An Empirical Evaluation of k-Means Coresets*

Abstract

Coresets are among the most popular paradigms for summarizing data. In particular, there exist many high performance coresets for clustering problems such as k-means in both theory and practice. Curiously, there exists little work on comparing the quality of available k-means coresets.

In this paper we perform such an evaluation. First, we show that it is computationally hard to compare the quality of not only two different coreset algorithms, but also of two different output of a (randomized) coreset algorithm. In order to perform an empirical evaluation, we therefore have to work with heuristics. To this end, we propose and analyse a benchmark for coreset comparison. Using this benchmark and real-world data sets, we conduct an exhaustive evaluation of the most commonly used coreset implementations.

1 Introduction

The design and analysis of scalable algorithms has become an important research area over the past two decades. This is particularly important in data analysis, where even polynomial running time might not be enough to handle proverbial *big data* sets. One of the main approaches to deal with the scalability issue is to compress or sketch large data sets into smaller, more manageable ones. The aim of such compression methods is to preserve the properties of the original data, up to some small error, while significantly reducing the number of data points.

Among the most popular and successful paradigms in this line of research are *coresets*. Informally, given a data set A, a coreset $S \subset A$ with respect to a given set of queries Q and query function $f : A \times Q \to \mathbb{R}_{\geq 0}$ approximates the behaviour of A for all queries up to some multiplicative distortion D via

$$\sup_{q \in Q} \max\left(\frac{f(S,q)}{f(A,q)}, \frac{f(A,q)}{f(S,q)}\right) \leq D.$$

Coresets have been applied to a number of problems such as computational geometry [2, 6], linear algebra [24, 28], and machine learning [30, 33]. But the by far most intensively studied an arguably most successful applications of the coreset framework are k-clustering problem.

Here we are given n points A with (potential unit) weights $w : A \to \mathbb{R}_{\geq 0}$ in some metric space with distance function dist and aim to find k centers C such that

$$\mathrm{cost}_A(C) := \frac{1}{n} \sum_{p \in A} \min_{c \in C} w(p) \cdot \mathrm{dist}^z(p, c)$$

is minimized. The most popular variant of this problem is probably the k-means problem in d-dimensional Euclidean space where $z = 2$ and $\mathrm{dist}(x, y) = \sqrt{\sum_{i=1}^{d}(x_i - y_i)^2}$.

A (k, ε)-coreset is now a subset $\Omega \subset A$ with weights $w : \Omega \to \mathbb{R}_{\geq 0}$ such that for any set of k centers C

$$\sup_{C} \max\left(\frac{\mathrm{cost}_A(C)}{\mathrm{cost}_\Omega(C)}, \frac{\mathrm{cost}_\Omega(C)}{\mathrm{cost}_A(C)}\right) \leq 1 + \varepsilon. \tag{1.1}$$

In a long line of work spanning the last 20 years[4, 5, 7, 14, 17, 21, 20, 23, 5, 26, 36], the size of coresets has been steadily improved with the current state of the art yielding a coreset with $\tilde{O}(k\varepsilon^{-4})$ points for a distortion $D \leq (1 + \varepsilon)$ due to Cohen-Addad, Saulpic, and Schwiegelshohn [11][1].

While we have a good grasp of the theoretical guarantees of these algorithms, our understanding of the empirical performance is somewhat lacking. This is due to two main reasons.

- Experiments are geared towards optimization: Often experiments on coresets are conducted as follows. First, compute coreset(s) with the available algorithm(s). Then run an optimization algorithm. The *best* coreset algorithm is considered to be the one resulting in the clustering with smallest cost.
- Evaluating the quality of a coreset is hard: Given two point sets A and B, it is computationally hard to determine the distortion when considering B as

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[1] We use $\tilde{O}(x)$ to hide $\log^c x$ terms for any constant c.

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a candidate coreset of A with respect to the k-means objective. Thus, while we can default to the worst case guarantees from theory, it is difficult to compare the output of two coreset algorithms for a given data set.

These two reasons are related. Due to the difficulty of evaluating coresets, comparing the outcome of an optimization algorithm is a simple and reasonable alternative. To some degree the fact that a clustering has low cost is also a global property of this clustering. Nevertheless, this method of comparison has the drawback that it is more likely to measure the performance of the underlying optimization problem, rather than evaluating coresets. Moreover, coresets as defined in Eq. (1.1) have a guarantee for *all* candidate solutions C. A relaxed guarantee that only preserves optimal or nearly optimal clusterings are known as weak coresets, which often are easier to compute. Thus, if a candidate coreset algorithm outputs a weak coreset, it may have a bad worst-case distortion which would not be visible when evaluating it on the outcome of an optimization algorithm.

Thus, the purpose of this paper is to systematically evaluate the distortion of various coreset algorithms. On real world data sets, we observe that while all coreset algorithms are generally able to find a solution with good cost, there is a stark difference in the distortion, which shows a differences between optimization and compression are readily observable in practise. In addition, we propose a benchmark for k-means coresets in Euclidean spaces. We argue why this benchmark has properties that make it both hard for all known coreset constructions. We also show how to efficiently estimate the distortion of a candidate coreset on the benchmark.

2 Coreset Algorithms

Though the algorithms vary in details, coreset constructions come in one of the following two flavours:

1. Movement-based constructions: Such algorithms compute a clustering with T points such that $\text{cost}_A(T) \ll \text{OPT}$, where OPT is the cost of an optimal k-means clustering. The coreset guarantee then follows as a consequence of the triangle inequality. These algorithms all have an exponential dependency on the dimension d, and therefore have been overtaken by sampling-based methods. Nevertheless, these constructions are more robust to various constrained clustering formulations [22, 35] and continue to be popular. Examples from theory include [19, 21].
2. Importance sampling: Points are sampled proportionate to their sensitivity which for a point p is defined as $sens(p) := \sup_C \frac{\min_{c\in C} \text{dist}^2(p,c)}{\text{cost}_A(C)}$ and weighted by their inverse sampling probability. In terms of theoretical performance, sensitivity sampling has largely replaced movement based constructions, see for example [15, 27].

Of course, there exist algorithms that draw on techniques from both, see for example [11]. In what follows, we will survey implementations of various coreset constructions that we will evaluate later.

StreamKM++ [1] The popular k-means++ algorithm [3] computes a set of centers K by iteratively sampling a point p in A proportionate to $\min_{q\in K} \text{dist}^2(p,q)$ and adding it to K. The procedure terminates once the desired number of centers has been reached. The first center is typically picked uniformly at random. The StreamKM++ paper runs the k-means++ algorithms for T iterations, where T is the desired coreset size. At the end, every point q in K is weighted by the number of points in A closest to it. While the construction has elements of important sampling, the analysis is largely movement-based. The provable bound required for the algorithm to compute a coreset is $O\left(\frac{k\log n}{\delta^{d/2}\varepsilon^d} \cdot \log^{d/2} \frac{k\log n}{\delta^{d/2}\varepsilon^d}\right)$.

BICO [18] Combines the very fast, but poor quality clustering algorithm BIRCH [40] with the movement-based analysis from [19, 21]. The clustering is organized by way of a hierarchical decomposition: When adding a point p to one of the coreset points Ω at level i, it first finds the closest point q in Ω. If p is too far away from q, a new center is opened at p. Otherwise p is either added to q, or, if adding p to q increases the clustering cost of q beyond a certain threshold, the algorithm attempts to add p to the child-clusters of q. The procedure then continues recursively. The provable bound required for the algorithm to compute a coreset is $O\left(k\log n\varepsilon^{-d-2}\right)$.

Sensitivity Sampling [14] The simplest implementation of sensitivity sampling first computes an $(O(1), O(1))$ bicriteria K approximation[2], for example by running k-means++ for $2k$ iterations [39]. Let K be the $2k$ clustering thus computed and let K_i be an arbitrary cluster of K with center q_i. Subsequently, the algorithm picks $T-2k$ points propor-

[2] An (α, β) bicriteria approximation computes an α approximation using $\beta \cdot k$ many centers.

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tionate to $\frac{\text{dist}^2(p,q)}{\text{cost}_{K_i}(\{q_i\})} + \frac{1}{|K_i|}$. Let $|\hat{K}_i|$ be the estimated number of points in the sample. Finally, the algorithm weighs each q_i by $(1+\varepsilon)\cdot|K_i| - |\hat{K}_i|$. The provable bound required for the algorithm to compute a coreset is $\tilde{O}\left(kd\varepsilon^{-4}\right)$ ([14]), $\tilde{O}\left(k\varepsilon^{-6}\right)$ ([23]), or $\tilde{O}\left(k^2\varepsilon^{-4}\right)$ ([5]).

Group Sampling [11] First, the algorithm computes an $O(1)$ approximation (or a bicriteria approximation) K. Subsequently, the algorithm preprocesses the input into groups such that (1) for any two points $p, p' \in K_i$, their cost is identical up to constant factors and (2) for any two clusters K_i, K_j, their cost is identical up to constant factors. In every group, Group-Sampling now samples points proportionate to their cost. The authors of [11] show that there always exist a partitioning into $\log^2 1/\varepsilon$ groups. Points not contained in a group are snapped to their closest center q in K. q is weighted by the number of points snapped to it. The provable bound required for the algorithm to compute a coreset is $\tilde{O}\left(k\varepsilon^{-4}\right)$ ([11]).

2.1 Dimension Reduction Finally, we also combine coreset constructions with a variety of dimension reduction techniques. Since the seminal paper by Feldman, Schmidt, and Sohler [16], most coreset algorithms have used some form of dimension reduction to eliminate the dependency on d, either by explicitly computing a low-dimensional embedding, see for example [16, 37], or by using the existence of a suitable embedding in the analysis [11, 23].

In particular, movement-based coresets often have an exponential dependency on the dimension, which can be alleviated with some form of dimension reduction, both in theory [35] and in practice [25].

Here the are two main techniques.

Principal Component Analysis: Feldman, Schmidt, and Sohler [16] showed that projecting an input A onto the first $O(k/\varepsilon^2)$ principal components is a coreset, albeit in low dimension. The analysis was subsequently tightened by [8] and extended to other center based cost functions by [36]. Although it's target dimension is generally worse than those based on random projections and terminal embeddings, there is nevertheless reasons for using PCA regardless: It removes noise and thus may make it easier to compute a high quality coreset.

Terminal Embeddings: Given a set of points A in $\mathbb{R}^d$, a terminal embedding $f : \mathbb{R}^d \to \mathbb{R}^m$ preserves the pairwise distance between any point $p \in A$ and any point $q \in \mathbb{R}^d$ up to a $(1 \pm \varepsilon)$ factor. The statement is related to the famous Johnson-Lindenstrauss lemma but it is stronger as it does not apply to only the pairwise distances of A. Nevertheless, the same target dimension is sufficient. Terminal embeddings were studied by [13, 29, 34], with Narayanan and Nelson [34] achieving an optimal target dimension of $O(\varepsilon^{-2}\log n)$, where n is the number of points. For applications to coresets, we refer to [4, 11, 23].

For an overview on practical aspects of dimension reduction, we refer to Venkatsubramanian and Wang [38].

3 Hardness of Coreset Evaluation and a Benchmark

In this section, we first show that it is in general co-NP hard to evaluate the coreset distortion, given two point sets A and B. Thereafter we describe the benchmark and it's properties.

PROPOSITION 3.1. *Given two point sets A and B in $\mathbb{R}^d$ and a sufficiently small (constant) $\varepsilon > 0$, it is co-NP hard to decide whether A is a (k,ε)-coreset of B.*

Proof. First, we recall that for some ε_0 and candidate clustering cost V, it is NP-hard to decide whether there exists a clustering C with cost in $\text{cost}_A(C) \leq V$ and $\text{cost}_B(C) \geq (1+\varepsilon_0)\cdot V$. Conversely, it is co-NP-hard to decide whether there exists no set of centers C such that $\text{cost}_A(C) \leq V$ and $\text{cost}_B(C) \geq (1+\varepsilon_0)\cdot V$. ∎

We remark that the possible values for ε_0 are determined by the current APX-hardness results. Assuming NP≠P, $\varepsilon_0 \approx 1.07$ and assuming UCG, $\varepsilon_0 \approx 1.17$ [10, 9] for k-means in Euclidean spaces.

3.1 Benchmark Construction In this section, we describe our benchmark. The benchmark has a parameters α which controls the number of points and dimensions. For a given value of k the benchmark consists of $n = k^\alpha$ points and $d = \alpha \cdot k$ dimensions. It is recursively constructed as follows.

Denote by $\mathbb{1}_k$ the k-dimensional all 1 vector and by v_i^1 the k dimensional vector with entries $(v_i^1)_j = \begin{cases} -\frac{1}{k} & \text{if } i \neq j \\ \frac{k-1}{k} & \text{if } i = j \end{cases}$. For $\ell \leq \alpha$, recursively define the k^ℓ dimensional vector $v_i^\ell = \begin{bmatrix} (v_i^{\ell-1})_1 \cdot \mathbb{1}_k \\ (v_i^{\ell-1})_2 \cdot \mathbb{1}_k \\ \vdots \\ (v_i^{\ell-1})_1 \cdot \mathbb{1}_k \end{bmatrix}$. Finally, set the

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column $t = a \cdot k + b$, $a \in \{0, \dots \alpha - 1\}$ and $b \in \{1, \dots k\}$, of A to be $k^{\alpha - a}$ stacks of v_b^{a+1}.

To get a better feel for the construction, we have given two example inputs in Figure 1.

3.2 Properties of the Benchmark We now summarize the key properties of the benchmark. To this end, we require a few notions. Let A be the input matrix. We slightly abuse notation an refer to A_i as both the ith point as well as the ith row of the matrix A. For a clustering $\mathcal{C} = \{C_1, \dots, C_k\}$, we define that the $n \times k$ indicator matrix $\tilde{X}$ induced by $\mathcal{C}$ via

$$\tilde{X}_{i,j} = \begin{cases} 1 & \text{if } A_i \in C_j \\ 0 & \text{else.} \end{cases}$$

Furthermore, we will also use the $n \times k$ normalized clustering matrix X defined as

$$X_{i,j} = \begin{cases} \frac{1}{\sqrt{|C_i|}} & \text{if } A_i \in C_j \\ 0 & \text{else.} \end{cases}$$

We also recall the following lemma which will allow us to express the k-means cost of a clustering $\mathcal{C}$ with optimally chosen centers in terms of the cost of X and A.

LEMMA 3.1. (FOLKLORE) *Let A be an arbitrary set of points and let $\mu(A) = \frac{1}{|A|} \sum_{p \in A} p$ be the mean. Then for any point c*

$$\sum_{p \in A} \|p - c\|^2 = \sum_{p \in A} \|p - \mu(A)\|^2 + |A| \cdot \|\mu(A) - c\|^2.$$

This lemma proves that for any given cluster C_j, the mean is the optimal choice of center. We also note that any two distinct columns of X are orthogonal. Furthermore $\frac{1}{n}\mathbf{1}\mathbf{1}^T A$ copies the mean into every entry of A. Combining these two observations, we see that the matrix XX^TA maps the ith row of A onto the mean of the cluster it is assigned to. Finally, define the Frobenius norm of an $n \times d$ A by $\|A\|_F = \sqrt{\sum_{i=1}^n \sum_{j=1}^d A_{i,j}^2}$. Then the k-means cost of the clustering $\mathcal{C}$ is precisely

$$\|A - XX^TA\|_F^2.$$

We also require the following distance measure on clusterings as proposed by Meila [31, 32]. Given two clusterings $\mathcal{C}$ and $\mathcal{C}'$, the $k \times k$ confusion matrix M is defined as

$$M_{i,j} = |C_i \cap C'_j|.$$

Furthermore for the indicator matrices $\tilde{X}$ and $\tilde{X}'$ induced by $\mathcal{C}$ and $\mathcal{C}'$ we have the identity $M = \tilde{X}^T \tilde{X}'$. Denote by Π_k the set of all permutations over k elements. Then the distance between $\mathcal{C}$ and $\mathcal{C}'$ is defined as

$$d(\mathcal{C}, \mathcal{C}') = 1 - \frac{1}{n} \max_{\pi \in \Pi_k} \sum_{i=1}^{k} M_{i,\pi(i)}.$$

Observe that for clusters that are identical, their distance is 0. The maximum distance between any two k clusterings is always $\frac{k-1}{k}$.

We are now ready to state the desired properties of our benchmark. The benchmark was designed to generate many clusterings such that

1. The distance between these clustering is maximized.
2. The clusterings have equal cost.
3. The clusterings are induced by a set of centers in $\mathbb{R}^d$.

The first and second property ensure that (equally good) solutions we use for evaluation are spread out through the solution space. In other words, we are less likely to only focus on a set of solutions $\mathcal{S}$ for which a low distortion on one $S \in \mathcal{S}$ implies a low distortion for all elements of $\mathcal{S}$. The third property is important as these are the only clusterings the (standard) coreset guarantee has to apply to.

The solutions we consider are given as follows. For the columns $a \cdot k + 1, \dots (a+1) \cdot k$, we define the clustering $\mathcal{C}^a = \{C_1^a, \dots C_k^a\}$ with $A_i \in C_j^a$ if and only if $A_{i,j} > 0$. Let $\tilde{X}^a$ and X^a denote the indicator matrix and clustering matrix, respectively, as induced by $\mathcal{C}^a$.

FACT 3.1. *For $a \neq a'$, we have $d(\mathcal{C}^a, \mathcal{C}^{a'}) = 1 - 1/k$.*

Proof. Consider an arbitrary vector v_i^ℓ. By construction, the positive entries of v_i^ℓ range from $k^{\ell-1} \cdot i + 1$ to $k^{\ell-1} \cdot (i+1)$. Similarly, the positive entries for the vector $v_j^{\ell-1}$ range from range from $k^{\ell-2} \cdot j + 1$ to $k^{\ell-2} \cdot (j+1)$. Therefore, concatenating $v_j^{\ell-1}$ k times into a vector v', v' and v_i^ℓ can share at most one positive coordinate. Inductively, the same holds true for any concatenation of vectors $v_j^{\ell-h}$. Thus, the two clusters induced by the columns formed by concatenating the vectors v can share only a $1/k$ fraction of the points. Since each cluster consists of exactly $k^\alpha/k = k^{\alpha-1}$ points, the confusion matrix M only has entries $\frac{n}{k^2}$ and for any permutation π, we have $d(\mathcal{C}^a, \mathcal{C}^{a'}) = 1 - 1/k$. ∎

FACT 3.2. *For any C_j^a, we have $cost_{C_j^a}(\{\mu(C_j^a)\}) = (\alpha - 1) \cdot k^{\alpha-2} \cdot (k-1)$.*

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$$\begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \qquad \begin{bmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \end{bmatrix}$$

Figure 1: Benchmark construction for $k = 2$ and $\alpha = 3$ (left) and $k = 3$ and $\alpha = 2$ (right).

Proof. Without loss of generality, we consider C_1^0; the proof is analogous for the other choices of j and a. We first note that for any point $A_i \in C_1^0$, the coordinates $A_{i,\ell}$ are identical for $\ell < k$. Furthermore for the column $\ell \geq k$, we have by construction $\sum_{A_i \in C_j} A_{i,\ell} = k^{\alpha-1} \cdot \frac{k-1}{k} + (k^\alpha - k^{\alpha-1})\frac{1}{k} = k^{\alpha-1} \cdot (\frac{k-1}{k} - (k-1)\frac{1}{k}) = 0$. Therefore, the mean of C_1^0 satisfies $\mu(C_1^0)_\ell = \begin{cases} A_{i,\ell} & \text{if } \ell < k \\ 0 & \text{else.} \end{cases}$. Thus, the cost is precisely $(\alpha-1) \cdot k^{\alpha-1} \cdot \left(\left(\frac{k-1}{k}\right)^2 + \left(\frac{1}{k}\right)^2\right) = (\alpha-1) \cdot k^{\alpha-2} \cdot (k-1)$. ∎

Finally, we show that the means for the clustering $\mathcal{C}^a$ also induce $\mathcal{C}^a$.

FACT 3.3. *For a clustering $\mathcal{C}^a$, let $\mu(C_j^a)$ denote the mean of cluster C_j^a. Then every point of is assigned to its closest center. Moreover, every point A_i of C_j^a has equal distance to any center $\mu(C_h^a)$ with $h \neq j$.*

Proof. Again, we assume without loss of generality $a = 0$. Let A_i be an arbitrary point of cluster C_h^a and consider the mean $\mu(C_j^a)_\ell = \begin{cases} A_{i,\ell} & \text{if } \ell < k \\ 0 & \text{else.} \end{cases}$ of cluster C_j^a. By definition, the positive coordinates of A_i are not equal to the positive coordinates of $\mu(C_j^a)$. The only difference in coordinates between the means of $\mu(C_j^a)$ and $\mu(C_h^a)$ are the first k coordinates, as the rest are 0. But here the coordinates of $\mu(C_h^a)$ and A_i are identical, hence $\mu(C_j^a)$ cannot be closer to A_i.

To prove that the distances between A_i and any $\mu(C_h^a)$ with $h \neq j$ are equal, again consider that any difference can only exist among the first k coordinates. Here, we have $\mu(C_h^a)_h = \frac{k-1}{k}$, and the remaining columns are $-\frac{1}{k}$. Since $A_{i,h} = -\frac{1}{k}$ for any $h \neq j$, the claim follows. ∎

3.3 Benchmark Evaluation We now describe how we use the benchmark to measure the distortion of a coreset. Assume that the coresets only consists of input point[3]

Consider the clustering $\mathcal{C}^a = \{C_1^a, \ldots C_k^a\}$ for some a and let Ω with weights $w : \Omega \to \mathbb{R}_{\geq 0}$ be the coreset. We use $w(C_i^a \cap \Omega) := \sum_{p \in C_i^a \cap \Omega} w(p)$ to denote the mass of points of C_i^a in Ω. For every cluster C_i^a with $w(C_i^a \cap \Omega) \geq |C_i|(1-\varepsilon)$, we place a center at $\mu(C_i^a)$. Conversely, if $w(C_i^a \cap \Omega) \leq |C_i|(1-\varepsilon)$, we do not place a center at $\mu(C_i^a)$. We call such clusters *deficient*. Let $\mathcal{S}$ be the total number of thus placed centers.

We now compare the cost as computed on the coreset and the true cost of $\mathcal{S}$. Due to Lemma 3.1 and Fact 3.3, we may write for any deficient cluster C_i^a $\text{cost}_{C_i^a}(\mathcal{S}) = \text{cost}_{C_j^a}(\{\mu(C_j^a)\}) + k^{\alpha-1}\|\mu(C_j^a) - \mu(C_h^a)\|_2^2$, where C_h^a is a non-deficient cluster. Thus, the cost is due to Fact 3.2

$$\begin{aligned} \text{cost}_{C_i^a}(\mathcal{S}) &= (\alpha-1) \cdot k^{\alpha-2} \cdot (k-1) + k^{\alpha-1} \cdot 2 \\ &\approx (1 + \frac{2}{\alpha}) \cdot \text{cost}_{C_j^a}(\{\mu(C_j^a)\}). \end{aligned}$$

Conversely, the cost on the coreset is

$$\begin{aligned} & \text{cost}_{\Omega \cap C_i^a}(\mathcal{S}) \\ = \; & w(C_i^a \cap \Omega)\left((\alpha-1) \cdot \left(\left(\frac{k-1}{k}\right)^2 + (k-1)\left(\frac{1}{k}\right)^2\right) + 2\right) \\ \approx \; & \frac{w(C_i^a \cap \Omega)}{\text{cost}_{C_j^a}(\{\mu(C_j^a)\})}(1 + \frac{2}{\alpha}) \cdot \text{cost}_{C_j^a}(\{\mu(C_j^a)\}). \end{aligned}$$

Thus for each deficient clustering individually, the distortion will be close to $\frac{k^{\alpha-1}}{w(C_i^a \cap \Omega)} \geq \frac{1}{1-\varepsilon}$. If there are many deficient clusters, then this will also be the overall distortion.

[3] It is not necessary for coreset constructions in general to consists of input points. One can adjust the evaluation in to account for this. But since all algorithms considered in this paper have the property and it makes the evaluation simpler, we will only consider coresets that are subsets of the original point set.

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3.4 Further Extensions On the benchmark we considered here, both Sensitivity Sampling, as well as Group Sampling are similar to uniform sampling and, indeed, uniform sampling could be used to construct a good coreset. We can eliminate uniform sampling as a viable algorithm for this instance by combining multiple benchmarks $B_1, \dots B_t$ with $\sum_{i=1}^{t} k_i = k$. Each benchmark then has size $\sum_{i=1}^{t} k_i^{\alpha}$. We then adding an additive offset to the coordinates of each benchmark such that they do not interfere. In this case, uniform sampling does not work if the values of the k_i are different enough. Since it is well known that uniform sampling is not a viable coreset algorithm in both theory and practice, we only used the basic benchmark for our evaluations.

4 Experiments

We now present the empirical evaluation of these corsets. We ran two kinds of experiments. On real-world data sets, we merely computed a coreset Ω, followed by running k-means++ on Ω. The k-means++ algorithm was repeated 10 times, each yielding a solution $\mathcal{S}_i$, and as the best lower bound on the distortion we used the largest ratio $\max_i \left(\max \left(\frac{\text{cost}_A(\mathcal{S}_i)}{\text{cost}_\Omega(\mathcal{S}_i)}, \frac{\text{cost}_\Omega(\mathcal{S}_i)}{\text{cost}_A(\mathcal{S}_i)} \right) \right)$. For the benchmark, we used the evaluation as proposed in Section **??**. In addition, we also determined the distortion via simply running the k-means++ algorithm.

Except for BICO, which is deterministic, this experiment was repeated for each coreset algorithm 10 times. We aggregated the reported distortions by taking the median over all 10 evaluations. In addition, we also preprocessed the data using the dimension reduction techniques described in Section **??**.

4.1 Datasets We use three common real-world datasets for evaluating k-means coresets — *Census*[4], *Covertype*[5], and *Tower*[6] — and several instances of the proposed benchmark. The *Census* dataset is a small subset of the Public Use Microdata Samples from 1990 US census. It consists of demographic information encoded as 68 categorical attributes of 2,458,285 individuals. *Covertype* is comprised of cartographic descriptions and forest cover type of four wilderness areas in the Roosevelt National Forest of Northern Colorado in the US. It consists of 581,012 records, 54 cartographic variables and one class variable. Although *Covertype* was originally made for classification tasks, it is often used for clustering tasks by removing the class variable [1]. *Tower* is a 2,560 by 1,920 picture of a tower on a hill where each pixel is represented by a RGB color value. This dataset consists of 4,915,200 rows and 3 columns. To evaluate how denoising effects the quality of the output, we apply SVD on *Census* and *Covertype* using the k largest singular values. Note that we do not reduce the number of dimensions of the original datasets. As for the benchmark dataset, instances are generated to match roughly the sizes of the real-world datasets. The chosen parameters values and the corresponding dataset sizes are shown in Table 2.

Table 1: The sizes of the real-world datasets used for the experimental evaluation

	Data points	Dimensions
Census	2,458,285	68
Covertype	581,012	54
Tover	4,915,200	3

Table 2: The parameter values and the sizes of the benchmark instances used for the experimental evaluation.

k	α	Data points	Dimensions
10	6	1,000,000	60
20	5	3,200,000	100
30	4	810,000	120
40	4	2,560,000	160

4.2 Algorithm Parameters We followed the same experimental procedure with respect to the choice of parameter values for the algorithms as prior works [18, 1]. For the target coreset size, we used $200k$ for all our experiments. On *Census* and *Covertype*, we used k values $\{10, 20, 30, 40, 50\}$, while for *Tower* we used larger cluster sizes $k \in \{20, 40, 60, 80, 100\}$ as in. On the benchmark instances, we settled on $k \in \{10, 20, 30, 40\}$ as a reasonable trade-off between running time and dataset size.

4.3 Setup We implemented Sensitivity Sampling, Group Sampling and StreamKM++ in C++17 using Boost and Blaze libraries. The source code can be found on GitHub[7]. For BICO, we used the authors' reference implementation[8]. We used gcc 9.3.0 to compile the source code. The experiments were performed on

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

[5] https://archive.ics.uci.edu/ml/datasets/covertype

[6] http://homepages.uni-paderborn.de/frahling/coremeans.html

[7] Link to repository will be provided later.

[8] https://ls2-www.cs.tu-dortmund.de/grav/en/bico

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an Intel i7 machine (8 core, 3.4 GHz and 32 GB RAM) and an Intel i9 server (14 core, 3.3 GHz and 256 GB RAM).

4.4 Results

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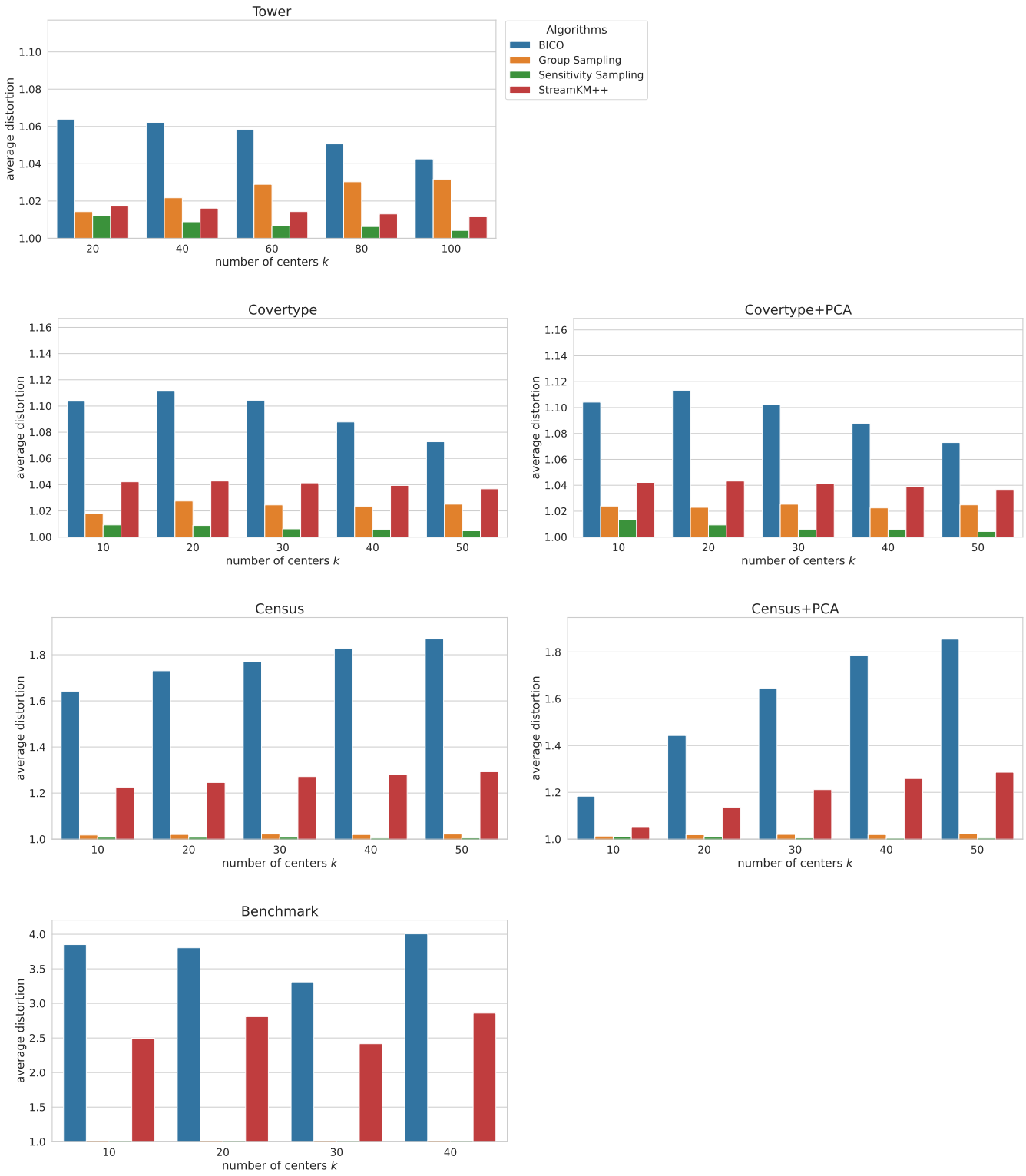

Figure 2: The average distortion of the evaluated algorithms on different datasets.

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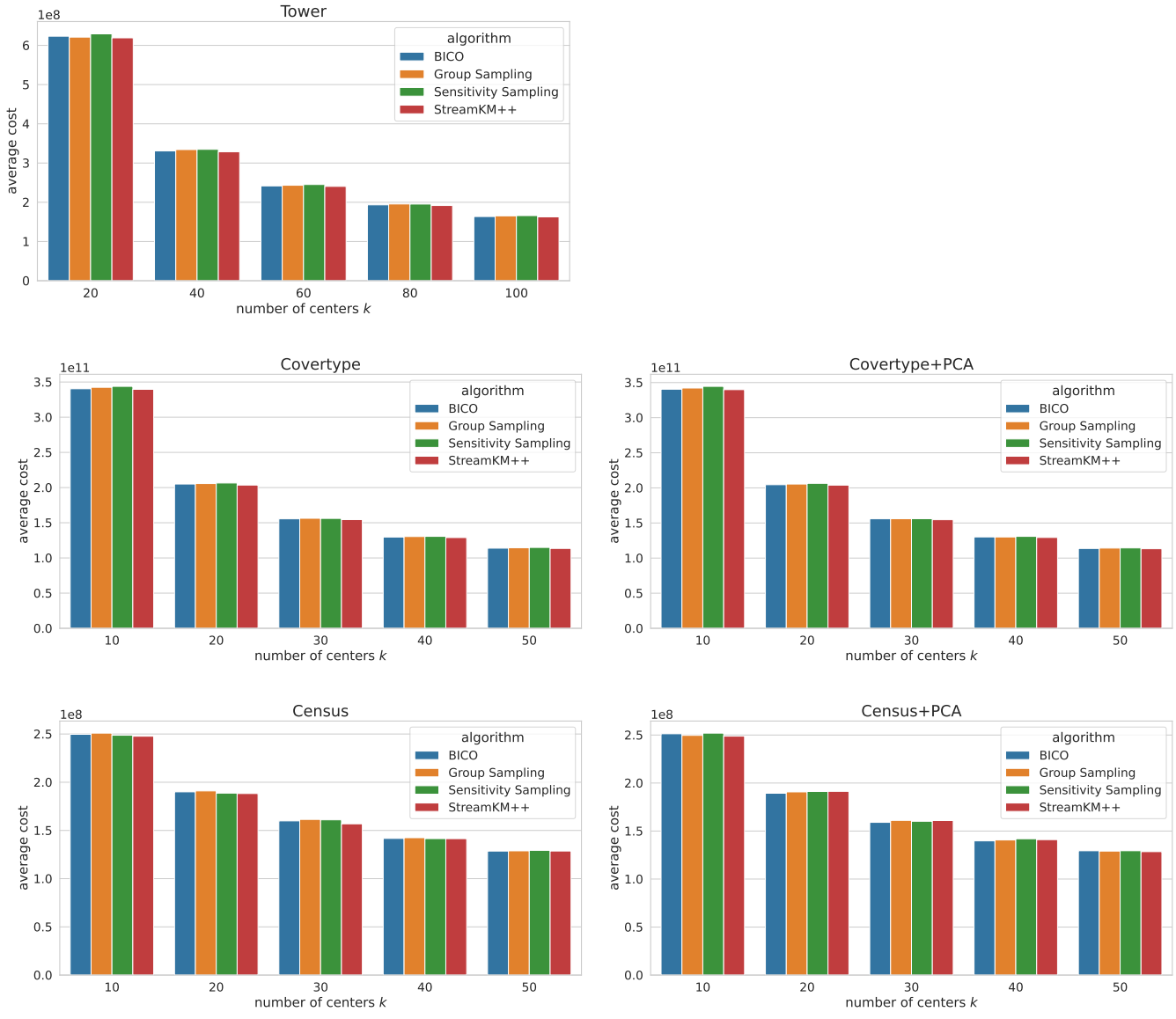

Figure 3: The costs of the evaluated algorithms on *Tower*, *Covertype*, and *Census* datasets.

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