Improved Coresets for Euclidean k-Means

Anonymous Author(s)
Affiliation
Address
email

Abstract

Given a set of n points in d dimensions, the Euclidean k-means problem consists of finding k centers such that the sum of squared distances from every point to its closest center is minimized. The arguably most popular way of dealing with this problem in the big data setting is to first compress the data by computing a weighted subset known as a coreset and then run any algorithm on this subset. The guarantee of the coreset is that for any candidate solution, the ratio between coreset cost and the cost of the original instance is less than a $(1 \pm \varepsilon)$ factor. The current state of the art coreset size for Euclidean k-means is $\tilde{O}(k\varepsilon^{-2} \cdot \min(k, \varepsilon^{-2}))$. This matches the lower bound of $\Omega(k\varepsilon^{-2})$ up to the $\min(k, \varepsilon^{-2})$ term. In this paper, we improve this bound to $\min(\sqrt{k}, \varepsilon^{-2})$. In the regime where $k \leq \varepsilon^{-2}$, this is a strict improvement over the state of the art. In particular, ours is the first provable bound that breaks through the k^2 barrier while retaining an optimal dependency on ε.

1 Introduction

Coresets have become a staple in the design of algorithms for large data sets. In the most general setting, a coreset compresses the data set in such a way that for any set of previously specified candidate queries, the cost of evaluating the query and the cost of the coreset are similar, up to an arbitrary small distortion.

A popular subject in coreset literature is the Euclidean k-means problem. Here, we are given n points P in d dimensions and our task is to find a set of k points C called centers minimizing $\text{cost}(P, C) := \sum_{p \in P} \min_{c \in C} \|p - c\|^2$, where $\|p - c\| = \sqrt{\sum_{i=1}^{d} (p_i - c_i)^2}$ denotes the Euclidean distance. In this case, a coreset is a weighted subset of the input such that difference between the cost for any set of k centers C on the coreset and the cost on the original point set P is at most $\varepsilon \cdot \text{cost}(P, C)$. Since its initial study by Har-Peled and Mazumdar [2004], the Euclidean k-means problem has received arguably the most attention out of any coreset problem. The current state of the art by Cohen-Addad et al. [2022] yields coresets of size $\tilde{O}(k\varepsilon^{-2} \min(k, \varepsilon^{-2}))$, where $\tilde{O}(x)$ hides multiplicative factors that are polylogarithmic in x. Unfortunately, there is still a gap towards the best known lower bound of $\Omega(k\varepsilon^{-2})$ by Cohen-Addad et al. [2022].

We thus have the option of obtaining either an optimal dependency on k, at the cost of a suboptimal dependency on ε^{-1}, or an optimal dependency on ε^{-1}, at the cost of a suboptimal dependency on k. While these bounds suggest that the lower bound is the correct answer, things are not as clear on closer inspection. Quadratic dependencies on k become necessary for many forms of analysis and so far, it is unknown how to avoid this loss while retaining an optimal dependency on the remaining parameters[1]. Moreover, the trade-off between the dependency on k and the dependency on ε^{-2} is natural. Specifically, if $k \approx \varepsilon^{-2}$ the two previous alternatives $\tilde{O}(k^2/\varepsilon^2)$ and $\tilde{O}(k/\varepsilon^4)$ are equal.

[1] As an alternative, coresets of size $\tilde{O}(kd/\varepsilon^2)$ are also known. This offers improvements in low dimensions, but generally a dependency on d is considered worse than a dependency on k or ε^{-2}.

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In this paper we break through this barrier. Specifically, we show that coresets of size $\tilde{O}(k^{1.5}\varepsilon^{-2})$ exist. In our view, this is further and arguably stronger evidence that the $k\varepsilon^{-2}$ bound will be the correct answer. Another contribution exists on a technical level. Previously, most coreset constructions for high dimensions heavily relied on terminal embeddings to facilitate the analysis. In this paper, we present a novel method that avoids terminal embeddings. We expect that our technique may have further applications for coreset constructions in Euclidean spaces.

1.1 Techniques

Starting point of our work is the framework introduced by Cohen-Addad et al. [2021a] and specifically Cohen-Addad et al. [2022]. Prior to Cohen-Addad et al. [2022], all coreset analyses required a dependency of at least $k \cdot d \cdot \varepsilon^{-2}$. To illustrate why, suppose we are sampling points from some distribution and wish to use the sampled points as an estimator for the true cost of any candidate solution. The analysis then consists of (1) a bound on the variance σ^2 of the estimator and (2) a bound on the number of solutions $|\mathbb{N}|$ to be approximated. This typically results in coresets of size $O(\varepsilon^{-2} \cdot \sigma^2 \cdot \log |\mathbb{N}|)$. When enumerating all (discretized) candidate solutions, henceforth called a *net*) in d dimensions, virtually all known techniques result in $|\mathbb{N}| \approx \exp(k \cdot d)$. The dependency on d may be reduced to $\log(k/\varepsilon)\varepsilon^{-2}$ using dimension reduction techniques.

To bypass this, Cohen-Addad et al. [2022] used the chaining to technique to define a sequence of discretized candidate solutions. Specifically, they showed that there exist discretizations $\mathbb{N}_\alpha$ of size $\exp(k\alpha^{-2})$ such that for any point p and any solution $\mathcal{S}$, there exists a solution $\mathcal{S}_\alpha$ with

$$|\text{cost}(p, \mathcal{S}_\alpha - \text{cost}(p, \mathcal{S})| \leq \alpha \cdot \text{cost}(p, \mathcal{S}),$$

where $\text{cost}(p, \mathcal{S}_\alpha) = \min_{s \in \mathcal{S}_\alpha} \|p - s\|^2$ and $\text{cost}(p, \mathcal{S}) = \min_{s \in \mathcal{S}} \|p - s\|^2)$. The idea of the analysis is then to write $\text{cost}(p, \mathcal{S})$ as a telescoping sum

$$\text{cost}(p, \mathcal{S}) = \sum_{h=1}^{\infty} \text{cost}(p, \mathcal{S}_{2^{-(h+1)}}) - \text{cost}(p, \mathcal{S}_{2^{-h}})$$

and show that the sampled points achieve concentration for each summand. The number of candidate solutions is now $|\mathbb{N}_{2^{-(h+1)}}| \cdot |\mathbb{N}_{2^{-h}}| \approx \exp(k \cdot 2^{2h})$ but the difference in cost is $2^{-h}\text{cost}(p, \mathcal{S})$. This directly leads to a variance of the order $2^{-2h}\sigma^2$, where σ^2 is the variance of the basic estimator. Thus, the increase in net size is countered by the decrease and variance. Using this technique, Cohen-Addad et al. [2022] obtained a coreset of size roughly $\varepsilon^{-2}k\sigma^2$.

To obtain a bound on σ^2, the framework by Cohen-Addad et al. [2021a] proposed an algorithm that first computes a solution $\mathcal{A}$ with strong structural properties and then samples any point p proportionate $\text{cost}(p, \mathcal{A})$. To simplify the exposition, we assume that $\mathcal{A}$ is the optimum, every cluster has identical cost and every point has identical cost. For this special case, the distribution of Cohen-Addad et al. [2021a] turns out to be equivalent to uniform sampling. For any given solution $\mathcal{S}$, let k_i be the number of clusters of $\mathcal{A}$ whose points are served at cost 2^i times their cost in $\mathcal{A}$ for $i > 2$[2], i.e. $2^i = \frac{\text{cost}(p,\mathcal{S})}{\text{cost}(p,\mathcal{A})}$. Cohen-Addad et al. [2021a] showed that their sampling distribution leads to a variance of the order $\sigma^2 \approx \left(\frac{k \cdot k_i 2^i}{(k + k_i \cdot 2^i)^2}\right) \cdot \min(\varepsilon^{-2}, 2^i, k)$, which yields the $\tilde{O}(k\varepsilon^{-2} \min(k, \varepsilon^{-2}))$ bound.

To improve either the variance or the net size has to reduced. Unfortunately, is unlikely that reducing σ^2 will be possible as the bounds on σ^2 obtained by Cohen-Addad et al. [2022] are tight up to constant factors. Our main goal is to find a net with an finer error of

$$|\text{cost}(p, \mathcal{S}_\alpha) - \text{cost}(p, \mathcal{S})| \leq 2^{-h} \cdot \sqrt{\text{cost}(p, \mathcal{S}), \text{cost}(p, \mathcal{A})}.$$

In the case of $\min(2^i, \varepsilon^{-2}, k) = 2^i$, this leads to a reduced variance for the h-th summand of the order $2^{-2h} \cdot \frac{(\sqrt{\text{cost}(p,\mathcal{S})\text{cost}(p,\mathcal{A})})^2}{\text{cost}(p,\mathcal{A})^2} \cdot \left(\frac{k \cdot k_i}{(k + k_i \cdot 2^i)^2}\right) \leq 2^{-2h} \cdot \left(\frac{k \cdot k_i \cdot 2^i}{(k + k_i \cdot 2^i)^2}\right)$. To find such a net, we now have two options. First, we can essentially use the previous nets and rescale 2^{-h} by a factor $2^{-i/2}$. Unfortunately, this leads to nets of size $\exp(k \cdot 2^{2h} 2^i)$, so any gain in reducing the variance is countered by an increase in the net size.

The novelty in our approach now lies in showing that a net of size $\exp(k \cdot k_i \cdot 2^{2h})$ exists. Combining the two net sizes with the improved variance bound results in a coreset of size roughly

[2]Observe that if one points of a cluster C_j of $\mathcal{A}$ costs 2^i times more, then all points from C_j do likewise up to constant factors.

$\varepsilon^{-2} \log\left(\exp(k \cdot \min(k_i, 2^i) \cdot 2^{2h})\right) \cdot 2^{-2h} \cdot \left(\frac{k \cdot k_i \cdot 2^i}{(k+k_i \cdot 2^i)^2}\right)$, which after some calculation is shown to be of the order $O(k^{1.5}\varepsilon^{-2})$.

For the remainder of this section we will illustrate how these improved nets can be obtained. The key idea already appears in the case of a single center. Suppose that s is a candidate center. Then we can show that there always exists a subspace with orthogonal basis U spanned by a set T of at most $O(\alpha^{-2})$ points of P such that

$$|p^T(I - UU^T)s| \leq \alpha \cdot \|(I - UU^T)p\| \cdot \|(I - UU^T)s\|.$$

We can then write

$$\|p - s\|^2 = \|U(p - s)\|^2 + \|(I - UU^T)p\|^2 + \|(I - UU^T)s\|^2 - 2p^T(I - UU^T)s.$$

The error for the terms $\|Up - s\|^2$ and $\|(I - UU^T)s\|^2$ can be made negligibly small using a net of size $\exp(\alpha^{-2})$. Thus the main loss in error comes from the $p^T(I - UU^T)s$ term. The key insight is that by adding the k_i centers of clusters that cost 2^i more in $\mathcal{S}$ to T, we have $\|(I - UU^T)p\|^2 \leq \sqrt{\text{cost}(p, \mathcal{A})}$. Thus, the net size becomes $\exp(\alpha^{-2} + k_i)$. By composing these nets for k candidate centers, we then obtain our desired bound.

1.2 Related Work

There has been a tremendous amount of work on coresets for Euclidean k-means following the work in Bachem et al. [2018a,b], Baker et al. [2020], Becchetti et al. [2019], Braverman et al. [2021b], Chen [2009], Cohen-Addad et al. [2021a,b], Feldman and Langberg [2011a], Feldman et al. [2020], Feng et al. [2021], Fichtenberger et al. [2013], Har-Peled and Kushal [2007], Har-Peled and Mazumdar [2004], Huang and Vishnoi [2020], Huang et al. [2018], Langberg and Schulman [2010], Sohler and Woodruff [2018]. Almost as prolific is the catalogue of work on dimension reduction for clustering problems in Euclidean spaces, see Boutsidis et al. [2009, 2010, 2015], Charikar and Waingarten [2022a,b], Cohen et al. [2015], Cohen-Addad and Schwiegelshohn [2017], Drineas et al. [2004], Feng et al. [2019], Makarychev et al. [2019]. The arguably most important dimension reduction technique for coresets are terminal embeddings, see Cherapanamjeri and Nelson [2021], Elkin et al. [2017], Mahabadi et al. [2018], Narayanan and Nelson [2019].

Further recent related work with a focus on Euclidean spaces deals with obtaining coresets for cardinality constrained clustering which includes capacitated and fair clustering, see Bandyapadhyay et al. [2021], Cohen-Addad and Li [2019], Huang et al. [2019], Schmidt et al. [2019] or considering objects other than points as centers Braverman et al. [2021a], Feldman and Langberg [2011b], Feldman et al. [2010], Huang et al. [2021].

1.3 Limitations and Societal Impact

The results do not extend to higher powers, i.e. for $\text{cost}(p, s) = \|p - s\|^z$ the bound $\tilde{O}(k\varepsilon^{-2} \cdot \min(k, \varepsilon^{-z}))$ remains the state of the art. For k-median the new bound also holds (discussed in the supplementary material). Arguably, the $\tilde{O}(k^{1.5}\varepsilon^{-2})$ bound also suggests that a $\tilde{O}(k \cdot \varepsilon^{-3})$ bound should be possible for k-means. We were not able to obtain this and $\tilde{O}(k\varepsilon^{-4})$ remains the state of the art if the dependency on k is required to be (nearly) linear.

Since this is mainly a theoretical work on a basic computational problem, we do not believe that there is any adverse societal impact.

2 Preliminaries and Setup

First, we require the following basic notions. For a point $p \in \mathbb{R}^d$, we denote $\|p\|_2 = \sqrt{\sum_{i=1}^d p_i^2}$ to be the Euclidean norm of p and $\|p\|_1 = \sum_{i=1}^d |p_i|$. The distinct number of points in a point set P is denoted by $\|P\|_0$. Note that the true number of points $|P|$ may be larger than $\|P\|_0$ as different points may lie on the same coordinates. Given a solution $\mathcal{S}$ consisting of at most k centers, and any subset $P' \subset P$ we use $\text{cost}(P', \mathcal{S}) := \sum_{p \in P'} \text{cost}(p, \mathcal{S}) = \sum_{p \in P} \min_{s \in \mathcal{S}} w_p \text{cost}(p, s)$, where $\text{cost}(p, s) = \|p - s\|^2$ for Euclidean k-means and w_p is a non-negative weight (in the basic case this simply 1 whereas for the coreset it can be any non-negative number). We also denote by $v^{\mathcal{S}} \in \mathbb{R}^{\|P\|_0}$ the cost vector associated with the point set P and solution $\mathcal{S}$, that is $v_p^{\mathcal{S}} := w_p \text{cost}(p, s)$. Note that

$\|v^{\mathcal{S}}\|_1 = \text{cost}(P, \mathcal{S})$. The classic coreset guarantee is to show that for any solution $\mathcal{S}$ the designated coreset Ω satisfies

$$|\text{cost}(\Omega, \mathcal{S}) - \text{cost}(P, \mathcal{S})| \leq \varepsilon \cdot \text{cost}(P, \mathcal{S}).$$

We will later introduce an equivalent statement that uses cost vectors. It will also be convenient to consider coresets with an additive error E which satisfy

$$|\text{cost}(\Omega, \mathcal{S}) - \text{cost}(P, \mathcal{S})| \leq \varepsilon \cdot \text{cost}(P, \mathcal{S}) + E.$$

Cohen-Addad et al. [2022] showed that any coreset algorithm that works for instances with the following assumptions can be extended to general instances:

Assumption 1: $\|P\|_0 \in \text{poly}(k, \varepsilon^{-1})$.

Assumption 2: $d \in O(\log(k/\varepsilon) \cdot \varepsilon^{-2})$.

Assumption 3: $w_p = 1$, for all $p \in P$. Note that this only applies to the weights of the original points; the coreset points will have different weights.

Assumption 4: There exists a solution $\mathcal{A}$ such that

1. $|\mathcal{A}| \in O(k)$.
2. For any two clusters C_i, C_j induced by $\mathcal{A}$, $\text{cost}(C_i, \mathcal{A}) \leq 2 \cdot \text{cost}(C_j, \mathcal{A})$.
3. For any cluster C_j induced by $\mathcal{A}$ and any two points $p, p' \in C_j$, $\text{cost}(p, \mathcal{A}) \leq 2 \cdot \text{cost}(p', \mathcal{A})$

To keep this paper self contained, we will detail the validity of these assumptions as well as the sufficiency of computing this relaxed coreset guarantee in the supplementary material.

The sampling procedure is now very simple. Given that these aforementioned assumptions hold, we sample a points $p \in C_j$ with probability $\mathbb{P}_p := \frac{1}{|C_j|} \cdot \frac{\text{cost}(C_j, \mathcal{A})}{\text{cost}(P, \mathcal{A})}$ and add it to the designated coreset Ω. Furthermore, p receives the weight $w_p = \frac{1}{\mathbb{P}_p}$. Overall, our basic cost estimator for any candidate solution $\mathcal{S}$ is therefore

$$\text{cost}(\Omega, \mathcal{S}) := \frac{1}{|\Omega|} \sum_{p \in \Omega} \text{cost}(p, \mathcal{S}) \cdot w_p.$$

It is routine to check that $\mathbb{E}[\text{cost}(\Omega, \mathcal{S})] = \text{cost}(P, \mathcal{S})$. The remainder of this section will be devoted to showing that Ω satisfies for all $\mathcal{S}$

$$|\text{cost}(\Omega, \mathcal{S}) - \text{cost}(P, \mathcal{S})| \leq \frac{\varepsilon}{\log^2 \varepsilon^{-1}} \cdot (\text{cost}(P, \mathcal{S}) + \text{cost}(P, \mathcal{A})) \tag{1}$$

Using the framework from Cohen-Addad et al. [2021a], this implies an $O(\varepsilon)$ coreset in general.

3 Analysis

In this section we prove the following theorem.

Theorem 1. *For any set of points in d dimensional Euclidean space, there exists a coreset for k-means clustering of size $\tilde{O}(k^{1.5}\varepsilon^{-2})$.*

We first describe the random process used to show concentration of the estimator.

3.1 Setting up the Chaining Analysis

First, we observe that Eq.1 is equivalent to showing

$$\sup_{\mathcal{S}} \frac{|\text{cost}(\Omega, \mathcal{S}) - \|v\|_1|}{(\text{cost}(P, \mathcal{S}) + \text{cost}(P, \mathcal{A}))} \leq \frac{\varepsilon}{\log^2 \varepsilon^{-1}}.$$

Our goal is to show that

$$\mathbb{E}_\Omega \left[\sup_{\mathcal{S}} \frac{|\text{cost}(\Omega, \mathcal{S}) - \|v\|_1|}{(\text{cost}(P, \mathcal{S}) + \text{cost}(P, \mathcal{A}))} \right] \leq \frac{\varepsilon}{\log^2 \varepsilon^{-1}},$$

where $\mathbb{E}_\Omega$ is meant to denote the expectation over the randomness of Ω. This implies that the desired guarantee holds with constant probability.

We now apply a standard symmetrization argument by Rudra and Wootters [2014].

Lemma 1 (Appendix B.3 of Rudra and Wootters [2014]). *Let g_p be independent standard Gaussian random variables. Then.*

$$\mathbb{E}_\Omega \sup_{\mathcal{S}} \left[\left| \frac{\frac{1}{|\Omega|}\sum_{p\in\Omega} cost(p,\mathcal{S})\cdot w_p - \|v\|_1}{(cost(P,\mathcal{S}) + cost(P,\mathcal{A}))} \right| \right] \leq \sqrt{2\pi}\mathbb{E}_\Omega \mathbb{E}_g \sup_{\mathcal{S}} \left[\left| \frac{\frac{1}{|\Omega|}\sum_{p\in\Omega} cost(p,\mathcal{S})\cdot w_p}{(cost(P,\mathcal{S}) + cost(P,\mathcal{A}))} \cdot g_p \right| \right].$$

It is therefore sufficient to show

$$\mathbb{E}_\Omega \mathbb{E}_g \sup_{\mathcal{S}} \left[\left| \frac{\frac{1}{|\Omega|}\sum_{p\in\Omega} \mathrm{cost}(p,\mathcal{S})\cdot w_p}{(\mathrm{cost}(P,\mathcal{S}) + \mathrm{cost}(P,\mathcal{A}))} \cdot g_p \right| \right] \leq \frac{\varepsilon}{\sqrt{2\pi}\log^2 \varepsilon^{-1}}. \tag{2}$$

We partition the clusters of any solution $\mathcal{S}$ by type. We consider a cluster C_j of type T_i if

$$2^i \min_{c\in\mathcal{A}} \|p-c\|^2 \leq \min_{p\in C_i} \min_{s\in\mathcal{S}} \|p-s\|^2 \leq 2^{i+1} \min_{c\in\mathcal{A}} \|p-c\|^2.$$

The number of clusters $C_j \in T_i$ are denoted by k_i. If C_j is of type $i \leq 3$, we say C_j is of type T_{small} and if C_j is of type $i \geq \log \gamma\varepsilon^{-2}$, for a sufficiently large absolute constant γ, we say that C_j is of type T_{large}. Then, we show

$$\mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{\mathcal{S}} \left| \frac{\frac{1}{|\Omega|}\sum_{C_j\in T_{small}} \sum_{p\in C_j\cap\Omega} \mathrm{cost}(p,\mathcal{S}) w_p}{(\mathrm{cost}(P,\mathcal{S}) + \mathrm{cost}(P,\mathcal{A}))} g_p \right| \right] \leq \frac{\varepsilon}{\sqrt{2\pi}\log^3 \varepsilon^{-1}} \tag{3}$$

$$\mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{\mathcal{S}} \left| \frac{\frac{1}{|\Omega|}\sum_{C_j\in T_i} \sum_{p\in C_j\cap\Omega} \mathrm{cost}(p,\mathcal{S}) w_p}{(\mathrm{cost}(P,\mathcal{S}) + \mathrm{cost}(P,\mathcal{A}))} g_p \right| \right] \leq \frac{\varepsilon}{\sqrt{2\pi}\log^3 \varepsilon^{-1}} \tag{4}$$

$$\mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{\mathcal{S}} \left| \frac{\frac{1}{|\Omega|}\sum_{C_j\in T_{large}} \sum_{p\in C_j\cap\Omega} \mathrm{cost}(p,\mathcal{S}) w_p}{(\mathrm{cost}(P,\mathcal{S}) + \mathrm{cost}(P,\mathcal{A}))} g_p \right| \right] \leq \frac{\varepsilon}{\sqrt{2\pi}\log^3 \varepsilon^{-1}} \tag{5}$$

Note that if Equation 4 holds for $i \in \{3, \ldots, \log 1/\varepsilon\}$, this also implies Equation 2, as the error from each type can only sum up in the worst case and there are at most $O(\log \varepsilon^{-1})$ many types.

The small and large types are comparatively simple to handle.

Lemma 2 (Lemmas 15 and 16 of Cohen-Addad et al. [2022]). *Let $|\Omega| \geq \kappa \frac{k}{\varepsilon^2} \log^{10}(k/\varepsilon)$ for some absolute constant κ. Then Equations 3 and 5 hold.*

Our main objective will be to prove the following lemma.

Lemma 3. *Let $|\Omega| \geq \kappa_1 \frac{k^{1.5}}{\varepsilon^2} \log^{10}(k/\varepsilon) \geq \kappa_2 \frac{k}{\varepsilon^2} \log^{10}(k/\varepsilon) \cdot \left(\frac{\min(k_i, 2^i)\cdot 2^i k\cdot k_i}{(k+k_i\cdot 2^i)^2} \right)$ for some absolute constants κ_1 and κ_2. Then Equation 4 holds.*

Combining Lemma 2 and Lemma 3 then implies Theorem 1.

3.2 Sketch of the Proof of Lemma 3

The proof of Lemma 3 mainly consists of defining a nested sequence of nets over cost vectors over which we apply a union bound. Roughly speaking, for any cost vector $v^{\mathcal{S}}$, we aim to find an approximating cost vector v' such that

$$\mathrm{cost}(p,\mathcal{S}) = v_p^{\mathcal{S}} - v'_p \leq \varepsilon \cdot \sqrt{\mathrm{cost}(p,\mathcal{S})\cdot \mathrm{cost}(p,\mathcal{A})}.$$

This analysis differs from the terminal-embedding-based nets one used in Cohen-Addad et al. [2022], which aimed for an error of the order $\varepsilon \cdot \mathrm{cost}(p,\mathcal{S})$.

Suppose we have, for every ε, a suitable collection of approximating cost vectors $\mathbb{N}_{\log 1/\varepsilon}$ with this guarantee for any candidate $\mathcal{S}$[3]. Let $v^{\mathcal{S},\varepsilon}$ be the cost vector approximating $v^{\mathcal{S}}$ in the net $\mathbb{N}_{\log 1/\varepsilon}$. Then we can write

$$v_p^{\mathcal{S}} = \sum_{h=0}^{\infty} v_p^{\mathcal{S},2^{-(h+1)}} - v_p^{\mathcal{S},2^{-h}},$$

[3]The reason for indexing the net by $\mathbb{N}_{\log 1/\varepsilon}$ and not by $\mathbb{N}_\varepsilon$ is to conveniently sum over $\sum_{i=1}^{\infty} \log |N_i|$, rather than $\sum_{i=1}^{\infty} \log |N_{2^i}|$.

with $v_p^{\mathcal{S},1} = 0$. Our goal is to now bound

$$
\begin{aligned}
& \mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{\mathcal{S}} \left| \frac{\sum_{C_j \in T_i} \sum_{p \in C_j \cap \Omega} \text{cost}(p, \mathcal{S}) w_p}{|\Omega| \cdot (\text{cost}(P, \mathcal{S}) + \text{cost}(P, \mathcal{A}))} g_p \right| \right] \\
= \; & \mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{v^{\mathcal{S}}} \left| \frac{\sum_{h=0}^{\infty} \sum_{C_j \in T_i} \sum_{p \in C_j \cap \Omega} (v_p^{\mathcal{S},2^{-(h+1)}} - v_p^{\mathcal{S},2^{-h}}) w_p}{|\Omega| \cdot (\text{cost}(P, \mathcal{S}) + \text{cost}(P, \mathcal{A}))} g_p \right| \right] \\
\leq \; & \sum_{h=0}^{\infty} \mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{v^{\mathcal{S},h+1} - v^{\mathcal{S},h} \in \mathbb{N}_{2^{-(h+1)}} \times \mathbb{N}_{2^{-h}}} \left| \frac{\sum_{C_j \in T_i} \sum_{p \in C_j \cap \Omega} (v_p^{\mathcal{S},2^{-(h+1)}} - v_p^{\mathcal{S},2^{-h}}) w_p}{|\Omega| \cdot (\text{cost}(P, \mathcal{S}) + \text{cost}(P, \mathcal{A}))} g_p \right| \right] \\
= \; & \mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{v^{\mathcal{S},1} \in \mathbb{N}_{2^{-1}}} \left| \frac{\sum_{C_j \in T_i} \sum_{p \in C_j \cap \Omega} v_p^{\mathcal{S},2^{-1}} w_p}{|\Omega| \cdot (\text{cost}(P, \mathcal{S}) + \text{cost}(P, \mathcal{A}))} g_p \right| \right] \qquad (6) \\
+ \; & \sum_{h=1}^{\log \varepsilon^{-2}} \mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{v^{\mathcal{S},h+1} - v^{\mathcal{S},h} \in \mathbb{N}_{h+1} \times \mathbb{N}_h} \left| \frac{\sum_{C_j \in T_i} \sum_{p \in C_j \cap \Omega} (v_p^{\mathcal{S},2^{-(h+1)}} - v_p^{\mathcal{S},2^{-h}}) w_p}{|\Omega| \cdot (\text{cost}(P, \mathcal{S}) + \text{cost}(P, \mathcal{A}))} g_p \right| \right] \qquad (7) \\
+ \; & \sum_{\log \varepsilon^{-2}}^{\infty} \mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{v^{\mathcal{S},h+1} - v^{\mathcal{S},h} \in \mathbb{N}_{h+1} \times \mathbb{N}_h} \left| \frac{\sum_{C_j \in T_i} \sum_{p \in C_j \cap \Omega} (v_p^{\mathcal{S},2^{-(h+1)}} - v_p^{\mathcal{S},2^{-h}}) w_p}{|\Omega| \cdot (\text{cost}(P, \mathcal{S}) + \text{cost}(P, \mathcal{A}))} g_p \right| \right] \qquad (8)
\end{aligned}
$$

For each, we aim for an error bound of the error $\frac{\varepsilon}{\log^3 \varepsilon^{-1}}$; the overall bound then follows by summing up the errors and rescaling by constant factors. Bounding each of the terms in Equations 6, 7 and 8 requires somewhat different arguments. For the sake of illustrating the key new ideas we focus on Eq. 7. A full proof is contained in the supplementary material.

The next section presents the nets for the cost vectors. The subsequent section bounds the variance. The final section combines these results and completes the proof of Lemma 3.

Cost Vector Nets

Definition 1. *Let I be a metric space, P a set of points, k a positive integer, and let $\alpha > 0$ be a precision parameters and let $\mathcal{A}$ be some solution with at most k' centers. Let $\mathbb{C} \subset I^k$ be a (potentially infinite) set of candidate k-clusterings. We say that a set of cost vectors $\mathbb{N} \subset \mathbb{R}^{|P|}$ is an (α, k)-clustering net if for every $\mathcal{S} \in \mathbb{C}$ there exists a vector $v' \in \mathbb{N}$ such that the following condition holds. For all $p \in P$,*

$$|v_p^{\mathcal{S}} - v'_p| \leq \alpha \cdot \sqrt{\textit{cost}(p, \mathcal{S}) \textit{cost}(p, \mathcal{A})}.$$

These clustering nets have a substantially smaller error than those proposed in Cohen-Addad et al. [2022], which had an error of the order $\alpha \cdot (\text{cost}(p, \mathcal{S}) + \text{cost}(p, \mathcal{A}))$.

Given a set of points X in Euclidean space, an ε-net is a subset $S \subset X$ such that for every $p \in X$ there exists a q in S with $\|p - q\| \leq \varepsilon$. Throughout this section, we will frequently use the fact that in d dimensions, there exists an ε-net of cardinality $(1 + 2/\varepsilon)^d$ (see for example Pisier [1999]). Our main goal in this section is to prove the following lemma.

Lemma 4. *Let P be a set of points in d dimensional Euclidean space, k a positive integer, $\mathcal{A}$ be a candidate solution with k_i clusters and κ and absolute constant. Define $\mathbb{C}$ to be the set of possible candidate centers such that the clusters induced by $\mathcal{A}$ are of type i, with $3 \leq i \leq \log 1/\varepsilon^2$. For all $\alpha \leq 1/2$, there exists an (α, k)-clustering net $\mathbb{N}$ of $\mathbb{C}$ with*

$$|\mathbb{N}| \leq \exp\left(\kappa \cdot k \cdot \log \|P\|_0 \cdot \min(k_i + \alpha^{-2}, \alpha^{-2} \cdot 2^i) \cdot i \log \frac{1}{\alpha}) \right).$$

Proof (Sketch). We first show that given a set of vectors P and any vector s, there always exists a small subset U of P such that all inner products between $p \in P$ and s are preserved by the span of U.

Lemma 5. *Let $P = \{p_1, ..., p_n\} \subseteq \mathbb{R}^d$. For any vector $p \in \mathbb{R}^d$, there exists $U \subseteq X$, with $|U| = O(\varepsilon^{-2})$ and orthogonal basis Π_U, such that*

$$\forall p \in P, |p^T (I - \Pi_U \Pi_U^T) s| \leq \varepsilon \|(I - \Pi_U \Pi_U^T) p\| \cdot \|(I - \Pi_U \Pi_U^T) s\| \qquad (9)$$

Proof. Without loss of generality let s be a vector with unit Euclidean norm. The proof for arbitrary s follows by scaling. Start with $U_0 = \text{argmin}_{p \in P} \|p - s\|$, and proceed in rounds. In each round i, we add a vector p_i such that Eq. 9 does not hold. Note that $(I - \Pi_U \Pi_U^T)p$ is orthogonal to the span Pi_U of all previously added vectors. Thus, due to the Pythagorean theorem, we have

$$\sum_i^t \left(\frac{(p^T(I - \Pi_{U_{i-1}} \Pi_{U_{i-1}}^T)s)}{\|(I - \Pi_{U_{i-1}} \Pi_{U_{i-1}}^T)p\| \cdot \|(I - \Pi_{U_{i-1}} \Pi_{U_{i-1}}^T)s\|} \right)^2 \geq t \cdot \varepsilon^2.$$

Therefore, after $t = \varepsilon^{-2}$ many rounds $(I - \Pi_U \Pi_U^T)s = 0$, which implies that after at most ε^{-2} rounds Eq. 9 has to hold. □

With this lemma, we can prove our net bound. Our objective is to generate a small set of cost vectors that satisfy the desired guarantee. We first define the cost vectors. For each subset U of size $O(\min(\alpha^{-2} 2^i, \alpha^{-2} + k_i)$, we consider the the subspace Π_U spanned by U. In this subspace we consider $(\alpha/2^i) \cdot \sqrt{\text{cost}(p, \mathcal{A})}$-nets of every ball centered around $\Pi_U p$ with radius $60 \cdot 2^i/2 \cdot \sqrt{\text{cost}(p, \mathcal{A})}$ for all $p \in P$. Such a net has size $\exp(\gamma \cdot \textbf{rank}(U) i \log \alpha)$, for some constant γ and there exist at most $\|P\|_0 \cdot \exp(\gamma \cdot |U| i \log \alpha)$ many such nets. Furthermore, there are at most $\binom{\|P\|_0}{|U|} = \|P\|_0^{|U|}$ such subsets.

Now, for every point p, define an exponential sequence $\alpha^2(1 + \alpha/2^i)^j$ for $j \in \{0, \ldots \log 102^i\}$. There exist at most $\|P\|_0$ such sequences and every such sequence consists of at most $O(\alpha^{-1} \cdot 2^i \cdot i)$ many values. We combine every net point in ever ball of every subspace with all values in the exponential sequence to obtain the evaluation for a single candidate center. The overall number of candidate centers is therefore of the order $\|P\|_0^{|U|} \cdot \exp(\gamma \cdot |U| i \log \alpha)$, for a sufficiently large γ. The overall number of candidate cost vectors is now the number of k subsets of candidate centers, i.e. $\|P\|_0^{k \cdot |U|} \cdot \exp(\gamma \cdot k \cdot |U| i \log \alpha)$. Combined with the bounds on U, this yields the desired size. What remains to be shown is that the thus constructed cost vectors are a (α, k)-clustering net.

Here, we use that for any center s in some candidate solution $\mathcal{S}$

$$\|p - s\|^2 = \|\Pi_U(p - s)\|^2 + \|(I - \Pi_U \Pi_U^T)p\|^2 + \|(I - \Pi_U \Pi_U^T)s\|^2 - 2p^T(I - \Pi_U \Pi_U^T)s.$$

The nets for the span of Π_U are so fine that the distance $\|Pi_U s - s'\|^2$ is essentially negligible, where s' is the point in the span of Π_U closest to $\Pi_U s$ and the same holds for the exponential sequence approximating the term $\|(I - \Pi_U \Pi_U^T)s\|^2$. Thus, the error is dominated by $2p^T(I - \Pi_U \Pi_U^T)s$. Now, we can assume that the input point closest to s is included in U. Thus $\|(I - \Pi_U \Pi_U^T)s\| \leq \sqrt{\text{cost}(p, \mathcal{S})} \leq O(1) \cdot 2^{i/2} \sqrt{\text{cost}(p, \mathcal{A})}$ and $\|(I - \Pi_U \Pi_U^T)p\| \leq \sqrt{\text{cost}(p, \mathcal{S})} \leq O(1) \cdot 2^{i/2} \sqrt{\text{cost}(p, \mathcal{A})}$. If $\alpha^{-2} \cdot 2^i < k_i + \alpha^{-2}$, we have

$$|p^T(I - \Pi_U \Pi_U^T)s| \leq \alpha \cdot 2^{-i/2} \cdot \|(I - \Pi_U \Pi_U^T)p\| \cdot \|(I - \Pi_U \Pi_U^T)s\| \leq O(1) \cdot \alpha \cdot \sqrt{\text{cost}(p, \mathcal{S}) \text{cost}(p, \mathcal{A})}$$

otherwise we have $\|(I - \Pi_U \Pi_U^T)p\| \leq \sqrt{\text{cost}(p, \mathcal{A})}$ which implies

$$|p^T(I - \Pi_U \Pi_U^T)s| \leq \alpha \cdot \|(I - \Pi_U \Pi_U^T)p\| \cdot \|(I - \Pi_U \Pi_U^T)s\| \leq \alpha \cdot \sqrt{\text{cost}(p, \mathcal{S}) \text{cost}(p, \mathcal{A})}.$$

□

Bounding the Variance

We now use the cost vectors to obtain an improved variance for the estimator $\frac{\sum_{C_j \in T_i} \sum_{p \in C_j \cap \Omega} (v_p^{\mathcal{S}, 2^{-(h+1)}} - v_p^{\mathcal{S}, 2^{-h}}) w_p}{(\text{cost}(P, \mathcal{S}) + \text{cost}(P, \mathcal{A}))} g_p$. The bounds on variance for any random variable $\sum a_p g_p$ with standard Gaussians g_p is Gaussian distributed with mean 0 and variance $\sum a_p^2$.

Before we do this, we require an additional notion. Let $\mathcal{E}$ denote the event that $\frac{1}{|\Omega|} \sum_{p \in C_j \cap \Omega} w_p = (1 \pm \varepsilon) \cdot |C_j|$. The following lemma bounds the probability of $\mathcal{E}$ occurring.

Lemma 6. *[Compare Lemma 19 of Cohen-Addad et al. [2022]] If Assumption 4 holds, then event $\mathcal{E}$ holds with probability $1 - k^{-2}$ if $|\Omega| > \kappa \cdot k \varepsilon^{-2} \log k$ for a sufficiently high absolute constant κ.*

Lemma 7. *Given Assumption 4, the variance of* $\frac{\sum_{C_j \in T_i} \sum_{p \in C_j \cap \Omega} (v_p^{\mathcal{S},2^{-(h+1)}} - v_p^{\mathcal{S},2^{-h}}) w_p}{|\Omega| \cdot (\mathit{cost}(P,\mathcal{S}) + \mathit{cost}(P,\mathcal{A}))} g_p$ *is at most*

$$\gamma \cdot \frac{2^{-2h}}{|\Omega|} \cdot \frac{k \cdot k_i \cdot 2^i}{(k + k_i \cdot 2^i)^2} \qquad \textit{conditioned on event } \mathcal{E}$$

$$\gamma \cdot \frac{2^{-2h} \cdot k}{|\Omega|} \cdot \frac{k \cdot k_i \cdot 2^i}{(k + k_i \cdot 2^i)^2} \qquad \textit{conditioned on event } \overline{\mathcal{E}}$$

for an absolute constant γ.

Completing the Proof (for Eq. 7)

Throughout this section, we use the bound on the expected maximum of independent Gaussians.

Lemma 8 (Lemma 2.3 of Massart [2007])**.** *Let* $g_i \sim \mathcal{N}(0, \sigma_i^2)$, $i \in [n]$ *be Gaussian random variables and suppose* $\sigma_i \leq \sigma$ *for all* i*. Then* $\mathbb{E}[\max_{i \in [n]} |g_i|] \leq 2\sigma \cdot \sqrt{2 \ln n}$.

The number of cost vectors in $\mathbb{N}_{h+1} \times \mathbb{N}_h$ is at most $\exp\left(\gamma \cdot k \cdot \log \|P\|_0 \cdot \min(k_i + 2^{2h}, 2^{2h} \cdot 2^i) \cdot i \cdot h)\right)$ for some absolute constant γ due to Lemma 4. With the bound on the variance (Lemma 7 and conditioned on event $\mathcal{E}$ we then have

$$\begin{aligned}
& \sum_{h=1}^{\log \varepsilon^{-2}} \mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{v^{\mathcal{S},h+1} - v^{\mathcal{S},h} \in \mathbb{N}_{h+1} \times \mathbb{N}_h} \left| \frac{\sum_{C_j \in T_i} \sum_{p \in C_j \cap \Omega} (v_p^{\mathcal{S},2^{-(h+1)}} - v_p^{\mathcal{S},2^{-h}}) w_p}{(\mathrm{cost}(P,\mathcal{S}) + \mathrm{cost}(P,\mathcal{A}))} g_p \right| \middle| \mathcal{E} \right] \\
\leq \; & \sum_{h=1}^{\log \varepsilon^{-2}} \sqrt{\gamma \cdot k \cdot \log \|P\|_0 \cdot \min(k_i + 2^{2h}, 2^{2h} \cdot 2^i) \cdot i \cdot h \cdot \frac{2^{-2h}}{|\Omega|} \cdot \frac{k \cdot k_i \cdot 2^i}{(k + k_i \cdot 2^i)^2}} \\
\leq \; & 2\sqrt{\gamma \cdot k \cdot \log \|P\|_0 \cdot \min(k_i, 2^i) \cdot i \cdot \log^3 \varepsilon^{-1} \cdot \frac{1}{|\Omega|} \cdot \frac{k \cdot k_i \cdot 2^i}{(k + k_i \cdot 2^i)^2}}. \qquad (10)
\end{aligned}$$

Conditioned on event $\mathcal{E}$ not holding, we then have using a similar calculation

$$\begin{aligned}
& \sum_{h=1}^{\log \varepsilon^{-2}} \mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{v^{\mathcal{S},h+1} - v^{\mathcal{S},h} \in \mathbb{N}_{h+1} \times \mathbb{N}_h} \left| \frac{\sum_{C_j \in T_i} \sum_{p \in C_j \cap \Omega} (v_p^{\mathcal{S},2^{-(h+1)}} - v_p^{\mathcal{S},2^{-h}}) w_p}{(\mathrm{cost}(P,\mathcal{S}) + \mathrm{cost}(P,\mathcal{A}))} g_p \right| \middle| \overline{\mathcal{E}} \right] \\
\leq \; & 2\sqrt{\gamma \cdot k^2 \cdot \log \|P\|_0 \cdot \min(k_i, 2^i) \cdot i \cdot \log^3 \varepsilon^{-1} \cdot \frac{1}{|\Omega|} \cdot \frac{k \cdot k_i \cdot 2^i}{(k + k_i \cdot 2^i)^2}}. \qquad (11)
\end{aligned}$$

We have $\mathbb{P}[\overline{\mathcal{E}}] \leq 1/k^2$ due to Lemma 6. Since $\|P\|_0 \leq \mathrm{poly}(k, \varepsilon^{-1})$, $2^i \leq O(1) \cdot \varepsilon^{-2}$ and by our choice of $|\Omega|$, we can combine Equations 10 and 11 with the law of total expectation to obtain

$$\begin{aligned}
& \sum_{h=1}^{\log \varepsilon^{-2}} \mathbb{E}_\Omega \mathbb{E}_g \left[\sup_{v^{\mathcal{S},h+1} - v^{\mathcal{S},h} \in \mathbb{N}_{h+1} \times \mathbb{N}_h} \left| \frac{\sum_{C_j \in T_i} \sum_{p \in C_j \cap \Omega} (v_p^{\mathcal{S},2^{-(h+1)}} - v_p^{\mathcal{S},2^{-h}}) w_p}{(\mathrm{cost}(P,\mathcal{S}) + \mathrm{cost}(P,\mathcal{A}))} g_p \right| \right] \\
\leq \; & 4\sqrt{\gamma \cdot k \cdot \log \|P\|_0 \cdot \min(k_i, 2^i) \cdot i \cdot \log^3 \varepsilon^{-1} \cdot \frac{1}{|\Omega|} \cdot \frac{k \cdot k_i \cdot 2^i}{(k + k_i \cdot 2^i)^2}} \leq O(1) \frac{\varepsilon^{-2}}{\log^3 \varepsilon^{-1}}.
\end{aligned}$$

4 Experimental Results

We complement our results with an empirical evaluation of coreset algorithms. Specifically, we ran the algorithm used in our analysis (Group Sampling) as well as the popular Sensitivity Sampling (Feldman and Langberg [2011b]) and uniform sampling on synthetic and real world data. Here,

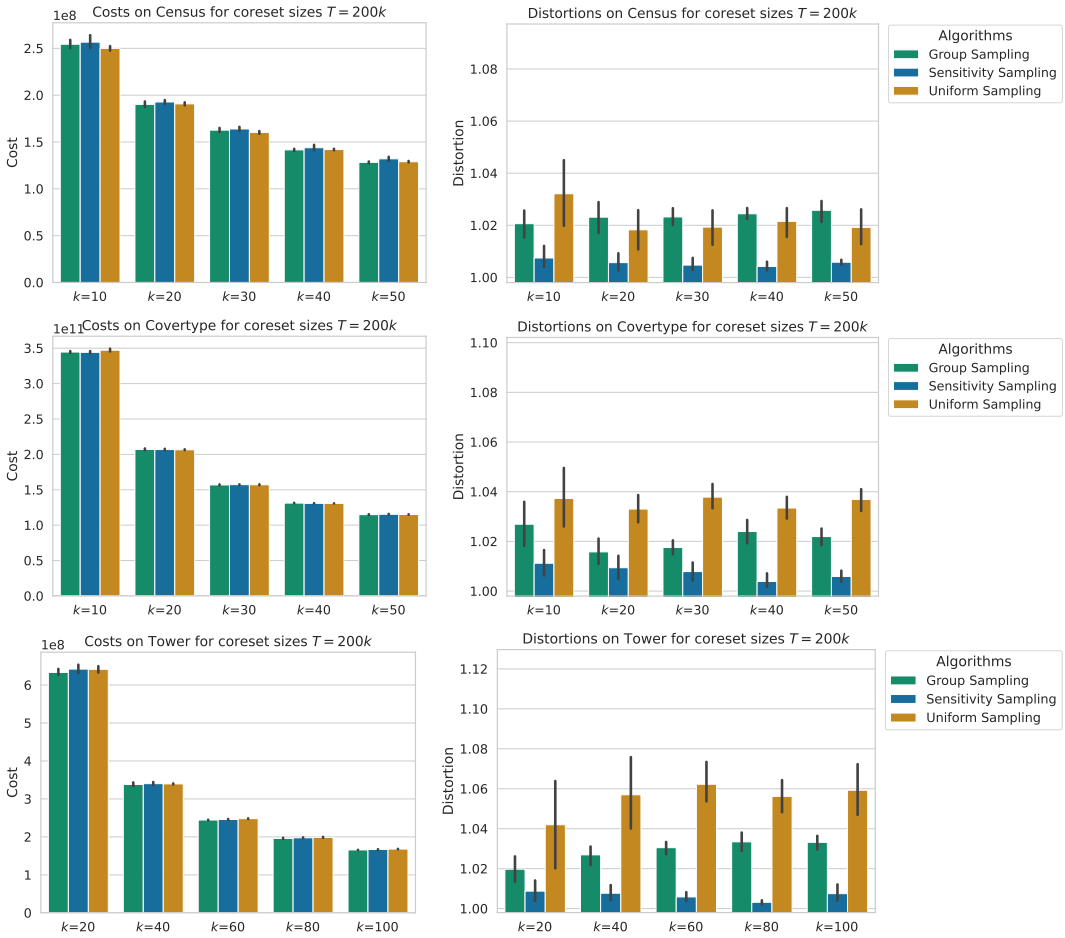

Figure 1: Costs and distortions on real-world data sets. Reported are mean values over the runs, as well as standard deviations indicated by the black bars.

we mainly focus on the performance of the three real world instances *Census*[4], *Covertype*[5] and *Tower*[6]. It is hard to compute the distortion of a given coreset, so for the real world data sets, we sampled $|\Omega| = 200k$ points from each distribution, followed by running k-means++ (see Arthur and Vassilvitskii [2007]) 10 times and compared the costs, as well as the distortion on the found solution (see Fig. 1). Every coreset was computed 10 times as well. The distortion is the maximum distortion over each run among all evaluated solutions.

In terms of cost, all algorithms computed solutions of roughly equal value. In terms of distortion, uniform sampling expectedly had the worst bounds. Somewhat interestingly, the Group Sampling algorithm which currently has a better worst case bound than Sensitivity Sampling tends to have a worse distortion. We leave it to future work to find an analysis of Sensitivity Sampling that matches (or outperforms) Group Sampling. Furthermore, there is a small increase in distortion with increasing k. While this suggests that a linear dependency in k is not the correct answer, the increase in distortion is too small to suggest that a $k^{1+\delta}$ dependency for some $\delta > 0$ will be the correct answer. It may also be too difficult to accurately measure distortion on real world instances as uniform sampling, which is known to be an extremely bad coreset algorithm in theory, performs moderately competitively.

Synthetic instances as well as numerical figures are discussed in the supplementary material.

[4] `https://archive.ics.uci.edu/ml/datasets/US+Census+Data+(1990)` (see Kohavi [1996])

[5] `https://archive.ics.uci.edu/ml/datasets/covertype` (see Blackard and Dean [1999])

[6] `http://homepages.uni-paderborn.de/frahling/coremeans.html` (see Frahling and Sohler [2006])

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [Yes]
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes] The complete proofs are in the supplementary material. Due to space constraints, we could not include them in the main body.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes]
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes]
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
   (b) Did you mention the license of the assets? [No] These data sets are unlimited.
   (c) Did you include any new assets either in the supplemental material or as a URL? [No]
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [No] We did not generate data sets ourselves.
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [No] We did not generate data sets ourselves.
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [No] Not applicable.
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [No] Not applicable.
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [No] Not applicable.