 0$, we have:

$$d(p, S) \leq d(p, q) + d(q, S)$$

$$d(p, t)^2 \leq (1 + c)d(p, q)^2 + (1 + 1/c)d(q, t)^2.$$

**Proof.** The first inequality follows since $d(p, S) = d(p, p^S) \leq d(p, q) + d(q, q^S) = d(p, q) + d(q, S)$.

The second inequality follows since $d(p, t)^2 \leq (d(p, q) + d(q, t))^2 = d(p, q)^2 + d(q, t)^2 + 2d(p, q)d(q, t)$ and $2d(p, q)d(q, t) \leq (1/c)d(p, q)^2 + cd(q, t)^2$, where the latter inequality holds since $((1/\sqrt{c})d(p, q) - \sqrt{c}d(q, t))^2 \geq 0$. 

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Table 1: Notations used throughout the paper: $P$ is a set of $|P|$ points, $S$ is a subset of $P$, and $0 < z < n$ is an integer parameter.
In the weighted variant of k-means, each point $p \in P$ carries a positive integer weight $w_p$. Letting $w : P \to \mathbb{Z}^+$ denote the weight function, the problem requires to determine a set $S \subset P$ of $k$ centers minimizing the cost function $\text{cost}(P, w, S) = \sum_{p \in P} w_p d(p, S)^2$. Likewise, the weighted variant of k-means with $z$ outliers requires to determine $S \subset P$ which minimizes the cost function $\text{cost}(P, \hat{w}, S)$, where $\hat{w}$ is obtained from $w$ by scaling the weights associated with the points of $P$ farthest from $S$, progressively until exactly $z$ units of weights overall are subtracted (again, with ties broken arbitrarily). We let $\text{OPT}_k(P, w)$ and $\text{OPT}_{k,z}(P, w)$ denote the cost of the optimal solutions of the two weighted variants above, respectively. (Table 1 summarizes the main notations used in the paper.)

**Doubling Dimension.** The algorithms presented in this paper are designed for general metric spaces, and their performance is analyzed in terms of the dimensionality of the dataset $P$, as captured by the well-established notion of doubling dimension defined as follows [10]. For any $p \in P$ and $r > 0$, let the ball of radius $r$ centered at $p$ be the set of points of $P$ at distance at most $r$ from $p$. The doubling dimension of $P$ is the smallest value $D$ such that for every $p \in P$ and $r > 0$, the ball of radius $r$ centered at $p$ is contained in the union of at most $2^{O(D)}$ balls of radius $r/2$, centered at suitable points of $P$. The doubling dimension can be regarded as a generalization of the Euclidean dimensionality to general spaces. In fact, it is easy to see that any $P \subset \mathbb{R}^\text{dim}$ under Euclidean distance has doubling dimension $O(\text{dim})$.

**Model of Computation.** We present and analyze our algorithms using the MapReduce model of computation [10, 22], which is one of the reference models for the distributed processing of large datasets, and has been effectively used for clustering problems (e.g., see [23, 6, 4]). A MapReduce algorithm specifies a sequence of rounds, where in each round, a multiset $X$ of key-value pairs is first transformed into a new multiset $X'$ of pairs by applying a given map function in parallel to each individual pair, and then into a final multiset $Y'$ of pairs by applying a given reduce function (referred to as reducer) in parallel to each subset of pairs of $X'$ having the same key. When the algorithm is executed on a distributed platform, the applications of the map and reduce functions in each round are (automatically) assigned to the available processors so to maximize parallelism. The data, maintained into a distributed storage system, are brought to the processors’ main memories in chunks, when needed by the map and reduce functions. Key performance indicators are the number of rounds and the maximum local memory required by individual executions of the map and reduce functions. Efficient algorithms typically target few (possibly, constant) rounds and substantially sublinear local memory. We remark that our algorithms can be straightforwardly rephrased for other distributed models, such as the popular Massively Parallel Computation (MPC) model [5].

### 3 MapReduce algorithm for k-means with $z$ outliers

In this section, we present a MapReduce algorithm for k-means with $z$ outliers running in $O(1)$ rounds with sublinear local memory. As typical of many efficient algorithms for clustering and related problems, our algorithm uses the following coreset-based approach. First, a suitably small weighted coreset $T$ is extracted from the input $P$, such that each point $p \in P$ has a “close” proxy $\pi(p) \in T$, and the weight $w_q$ of each $q \in T$ is the number of points of $P$ for which $q$ is proxy. Then, the final solution is obtained by running on $T$ the best (possibly slow) sequential approximation algorithm for weighted k-means with $z$ outliers. Essential to the success of this strategy is that $T$ can be computed efficiently in a distributed fashion, its size is much smaller than $|P|$, and it represents $P$ well, in the sense that: (i) the cost of any solution with respect to $P$ can be approximated well in $T$; and (ii) $T$ contains a good solution to $P$.

In Subsection 3.1 we describe a coreset construction, building upon the one presented in [15, 21] for the case without outliers, but with crucial modifications and a new analysis needed to handle the more general cost function, and to allow the use of bicriteria approximation algorithms on the coreset. In Subsection 3.2 we present and analyze the final algorithm, while in Subsection 3.3 we outline how a refined coreset construction can yield substantially lower local memory requirements.

#### 3.1 Flexible coreset construction

We first formally define two properties that capture the quality of the coreset computed by our algorithm. Let $T$ be a subset of $P$ weighted according to a proxy function $\pi : P \to T$, where the weight of each $q \in T$ is $w_q = |\{p \in P : \pi(p) = q\}|$.

**Definition 1.** For $\gamma \in (0, 1)$, $(T, w)$ is a $\gamma$-approximate coreset for $P$ with respect to $k$ and $z$ if for every $S, Z \subset P$, with $|S| \leq k$ and $|Z| \leq z$, we have:

$$|\text{cost}(P \setminus Z, S) - \text{cost}(T, \hat{w}, S)| \leq \gamma \cdot \text{cost}(P \setminus Z, S),$$

where $\hat{w}$ is such that for each $q \in T$, $\hat{w}_q = w_q - |\{p \in Z : \pi(p) = q\}|$.  


Definition 2. For $\gamma \in (0, 1)$, $(T, w)$ is a $\gamma$-centroid set for $P$ with respect to $k$ and $z$ if there exists a set $X \subseteq T$ of at most $k$ points such that
\[
\text{cost}(P \setminus \text{out}_{z}(P, X), X) \leq (1 + \gamma) \cdot \text{OPT}_{k,z}(P).
\]

In other words, a $\gamma$-approximate coreset can faithfully estimate (within relative error $\gamma$) the cost of any solution with respect to the entire input dataset $P$, while a $\gamma$-centroid set is guaranteed to contain one good solution for $P$. The following technical lemma states a sufficient condition for a weighted set to be an approximate coreset.

Lemma 1. Let $(T, w)$ be such that $\sum_{p \in P} d(p, \pi(p))^2 \leq \delta \cdot \text{OPT}_{k,z}(P)$. Then, $(T, w)$ is a $\gamma$-approximate coreset for $P$ with respect to $k$ and $z$, with $\gamma = \delta + 2\sqrt{3}$.

Proof. Consider two arbitrary subsets $S, Z \subseteq P$ with $|S| = k$ and $|Z| = z$, and let $\hat{w}$ be obtained from $w$ by subtracting the contributions of the elements in $Z$ from the weights of their proxies. We have:

\[
|\text{cost}(P \setminus Z, S) - \text{cost}(T, \hat{w}, S)| = | \sum_{p \in P \setminus Z} d(p, S)^2 - \sum_{q \in T} \hat{w}_q d(q, S)^2 |
\]

\[
= | \sum_{p \in P \setminus Z} d(p, S)^2 - \sum_{p \in P \setminus Z} d(\pi(p), S)^2 |
\]

\[
\leq \sum_{p \in P \setminus Z} |d(p, S)^2 - d(\pi(p), S)^2 |
\]

\[
= \sum_{p \in P \setminus Z} (d(p, S) + d(\pi(p), S))d(p, S) - d(\pi(p), S)|
\]

\[
\leq \sum_{p \in P \setminus Z} (d(p, \pi(p)) + 2d(p, S))d(p, \pi(p))
\]

(since, by Fact 2) $d(p, \pi(p) \leq d(p, S) - d(\pi(p), S) \leq d(p, \pi(p))$

\[
= \sum_{p \in P \setminus Z} d(p, \pi(p))^2 + 2 \sum_{p \in P \setminus Z} d(p, S) \cdot d(p, \pi(p)).
\]

By the hypothesis, we have that $\sum_{p \in P} d(p, \pi(p))^2 \leq \delta \cdot \text{OPT}_{k,z}(P)$, and since $\text{OPT}_{k,z}(P) \leq \text{cost}(P \setminus Z, S)$, the first sum is upper bounded by $\delta \cdot \text{cost}(P \setminus Z, S)$. Let us now concentrate on the second summation. As observed in the proof of Fact 2 for any $a, b, c > 0$, we have that $2ab \leq ca^2 + (1/c)b^2$. Therefore,

\[
2 \sum_{p \in P \setminus Z} d(p, S) \cdot d(p, \pi(p)) \leq \sqrt{3} \sum_{p \in P \setminus Z} d(p, S)^2 + \left(1/\sqrt{3}\right) \sum_{p \in P \setminus Z} d(p, \pi(p))^2 \]

\[
\leq \sqrt{3} \sum_{p \in P \setminus Z} d(p, S)^2 + \sqrt{3} \cdot \text{OPT}_{k,z}(P) \]

\[
\leq 2\sqrt{3} \cdot \text{cost}(P \setminus Z, S).
\]

The lemma follows since $\gamma = \delta + 2\sqrt{3}$. 

The first ingredient of our coreset construction is a primitive, called CoverWithBalls, which, given any set $X \subseteq P$, a precision parameter $\delta$, and a distance threshold $R$, builds a weighted set $Y \subseteq P$ whose size is not much larger than $X$, such that for each $p \in P$, $d(p, Y) \leq \delta \cdot \max\{R, d(q, X)\}$. Specifically, the primitive identifies, for each $p \in P$, a proxy $\pi(p) \in Y$ such that $d(p, \pi(p)) \leq \delta \cdot \max\{R, d(p, X)\}$. For every $q \in Y$, the returned weight $w_q$ is set equal to the number of points of $P$ for which $q$ is proxy. Primitive CoverWithBalls has been originally introduced in [21] and is based on a simple greedy procedure. For completeness, we report the pseudocode below, as Algorithm 1. We wish to remark that the proxy function $\pi$ is not explicitly represented and is reflected only in the vector $w$. In our coreset construction, CoverWithBalls will be invoked multiple times to compute coresets of increasingly higher quality. Observe that the output $(Y, w)$ of CoverWithBalls $(P, X, \delta, R)$ is implicitly associated with a map $\pi : P \rightarrow Y$ such that:

- for every $q \in Y$, $w_q = |\{p \in P : \pi(p) = q\}|$;
- for every $p \in P \setminus Y$, $d(p, \pi(p)) \leq \delta \cdot \max\{R, d(p, X)\}$.
Algorithm 1: CoverWithBalls\(\mathcal{P}, X, \delta, R\)

\begin{algorithmic}[1]
\STATE \(Y \leftarrow \emptyset;\)
\WHILE {\(P \neq \emptyset\)}
    \STATE \(q \leftarrow\) arbitrarily selected point in \(P;\)
    \STATE \(Y \leftarrow Y \cup \{q\}; w_q \leftarrow 1;\)
    \FOR EACH \(p \in P\)
        \IF {\(d(p,q) \leq \delta \max\{R, d(p, X)\}\)}
            \STATE remove \(p\) from \(P;\)
            \STATE \(w_q \leftarrow w_q + 1\); \{implicitly, \(q\) becomes the proxy \(\pi(p)\) of \(p\)\} \\
        \ENDIF
    \ENDFOR
\ENDWHILE
\RETURN \((Y, w)\)
\end{algorithmic}

The second ingredient of our distributed coreset construction is some sequential algorithm, referred to as SeqkMeans in the following, which, given in input a dataset \(Q\) and an integer \(k\), computes a \(\beta\)-approximate solution to the standard k-means problem without outliers with respect to \(Q\) and \(k\).

We are now ready to present a 2-round MapReduce algorithm, dubbed MRcoreset, that, on input a dataset \(P\), the values \(k\) and \(z\), and a precision parameter \(\gamma\), combines the two ingredients presented above to produce a weighted coreset which is both an \(O(\gamma)\)-approximate coreset and an \(O(\gamma)\)-centroid set with respect to \(k\) and \(z\). The computation performed by \(\text{MRcoreset}(P, k, z, \gamma)\) in each round is described below.

First Round The dataset \(P\) is evenly partitioned into \(L\) equally sized subsets, \(P_1, P_2, \ldots, P_L\), through a suitable map function. Then, in parallel, the following steps are performed by a distinct reducer on each \(P_i\), with \(1 \leq i \leq L\):

1. SeqkMeans is invoked with input \((P_i, k')\), where \(k'\) is a suitable function of \(k\) and \(z\) that will be fixed later in the analysis, returning a solution \(S_i \subset P_i\).
2. Let \(R_i = \sqrt{\text{cost}(P_i, S_i)/|P_i|}\). The primitive \(\text{CoverWithBalls}(P_i, S_i, \gamma/\sqrt{2\beta}, R_i)\) is invoked, returning a weighted set of points \((C_i, w^C_i)\).

Second Round The same partition of \(P\) into \(P_1, P_2, \ldots, P_L\) is used. A suitable map function is applied so that each reducer receives a distinct \(P_i\) and the triplets \((|P_j|, R_j, C_j)\) for all \(1 \leq j \leq L\) from Round 1 (the weights \(w^C_i\) are ignored). Then, for \(1 \leq i \leq L\), in parallel, the reducer in charge of \(P_i\) sets \(R = \sqrt{\sum_{j=1}^{L} |P_j| \cdot R_j^2 / |P|}\), \(C = \bigcup_{j=1}^{L} C_j\), and invokes \(\text{CoverWithBalls}(P_i, C, \gamma/\sqrt{2\beta}, R)\). The invocation returns the weighted set \((T_i, w^{T_i})\).

The final coreset returned by the algorithm is \((T, w^{T})\), where \(T = \bigcup_{i=1}^{L} T_i\) and \(w^{T}\) is the weight function such that \(w^{T_i}\) is the projection of \(w^{T}\) on \(P_i\), for \(1 \leq i \leq L\).

We now analyze the main properties of the weighted coreset returned by \(\text{MRcoreset}\), which will be exploited in the next subsection to derive the performance-accuracy tradeoffs featured by our distributed solution to k-means with \(z\) outliers. Recall that we assumed that SeqkMeans is instantiated with an approximation algorithm that, when invoked on input \((P_i, k')\), returns a set \(S_i \subset P_i\) of \(k'\) centers such that \(\text{cost}(P_i, S_i) \leq \beta \cdot \text{OPT}_{k'}(P_i)\), for some \(\beta \geq 1\). Let \(D\) denote the doubling dimension of \(P\). The following lemma is a consequence of the analysis in [21] for the case without outliers, and its proof (omitted) is a simple composition of the proofs of Lemmas 3.6, 3.11, and 3.12 in that paper.

**Lemma 2.** Let \((C, w^C)\) and \((T, w^{T})\) be the weighted coresets computed by \(\text{MRcoreset}(P, k, z, \gamma)\), and let \(\pi^C, \pi^T\) be the corresponding proxy functions. We have:

\[
\sum_{p \in P} d(p, \pi^X(p))^2 \leq 4\gamma^2 \cdot \text{OPT}_{k'}(P), \quad \text{(with } X = C, T)\]

and

\[
|C| = O\left(|L| \cdot (8\sqrt{2\beta}/\gamma)^D \cdot \log |P|\right),
\]
\[
|T| = O\left(|L|^2 \cdot (8\sqrt{2\beta}/\gamma)^{2D} \cdot \log^2 |P|\right).
\]
As noted in the introduction, while the doubling dimension \( D \) appears in the above bounds, the algorithm does not require the knowledge of this value, which would be hard to compute. The next theorem establishes the main result of this section regarding the quality of the coreset \((T, w^T)\) with respect to the k-means problem with \( z \) outliers.

**Theorem 1.** Let \( \gamma \) be such that \( 0 < \gamma \leq \sqrt{3/8} - 1/2 \). By setting \( k' = k + z \) in the first round, \( \mathcal{MRcoreset}(P, k, z, \gamma) \) returns a weighted coreset \((T, w^T)\) which is a \((4\gamma + 4\gamma^2)\)-approximate coreset and a \(2\gamma^2\)-centroid set for \( P \) with respect to \( k \) and \( z \).

**Proof.** Define \( \sigma = 4\gamma + 4\gamma^2 \) and, by the hypothesis on \( \gamma \), note that \( \sigma \leq 1/2 \). The fact that \((T, w^T)\) is a \(\sigma\)-approximate coreset for \( P \) with respect to \( k \) and \( z \), follows directly from Fact 1, Lemma 1 (setting \( \delta = 4\gamma^2 \)), and Lemma 2. We are left to show that \((T, w^T)\) is a \(2\gamma^2\)-centroid set for \( P \) with respect to \( k \) and \( z \). Let \( S^* \subseteq P \) be the optimal set of \( k \) centers and let \( Z^* = \text{out}_z(P, S^*) \). Hence, \( \text{cost}(P \setminus Z^*, S^*) = \text{OPT}_{k,z}(P) \). Define \( X = \{ p^T : p \in S^* \} \subseteq T \). We show that \( X \) is a good solution for the k-means problem with \( z \) outliers for \( P \). Clearly, \( \text{cost}(P \setminus Z^*, X) \leq \text{cost}(P \setminus Z^*, S^*) \), hence it is sufficient to upper bound the latter term. To this purpose, consider the weighted set \((C, w^C)\) computed at the end of Round 1, and let \( \mathcal{MRcoreset}(P, k, z, \gamma) \) be the proxy function defining the weights \( w^C \). Arguing as before, we can conclude that \((C, w^C)\) is also a \(\sigma\)-approximate coreset for \( P \) with respect to \( k \) and \( z \). Therefore, since \( \sigma \leq 1/2 \),

\[
\text{cost}(P \setminus Z^*, X) \leq \frac{1}{1 - \sigma} \text{cost}(C, w^C, X) \leq (1 + 2\sigma)\text{cost}(C, w^C, X),
\]

where \( \hat{w}^C \) is obtained from \( w^C \) by subtracting the contributions of the elements in \( Z^* \) from the weights of their proxies. Then, we have:

\[
\text{cost}(C, \hat{w}^C, X) = \sum_{q \in C} \hat{w}^C_q d(q, X)^2 \\
\leq (1 + \gamma) \sum_{q \in C} \hat{w}^C_q d(q, q^{S^*})^2 + (1 + (1/\gamma)) \sum_{q \in C} \hat{w}^C_q d(q^{S^*}, X)^2 \\
\text{(by Fact 1)} = (1 + \gamma)\text{cost}(C, \hat{w}^C, S^*) + (1 + (1/\gamma)) \sum_{q \in C} \hat{w}^C_q d(q^{S^*}, X)^2 \\
\leq (1 + \gamma)(1 + \sigma)\text{OPT}_{k,z}(P) + (1 + (1/\gamma)) \sum_{q \in C} \hat{w}^C_q d(q^{S^*}, X)^2 \\
\text{(since \((C, w^C)\) is a \(\sigma\)-approximate coreset)}.
\]

We now concentrate on the term \( \sum_{q \in C} \hat{w}^C_q d(q^{S^*}, X)^2 \). First observe that, since \( X \subseteq T \) contains the point in \( T \) closest to \( q^{S^*} \), we have \( d(q^{S^*}, X) = d(q^{S^*}, T) \) and \( \text{CoverWithBalls} \) guarantees that \( d(q^{S^*}, T) \leq (\gamma/\sqrt{2\beta})(R + d(q^{S^*}, C)) \), where \( R \) is the parameter used in \( \text{CoverWithBalls} \). Also, for \( q \in C, d(q^{S^*}, C) \leq d(q^{S^*}, q) \). Now,

\[
\sum_{q \in C} \hat{w}^C_q d(q^{S^*}, X)^2 \leq (\gamma^2/(2\beta)) \sum_{q \in C} \hat{w}^C_q (R^2 + d(q, S^*)^2) \\
\leq (\gamma^2/(2\beta)) \left( \frac{|P| - z}{|P|} \sum_{i=1}^L |P_i| \cdot R^2 + \sum_{q \in C} \hat{w}^C_q d(q, S^*)^2 \right) \\
\leq (\gamma^2/(2\beta)) \left( \sum_{i=1}^L \text{cost}(P_i, S_i) + \sum_{q \in C} \hat{w}^C_q d(q, S^*)^2 \right) \\
\leq (\gamma^2/(2\beta)) \left( \beta \sum_{i=1}^L \text{OPT}_{k+z}(P_i) + \text{cost}(C, \hat{w}^C, S^*) \right) \\
\leq (\gamma^2/2) \left( \sum_{i=1}^L \text{OPT}_{k+z}(P_i) + \text{cost}(C, \hat{w}^C, S^*) \right) \text{(since } \beta \geq 1). \]

Using the triangle inequality and Fact 1, it is easy to show that \( \sum_{i=1}^L \text{OPT}_{k+z}(P_i) \leq 4 \cdot \text{OPT}_{k,z}(P) \). Moreover, since \((C, w^C)\) is a \(\sigma\)-approximate coreset for \( P \) with respect to \( k \) and \( z \), \( \text{cost}(C, w^C, S^*) \leq (1 + \sigma)\text{OPT}_{k,z}(P) \).
Consequently, \( \sum_{q \in C} w_q^C d(q^C, X)^2 \leq (\gamma^2/2)(5 + \sigma)\text{OPT}_{k,z}(P) \). Putting it all together and recalling that \( \sigma = 4\gamma + 4\gamma^2 \leq 1/2 \), we conclude that

\[
\text{cost}(P \setminus Z^*, X) \\
\leq (1 + 2\sigma)((1 + \gamma)(1 + \sigma) + (1 + 1/\gamma)(\gamma^2/2)(5 + \sigma)) \cdot \text{OPT}_{k,z}(P) \\
\leq (1 + 27\gamma)\text{OPT}_{k,z}(P).
\]

\[\square\]

### 3.2 Complete algorithm

Let Seq\text{WeightedOut} be a sequential algorithm for weighted k-means with \( z \) outliers, which, given in input a weighted set \((T, w^T)\) returns a (possibly bicriteria) solution \( S \) of \( \rho k \) centers such that cost\((T, \hat{w}^T, S) \leq \alpha \cdot \text{OPT}_{k,z}(T, w)\), where \( \rho \geq 1 \) and \( \hat{w}^T \) is obtained from \( w^T \) by scaling \( \tau z \) units of weight from the points of \( T \) farthest from \( S \), for some \( \tau \geq 1 \). For \( \gamma > 0 \), the complete algorithm first runs the 2-round \( \text{MRcoreset}(P, \rho k, \tau z, \gamma) \) algorithm, to extract a weighted coreset \((T, w^T)\). Then, in a third round, the coreset is gathered in a single reducer which runs Seq\text{WeightedOut}(T, w^T, k, z) to compute the final solution \( S \). We have:

**Theorem 2.** For \( 0 < \gamma \leq \sqrt{3/8} - 1/2 \), the above 3-round MapReduce algorithm computes a solution \( S \) of at most \( \rho k \) centers such that

\[
\text{cost}(P \setminus \text{out}_{\tau z}(P, S), S) \leq (\alpha + O(\gamma)) \cdot \text{OPT}_{k,z}(P),
\]

and requires \( O\left(|P|^{2/3} \cdot (\rho k + \tau z)^{1/3} \cdot (8\sqrt{23}/\gamma)^{2D} \cdot \log^2 |P|\right) \) local memory.

**Proof.** Let \( T \) be the coreset computed at Round 2, and let \( \hat{Z} \subseteq P \) be such that the scaled weight function \( \hat{w}^T \), associated to the solution \( S \) computed in Round 3, can be obtained from \( w^T \) by subtracting the contribution of each point in \( \hat{Z} \) from the weight of its proxy in \( T \). Clearly, \(|Z| \leq \tau z \) and \( \text{cost}(P \setminus \text{out}_{\tau z}(P, S), S) \leq \text{cost}(P \setminus \hat{Z}, S) \). Now, let \( \sigma = 4\gamma + 4\gamma^2 \leq 1/2 \). We know from Theorem 1 that \((T, w^T)\) is a \( \sigma \)-approximate coreset for \( P \) with respect to \( \rho k \) and \( \tau z \). We have:

\[
\text{cost}(P \setminus \hat{Z}, S) \leq \frac{1}{1 - \sigma} \text{cost}(T, \hat{w}^T, S) \\
\leq (1 + 2\sigma) \text{cost}(T, \hat{w}^T, S) \leq (1 + O(\gamma)) \cdot \alpha \cdot \text{OPT}_{k,z}(T, w).
\]

Since \( \text{OPT}_{\rho k, \tau z}(P) \leq \text{OPT}_{k,z}(P) \). Fact 1 and Lemma 2 can be used to prove that both \((C, w^C)\) (computed in Round 1) and \((T, w^T)\) are \( \sigma \)-approximate coresets for \( P \) with respect to \( k \) and \( z \). A simple adaptation of the proof of Theorem 1 shows that \((T, w^T)\) is a \( 27\gamma \)-centroid set for \( P \) with respect to \( k \) and \( z \). Now, let \( X \subseteq T \) be the set of at most \( k \) points of Definition 2, and let \( \hat{w}^T \) be obtained from \( w^T \) by subtracting the contributions of the elements in \( \text{out}_{\tau z}(P, X) \) from the weights of their proxies. By the optimality of \( \text{OPT}_{k,z}(T, w) \) we have that

\[
\text{OPT}_{k,z}(T, w) \leq \text{cost}(T, w^T, X) \\
\leq (1 + \sigma) \text{cost}(P \setminus \text{out}_{\tau z}(P, X), X) \\
\leq (1 + \sigma)(1 + 27\gamma) \cdot \text{OPT}_{k,z}(P) = (1 + O(\gamma)) \cdot \text{OPT}_{k,z}(P).
\]

Putting it all together, we conclude that

\[
\text{cost}(P \setminus \text{out}_{\tau z}(P, S), S) \leq \text{cost}(P \setminus \hat{Z}, S) \leq (\alpha + O(\gamma)) \cdot \text{OPT}_{k,z}(P).
\]

The local memory bound follows from Lemma 2 setting \( L = (|P|/(\rho k + \tau z))^{1/3} \).

\[\square\]

### 3.3 Improved local memory

The local memory of the algorithm presented in the previous subsections can be substantially improved by modifying Round 2 of \( \text{MRcoreset}(P, k, z, \gamma) \) as follows. Now, each reducer first determines a \( \beta \)-approximate solution \( S_C \) to weighted k-means (without outliers) on \((C, w^C)\) with \( k' = k + z \) centers, and then runs \( \text{CoverWithBalls}(C, S_C, \gamma/\sqrt{23}, R) \), yielding a weighted set \( C' \), whose size is a factor \(|L|\) less than the size of \( C \). Finally, the reducer runs \( \text{CoverWithBalls}(P, C', \gamma/\sqrt{23}, R) \). A small adaptation to \( \text{CoverWithBalls} \) is required in this case: when point \( p \in C \) is mapped to a proxy \( q \in C' \), the weight of \( q \) is increased by \( w_q^C \) rather than by one. The analysis of this modified construction is given below.
Lemma 3. Let \((C', w^{C'})\) be the weighted coreset computed by CoverWithBalls\((C, S_C, \gamma / \sqrt{2}\beta, R)\) with \(0 < \gamma \leq \sqrt{3}/8 - 1/2\). Then, there exists a proxy function \(\pi^{C'}: P \rightarrow C'\) such that
\[
\sum_{p \in P} d(p, \pi^{C'}(p))^2 \leq 18\gamma^2 \cdot \text{OPT}_{k'}(P).
\]

Proof. Let \(\pi^C: P \rightarrow C\) be the proxy function of Lemma 2 and let \(\phi^{C'}: C \rightarrow C'\) be the map induced by CoverWithBalls\((C, S_C, \gamma / \sqrt{2}\beta, R)\). Define \(\pi^{C'}: P \rightarrow C'\) as \(\phi^{C'} \circ \pi^C\). By the triangle inequality and Lemma 2, we have that
\[
\sum_{p \in P} d(p, \pi^{C'}(p))^2 \leq 2 \sum_{p \in P} d(p, \pi^C(p))^2 + 2 \sum_{p \in P} d(\pi^C(p), \pi^{C'}(p))^2
\]
\[
\leq 8\gamma^2 \cdot \text{OPT}_{k'}(P) + 2 \sum_{q \in C} w_q \cdot d(q, \phi^{C'}(q))^2.
\]

The latter term can be bounded by using the properties of CoverWithBalls as follows. Let \(\overline{S}^*\) be the optimal centers for \(P\) with respect to \(k\). We have that
\[
\sum_{q \in C} w_q \cdot d(q, \phi^{C'}(q))^2 \leq (\gamma^2/(2\beta)) \sum_{q \in C} w_q \cdot (R^2 + d(q, S_C))^2
\]
\[
\leq (\gamma^2/(2\beta)) \left( \sum_{i=1}^L |P_i| \cdot R_i^2 + \text{cost}(C, w^C, S_C) \right)
\]
\[
\leq (\gamma^2/(2\beta)) \left( \sum_{i=1}^L \text{cost}(P_i, S_i) + \text{cost}(C, w^C, S_C) \right)
\]
\[
\leq (\gamma^2/(2\beta)) \left( 4\beta \sum_{i=1}^L \text{cost}(P_i, \overline{S}^*) + \beta \cdot \text{OPT}_{k'}(C, w^C) \right)
\]
\[
\leq (\gamma^2/2) \left( 4 \cdot \text{OPT}_{k'}(P) + \text{OPT}_{k'}(C, w^C) \right).
\]

By combining the arguments of Lemma 1 and Lemma 2, we obtain that \((C, w^C)\) is a \(\sigma\)-approximate coreset for \(P\) with respect to \(k\) and \(z = 0\), with \(\sigma = 4\gamma + 4\gamma^2 \leq 1/2\). Thus, using again the triangle inequality
\[
\text{OPT}_{k'}(C, w^C) \leq 4\text{cost}(C, w^C, \overline{S}^*)
\]
\[
\leq 4(1 + \sigma)\text{cost}(P, \overline{S}^*)
\]
\[
\leq 6 \cdot \text{OPT}_{k'}(P).
\]

Putting it all together, we conclude that
\[
\sum_{p \in P} d(p, \pi^{C'}(p))^2 \leq 18\gamma^2 \cdot \text{OPT}_{k'}(P).
\]

\[\square\]

Lemma 4. Let \((T, w^T)\) be the weighted coreset computed by \(\text{MRcoreset}(P, k, z, \gamma)\), and let \(\pi^T\) be the corresponding proxy function. We have:
\[
\sum_{p \in P} d(p, \pi^T(p))^2 \leq 11\gamma^2 \cdot \text{OPT}_{k'}(P).
\]

Proof. By the properties of the output of CoverWithBalls and Lemma 3, we have that
\[
\sum_{p \in P} d(p, \pi^T(p))^2 \leq (\gamma^2/(2\beta)) \left( \sum_{i=1}^L |P_i| \cdot R_i^2 + \sum_{p \in P} d(p, \pi^{C'}(p))^2 \right)
\]
\[
\leq (\gamma^2/(2\beta))(4\beta + 18\gamma^2) \cdot \text{OPT}_{k'}(P)
\]
\[
\leq 11\gamma^2 \cdot \text{OPT}_{k'}(P).
\]

\[\square\]
From Fact 1 and Lemmas 1 and 4, it follows that \((T, w^T)\) is an \((11\gamma^2 + 2\sqrt{11}\gamma)\)-approximate coreset for \(P\) with respect to \(k\) and \(z\). Moreover, by a slight adaptation of the proof of Theorem 1 and by setting \(\gamma \leq (\sqrt{3} - \sqrt{2})/6\), we have that \((T, w^T)\) is also a \(47\gamma\)-centroid set for \(P\) with respect to \(k\) and \(z\).

The main result is stated in the following theorem.

**Theorem 3.** For \(0 < \gamma \leq (\sqrt{3} - \sqrt{2})/6\), the modified 3-round MapReduce algorithm computes a solution \(S\) of at most \(pk\) centers such that

\[
\text{cost}(P, \text{out}_{z}(P, S), S) \leq (\alpha + O(\gamma)) \cdot \text{OPT}_{k,z}(P).
\]

The algorithm requires \(O\left(|P|^{1/2} \cdot (pk + \tau z)^{1/2} \cdot (8\sqrt{3}/\gamma)^{2D} \cdot \log^2 |P|\right)\) local memory.

**Proof.** The bound on the approximation factor is obtained as a straightforward adaptation of the proof of Theorem 2. For what concerns the local memory requirements, the result in [21] concerning the size of the output of CoverWithBalls yields:

\[
|C'| = O \left((pk + \tau z) \cdot (8\sqrt{3}/\gamma)^D \cdot \log |P|\right),
\]

\[
|T| = O \left(|L| \cdot (pk + \tau z) \cdot (8\sqrt{3}/\gamma)^{2D} \cdot \log^2 |P|\right).
\]

Setting \(L = (|P|/(pk + \tau z))^{1/2}\), we get the desired upper bound.

\[]

\section{Instantiation with different sequential algorithms for weighted k-means}

We briefly outline how to adapt two state-of-the-art sequential algorithms for \(k\)-means with \(z\) outliers in general metrics, namely, LS-Outlier [14] and \(\text{k-Means-Out}\) by [12], to handle the weighted variant of the problem. The algorithms are bicriteria, in the sense that the approximation guarantee is obtained at the expense of a larger number of outliers (LS-Outlier), or a larger number of centers (\(\text{k-Means-Out}\)). Then, we assess the accuracy-resource tradeoffs attained by the MapReduce algorithm of Section 3 when these algorithms are employed in its final round.

Given a set of points \(P\) and parameters \(k\) and \(z\), LS-Outlier starts with a set \(C = \text{out}_{z}(P, C)\) of outliers. Then, for a number of iterations, it refines the selection \((C, Z)\) to improve the value \(\text{cost}(P \setminus Z, C)\) by a factor at least \(1 - \epsilon/k\), for a given \(\epsilon > 0\), until no such improvement is possible. In each iteration, first a new set \(C'\) is computed through a standard local-search [13] on \(P\setminus Z\), and then a new pair \((C_{\text{new}}, Z_{\text{new}})\) with minimal \(\text{cost}(P \setminus Z_{\text{new}}, C_{\text{new}})\) is identified among the following ones: \((C', Z \cup \text{out}_{z}(P \setminus Z, C'))\) and \((C'_{\text{new}}, Z \cup \text{out}_{z}(P, C'_{\text{new}}))\), where \(C'_{\text{new}}\) is obtained from \(C'\) with the most profitable swap between a point of \(P\) and a point of \(C'_{\text{new}}\).

It is shown in [14] that LS-Outlier returns a pair \((C, Z)\) such that \(\text{cost}(P \setminus Z, C) \leq 274 \cdot \text{OPT}_{k,z}(P)\) and \(|Z| = O\left((1/\epsilon)kz\log(|P|\Delta)\right)\), where \(\Delta\) is the ratio between the maximum and minimum pairwise distances in \(P\). LS-Outlier can be adapted for the weighted variant of the problem as follows. Let \((P, w)\) denote the input pointset. In this weighted setting, the role of a set \(Z\) of \(m\) outliers is played by a weight function \(w^Z\) such that \(0 \leq w^Z_p \leq w_p\) for each \(p \in P\), and \(\sum_{p \in P} w^Z_p = m\). The union of two sets of outliers in the original algorithm is replaced by the pointwise sum or pointwise maximum of the corresponding weight functions, depending on whether the two sets are disjoint (e.g., \(Z\) and \(\text{out}_{z}(P \setminus Z, C')\)) or not (e.g., \(Z\) and \(\text{out}_{z}(P, C'_{\text{new}})\)). It can be proved that with this adaptation the algorithm returns a pair \((C, w^C)\) such that \(\text{cost}(P, w - w^Z, C) \leq 274 \cdot \text{OPT}_{k,z}(P, w)\) and \(\sum_{p \in P} w^Z_p = O\left((1/\epsilon)kz\log(|P|\Delta)\right)\).

Algorithm \(\text{k-Means-Out}\) also implements a local search. For given \(\rho, \epsilon > 0\), the algorithm starts from an initial set \(C \subseteq P\) of \(k\) centers and performs a number of iterations, where \(C\) is refined into a new set \(C'\) by swapping a subset \(Q \subseteq C\) with a subset \(U \subseteq P \setminus C\) (possibly of different size), such that \(|Q|, |U| \leq \rho \cdot |C| \leq (1 + \epsilon)k\), as long as \(\text{cost}(P \setminus \text{out}_{z}(P, C), C') < (1 - \epsilon/k) \cdot \text{cost}(P \setminus \text{out}_{z}(P, C), C)\). It is argued in [12] that for \(\rho = \left(D/\epsilon\right)^{(D/\epsilon)}\), \(\text{k-Means-Out}\) returns a set \(C\) of at most \((1 + \epsilon)k\) centers such that \(\text{cost}(P \setminus \text{out}_{z}(P, C), C) \leq (1 + \epsilon) \cdot \text{OPT}_{k,z}(P)\), where \(D\) is the doubling dimension of \(P\). The running time is exponential in \(\rho\), so the algorithm is polynomial when \(D\) is constant.

The adaptation of \(\text{k-Means-Out}\) for the weighted variant for an input \((P, w)\) is straightforward and concerns the cost function only. It is sufficient to substitute \(\text{cost}(P \setminus \text{out}_{z}(P, C), C)\) with \(\text{cost}(P, w - w^Z, C)\), where \(w\) is obtained from \(w\) by scaling the weights associated with the points of \(P\) farthest from \(C\), progressively until exactly \(z\) units of weights overall are subtracted. It can be proved that with this adaptation the algorithm returns a set \(C\) of at most \((1 + \epsilon)k\) centers such that \(\text{cost}(P, w, C) \leq (1 + \epsilon) \cdot \text{OPT}_{k,z}(P)\).

By Theorems 2 and 3, these two sequential strategies can be invoked in Round 3 of our MapReduce algorithm to yield bicriteria solutions with an additive \(O(\gamma)\) term in the approximation guarantee, for any sufficiently small \(\gamma > 0\).
5 Conclusions

We presented a flexible, coreset-based framework able to yield a scalable, 3-round MapReduce algorithm for k-means with $z$ outliers, featuring an approximation quality which can be made arbitrarily close to the one of any sequential (bicriteria) approximation algorithm for the weighted variant of the problem, and requiring local memory substantially sublinear in the size of the input dataset, when this dataset has bounded dimensionality. Our approach naturally extends to the case of k-median clustering with outliers, where the cost function is the sum of distances rather than of squared distances. Future research will target the adaptation of the state-of-the-art non-bicriteria LP-based algorithm of [19] to the weighted case, and the generalization of our approach to other clustering problems.

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