Scalable and Distributed Clustering via Lightweight Coresets

Olivier Bachem
Mario Lucic
Andreas Krause
Department of Computer Science, ETH Zurich

Abstract

Coresets are compact representations of data sets such that models trained on a coreset are provably competitive with models trained on the full data set. As such, they have been successfully used to scale up clustering models to massive data sets. While existing approaches generally only allow for multiplicative approximation errors, we propose a novel notion of coresets called lightweight coresets that allows for both multiplicative and additive errors. We provide a single algorithm to construct light-weight coresets for $k$-Means clustering, Bregman clustering and maximum likelihood estimation of Gaussian mixture models. The algorithm is substantially faster than existing constructions, embarrassingly parallel and resulting coresets are smaller. In an extensive experimental evaluation, we demonstrate that the proposed method outperforms existing coreset constructions.

1. Introduction

A recent, unprecedented increase in the size of data sets has led to new challenges for scalable machine learning. In particular, such massive data sets may not fit on single machines anymore but must be distributed. At the same time, many algorithms require several passes through the full data set and have a potentially even superlinear computational complexity. As a result, traditional algorithms optimized for single machines and small data set sizes are not suitable for this setting.

Coresets are a proven way to scale clustering problems. They are small, weighted subsets of an original data set such that models trained on the coreset are provably competitive with models trained on the full data set. They can be used to speed up inference while retaining strong theoretical guarantees on the solution quality. One first constructs a coreset — usually in linear time — and then uses any algorithm to solve the clustering problem on the coreset. As the coreset size is usually sublinear in or even independent of the number of data points, computationally intensive inference algorithms with superlinear complexity may be applied on the coresets.

Coresets have been successfully constructed for a wide variety of clustering problems. Yet, even linear-time coreset constructions can be hard to scale to massive data sets in a distributed setting. For example, the state-of-the-art construction for $k$-Means (Lucic et al., 2016) requires $k$ sequential passes through the data. While there are approaches to construct coresets in a distributed fashion (discussed in Section 2), they increase the total computational effort and still require several passes through the data. Consequently, existing approaches are unsuitable for the practical setting where one can process the full data set only once or twice in parallel.

Our contributions. We propose a novel approach to coreset construction for $k$-Means clustering that retains the benefits of previous coreset constructions at a fraction of the cost. In particular, we

1. introduce and motivate the novel notion of lightweight coresets,
2. provide a simple and embarrassingly parallel algorithm to construct such lightweight coresets using only two passes through the full data set,
3. prove that the required coreset size is only linear in the dimension and near-linear in the number of the clusters,
4. extend the results to hard and soft clustering with a large class of Bregman divergences, and
5. empirically confirm the proposed method’s effectiveness on a variety of data sets.

2. Background and related work

$k$-Means clustering. Let $\mathcal{X}$ denote a set points in $\mathbb{R}^d$. The $k$-Means clustering problem is to find a set $Q$ of $k$ cluster centers in $\mathbb{R}^d$ such that the quantization error $\phi_{\mathcal{X}}(Q)$ is minimized, where

$$\phi_{\mathcal{X}}(Q) = \sum_{x \in \mathcal{X}} d(x, Q)^2 = \sum_{x \in \mathcal{X}} \min_{q \in Q} \|x - q\|^2.$$ 

For general $k$-clustering the squared Euclidean distance is replaced with the corresponding divergence measure $d$. For a weighted set $\mathcal{C}$ with corresponding weights
Scalable and Distributed Clustering via Lightweight Coresets

$w : \mathcal{C} \to \mathbb{R}_{\geq 0}$, the quantization error is defined as

$$\phi_C(Q) = \sum_{x \in \mathcal{C}} w(x) d(x, Q)^2.$$ The quantization error of the optimal solution with $k$ centers is denoted by $\phi_{OPT}^k(\mathcal{X})$.

**Coresets.** A coreset is a weighted subset of the data such that the quality of any clustering evaluated on the coreset closely approximates the true quality on the full data set. For the $k$-Means clustering problem, this is generally formalized as follows (Har-Peled & Mazumdar, 2004; Lucic et al., 2016): A weighted set $\mathcal{C}$ is a $(\varepsilon, k)$-coreset for $\mathcal{X}$ if for any $Q \in \mathbb{R}^d$ of cardinality $k$

$$|\phi_X(Q) - \phi_C(Q)| \leq \varepsilon \phi_X(Q). \quad (1)$$

This is a strong theoretical guarantee as the cost evaluated on the coreset $\phi_C(Q)$ has to approximate the cost on the full data set $\phi_X(Q)$ up to a $1 \pm \varepsilon$ multiplicative factor uniformly for all possible sets of cluster centers. As a direct consequence, solving on the coreset yields provably competitive solutions when evaluated on the full data set (Lucic et al., 2016). More formally, if $\mathcal{C}$ is a $(\varepsilon, k)$-coreset of $\mathcal{X}$ with $\varepsilon \in (0, 1/3)$, it is easily shown that

$$\phi_X(Q^*_C) \leq (1 + 3\varepsilon)\phi_X(Q^*_\mathcal{X}) \quad (2)$$

where $Q^*_C$ denotes the optimal solution of $k$ centers on $\mathcal{C}$ and $Q^*_\mathcal{X}$ denotes the optimal solution on $\mathcal{X}$. Moreover, any $\alpha$ approximation can be used on the $\varepsilon$-coreset to produce a $(1 + 3\varepsilon)\alpha$ approximation on the original data. As a result, any solver that works on weighted data may be used to solve the clustering problem on the coreset while retaining strong theoretical guarantees.

Coresets are usually small, i.e., their size is logarithmic in or even independent of the number of data points. Hence, one may obtain a fast approximation of the optimal solution, even if the solver used on the coreset has superlinear complexity in the number of data points.

**Coresets for k-Means.** There is a rich history of coreset constructions for $k$-Means (Har-Peled & Mazumdar, 2004; Har-Peled & Kushal, 2005; Chen, 2009; Langberg & Schulman, 2010; Feldman & Langberg, 2011; Lucic et al., 2016). The construction by Lucic et al. (2016) with both state-of-the-art theoretical and experimental results works as follows:

In a first step, a rough approximation of the optimal solution is obtained using the seeding step of the well known $k$-means++ algorithm (Arthur & Vassilvitskii, 2007). In a second step, this solution is then used to construct an importance sampling scheme that provides $(\varepsilon, k)$-coresets if $m \in \Omega((dk^3 \log k + k^2 \log \frac{1}{\varepsilon} \varepsilon^{-2})$ points are sampled.\(^1\)

There is one key drawback to this approach: The coreset construction requires $k$ sequential passes through the full data set. Constructing coresets for massive data sets can hence become prohibitively expensive even for moderate $k$ despite the linearity in the number of data points. Furthermore, if the data set does not fit on a single machine, the seeding step of $k$-means++ cannot be run efficiently and the coreset has to be constructed in a distributed setting. This can be achieved using a generic approach by Feldman et al. (2011) based on partitioning the data, computing independent coresets and merging them. Alternatively, the seeding step of $k$-means++ can be replaced by $k$-means|| (Bahmani et al., 2012). However, both these approaches do not decrease the total computational effort. In fact, they increase it from $O(nkd)$ to $O(nkd \log n)$ where $n$ denotes the number of data points and $d$ their dimensionality.

Balcan et al. (2013) provide a low-communication distributed algorithm for $k$-Means and $k$-Median clustering on general network topologies and provide coresets for $k$-Means of size $\Omega(dk \log k/\varepsilon^4)$ with $O(Mpd)$ communication cost, where $p$ is the number of machines and $M$ is the number of edges in the network.\(^2\) In contrast, our algorithm produces coresets of size $\Omega(dk \log k/\varepsilon^2)$ and can be implemented with only $\Omega(pd)$ communication.

**Other related work.** Ccoresets were originally studied in computational geometry. Previous constructions for $k$-Means are based upon exponential grids (Har-Peled & Mazumdar, 2004) and building coresets along lines (Har-Peled & Kushal, 2005). These geometrically inspired constructions suffer from coreset sizes exponential in the number of dimensions and are rarely practical. The use of sampling-based approaches was investigated by Chen (2009) and Feldman et al. (2007). The latter uses weak coresets to construct a polynomial time approximation scheme. A general framework for constructing coresets was proposed by Langberg & Schulman (2010) and Feldman & Langberg (2011). Feldman et al. (2011) applied this framework to construct coresets for the estimation of Gaussian mixture models and Rosman et al. (2014) to the $k$-segmentation of streaming data. Recently, Bachem et al. (2015) constructed coresets for nonparametric clustering, Reddi et al. (2015) for empirical risk minimization in supervised learning and Huggins et al. (2016) for Bayesian logistic regression.

### 3. Lightweight coresets for $k$-Means

In this section, we propose and motivate lightweight coresets — a novel notion of coresets for $k$-Means. In Section 6, we will then show how to extend the results to other divergence measures.

\(^1\)The original paper states a required sample size of $m \in \Omega((dk^3 + k^2 \log \frac{1}{\varepsilon} \varepsilon^{-2})$. We refer to the discussion on the pseudo-dimension in Section 5 as to why the additional $\log k$ factor is required.

\(^2\)The original paper does not include a $\log k$ factor in the coreset size. We refer to the discussion on the pseudo-dimension in Section 5 as to why an additional $\log k$ factor is required.
Definition 1 (Lightweight coreset for $k$-Means). Let $\varepsilon > 0$ and $k \in \mathbb{N}$. Let $\mathcal{X} \subset \mathbb{R}^d$ be a set of points with mean $\mu(\mathcal{X})$. The weighted set $\mathcal{C}$ is an $(\varepsilon,k)$ lightweight coreset of $\mathcal{X}$ if for any set $Q \subset \mathbb{R}^d$ of cardinality at most $k$

$$|\phi_{\mathcal{X}}(Q) - \phi_{\mathcal{C}}(Q)| \leq \frac{\varepsilon}{2} \phi_{\mathcal{X}}(Q) + \frac{\varepsilon}{2} \phi_{\mathcal{C}}(\{\mu(\mathcal{X})\}).$$

(3)

The notion of lightweight coresets may be interpreted as a relaxation of “traditional” coresets as defined in (1) that allows for both an additive and multiplicative error. The $\frac{\varepsilon}{2} \phi_{\mathcal{X}}(Q)$ term allows the approximation error to scale with the quantization error and constitutes the “traditional” multiplicative part. The $\frac{\varepsilon}{2} \phi_{\mathcal{C}}(\{\mu(\mathcal{X})\})$ term scales with the variance of the data and corresponds to an additive approximation error that is invariant of the scale of the data.

We argue that the “additive” $\frac{\varepsilon}{2} \phi_{\mathcal{C}}(\{\mu(\mathcal{X})\})$ term is adequate in the machine learning setting for the following reason: In machine learning, one often tries to minimize the generalization error by performing empirical risk minimization on a finite sample. Yet, state-of-the-art deviation bounds for finite samples only provide an additive error guarantee (Telgarsky & Dasgupta, 2013).3 Given that one already incurs an additive error, one may thus accept the same additive error when optimizing on the finite sample.

The “multiplicative” $\frac{\varepsilon}{2} \phi_{\mathcal{C}}(\{\mu(\mathcal{X})\})$ term is required for the following (technical) reason: Equation (3) needs to hold uniformly for all possible sets $Q$ of $k$ centers in $\mathbb{R}^d$. As such, with only the $\frac{\varepsilon}{2} \phi_{\mathcal{X}}(\{\mu(\mathcal{X})\})$ term, one would be able to construct the following adverse solution for any coreset $\mathcal{C}$. If the cluster centers are placed arbitrarily far away from the data points, any difference on the left hand side in (3) would be arbitrarily large while the variance of the data would still bounded on the right hand side. Hence, without the multiplicative error term, there would exist no coreset $\mathcal{C}$ satisfying (3) for all possible sets $Q$.

The primary motivation behind coresets is that the optimal solution obtained on the coreset is provably competitive with the optimal solution of the full dataset. For “traditional” data sets, this guarantee is multiplicative as defined in (2). In Theorem 1, we show that lightweight coresets directly imply a corresponding additive guarantee on the solution quality.

Theorem 1. Let $\varepsilon \in (0, 1]$. Let $\mathcal{X}$ be any data set and $\mathcal{C}$ be a $(\varepsilon,k)$ lightweight coreset of $\mathcal{X}$. Denote by $Q^*_X$ an optimal $k$-Means solution on $\mathcal{X}$ and by $Q^*_C$ the optimal solution on $\mathcal{C}$. Then, it holds that

$$\phi_{\mathcal{X}}(Q^*_C) \leq \phi_{\mathcal{X}}(Q^*_X) + 4\varepsilon \phi_{\mathcal{X}}(\{\mu(\mathcal{X})\}).$$

Proof. By the lightweight coreset property, we have

$$\phi_{\mathcal{C}}(Q^*_C) \leq \frac{1 + \varepsilon}{2} \phi_{\mathcal{X}}(Q^*_C) + \frac{\varepsilon}{2} \phi_{\mathcal{C}}(\{\mu(\mathcal{X})\}),$$

and

$$\phi_{\mathcal{C}}(Q^*_C) \geq \frac{1 - \varepsilon}{2} \phi_{\mathcal{X}}(Q^*_C) - \frac{\varepsilon}{2} \phi_{\mathcal{C}}(\{\mu(\mathcal{X})\}).$$

Since $\phi_{\mathcal{C}}(Q^*_C) \leq \phi_{\mathcal{C}}(Q^*_X)$ and $1 - \frac{\varepsilon}{2} \geq \frac{1}{2}$ by definition, it holds that

$$\phi_{\mathcal{X}}(Q^*_C) \leq \frac{1 + \varepsilon}{2} \phi_{\mathcal{X}}(Q^*_X) + \frac{\varepsilon}{2} \phi_{\mathcal{X}}(\{\mu(\mathcal{X})\})$$

$$\leq (1 + 2\varepsilon)\phi_{\mathcal{X}}(Q^*_X) + 2\varepsilon \phi_{\mathcal{X}}(\{\mu(\mathcal{X})\}).$$

The claim then follows as $\phi_{\mathcal{X}}(Q^*_X) \leq \phi_{\mathcal{X}}(\{\mu(\mathcal{X})\})$. $$\square$$

Theorem 1 implies that as we decrease $\varepsilon$, the true cost of the optimal solution obtained on the coreset approaches the true cost of the optimal solution on the full data set in an additive manner. In Section 4 we show that lightweight coresets allows us to obtain a more efficient coreset construction while retaining the empirical benefits of “traditional” coresets as evidenced in Section 7.

4. Construction of lightweight coresets

Our coreset construction is based on importance sampling. Let $q(x)$ be any probability distribution on $\mathcal{X}$ and $Q$ any set of $k$ centers in $\mathbb{R}^d$. Then the quantization error may be rewritten as

$$\phi_{\mathcal{X}}(Q) = \sum_{x \in \mathcal{X}} q(x) \frac{d(x, Q)}{q(x)}.$$  

The quantization error can hence be approximated by sampling $m$ points from $\mathcal{X}$ using $q(x)$ and assigning them weights inversely proportional to $q(x)$. For any number of samples $m$ and any distribution $q(x)$, this yields an unbiased estimator of the quantization error. However, unbiasedness is not sufficient to guarantee a lightweight coreset as defined in Definition 1. In particular, (3) has to hold with probability $1 - \delta$ uniformly across all $k$-sized sets of centers $Q$. Obtaining such a stronger bound requires a suitable distribution $q(x)$ and a corresponding lower bound on the number of samples $m$. We suggest the following proposal distribution

$$q(x) = \frac{1}{2} \frac{1}{|\mathcal{X}|} + \frac{1}{2} \sum_{x' \in \mathcal{X}} \frac{d(x', \mu(\mathcal{X}))^2}{\sum_{x'' \in \mathcal{X}} d(x'', \mu(\mathcal{X}))^2}.$$ 

that has a natural interpretation as a mixture of two components. The first component (A) is the uniform distribution and ensures that all points can be sampled. The second component (B) ensures that points are sampled proportionally to the squared distance to the mean of the data. The intuition is that the points that are far from the mean of the data...
have a potentially large impact on the quantization error of a clustering. The component (B) ensures that these points are sampled more frequently.

4.1. A practical algorithm

The resulting coreset construction is provided as pseudo code in Algorithm 1 and is extremely simple and practical: One calculates the mean of the data and then uses it to compute the importance sampling distribution \(q(x)\). Finally, \(m\) points are sampled with probability \(q(x)\) from \(X\) and assigned the weight \(\frac{1}{m-q(x)}\). The algorithm only requires two passes through the full data set resulting in a total computational complexity of \(O(nd)\). There is no additional linear dependence on the number of clusters \(k\) as in previous constructions (Lucic et al., 2016) which becomes paramount in the setting where \(k\) even moderately large as demonstrated in Section 7.

4.2. Distributed implementation

Algorithm 1 is embarrassingly parallel and can be implemented in a two-round distributed procedure. Let \(X\) be partitioned across \(p\) machines and let \(X_i\) denote the points on the \(i\)-th machine. For each \(x \in X\), let \(x_j\) denote the \(j\)-th coordinate of \(x\). We first compute the mean as follows. In the first round, each machine computes \(|X_i|\), \(U_{ij} = \sum_{x \in X} x_j\) and \(V_{ij} = \sum_{x \in X_i} (x_j)^2\) and sends them back to the central machine. The central machine can then easily compute the global mean \(\mu\), the quantization errors \(\phi_{X_i}({\mu})\) and the total quantization error \(\phi_{X}({\mu})\). For each machine \(i\), we further keep track of the number of points \(u_i\) to be sampled uniformly using (A) and the number of points \(v_i\) to be sampled nonuniformly using (B). The central machine distributes the \(m\) points to be sampled iteratively as follows: In each round, with probability \(1/2\), it samples the machine \(i\) with probability proportional to \(|X_i|\) and increases the corresponding \(u_i\) by one. Otherwise, it samples the machine \(i\) with probability proportional to \(\phi_{X_i}({\mu})\) and increases \(v_i\) by one. Each machine \(i\) then obtains \(u_i\), \(v_i\), \(\phi_{X_i}({\mu})\) and \(\phi_{X}({\mu})\) and samples \(u_i\) points uniformly at random and \(v_i\) points proportionally to \(d(x, \mu)^2\). For each sampled point, it further computes its weight and outputs the weight-point pair. Hence, there is no loss in approximation with respect to the single-machine implementation. It is easy to see that the total computation cost is bounded by \(O(pd)\).

Algorithm 1 Light-weight coreset construction

Require: Set of data points \(X\), coreset size \(m\)
for \(x \in X\) do
\[
q(x) \leftarrow \frac{1}{2 \frac{1}{|X|}} + \frac{1}{2} \frac{d(x, \mu)^2}{\sum_{x' \in X} d(x', \mu)^2}
\]
\(C \leftarrow \text{sample } m\text{ weighted points from } X\) where each point \(x\) has weight \(\frac{1}{m-q(x)}\) and is sampled with probability \(q(x)\).
Return coreset \(C\).

Theorem 2. Let \(\varepsilon > 0, \delta > 0\) and \(k \in \mathbb{N}\). Let \(X\) be a set of points in \(\mathbb{R}^d\) and let \(C\) be the output of Algorithm 1 with \(m \in \Omega\left(\frac{dk+\log \frac{1}{\varepsilon}}{\varepsilon^2}\right)\). Then, with probability at least \(1 - \delta\), the set \(C\) is a \((\varepsilon, k)\) lightweight coreset of \(X\).

Proof of Theorem 2. We first derive an importance sampling distribution over \(x \in X\). Then, we show that by sampling a sufficient number of points from this importance sampling distribution one obtains \((\varepsilon, k)\) lightweight coreset of \(X\). We first bound the importance of each data point \(x \in X\). We define
\[
\tilde{f}(Q) = \frac{1}{2|X|} \phi_{X}(Q) + \frac{1}{2|X|} \phi_{X}({\mu}(X))
\]
\[
= \frac{1}{2|X|} \sum_{x' \in X} d(x', Q)^2 + \frac{1}{2|X|} \sum_{x' \in X} d(x', \mu)^2.
\]

and prove the following Lemma.

Lemma 1. Let \(X\) be a set of \(n\) points in \(\mathbb{R}^d\). For all \(Q \subset \mathbb{R}^d\) of cardinality \(k\) and \(x \in X\), we have
\[
\frac{d(x, Q)^2}{f(Q)} \leq \frac{16 d(x, \mu)^2}{|X|} \sum_{x' \in X} d(x', \mu)^2 + 16.
\]

Proof. By the triangle inequality and since \(|a| + |b| \leq 2a^2 + b^2\), we have for any \(x \in X\) and any \(Q \subset \mathbb{R}^d\) of cardinality \(k\)
\[
d(\mu, Q)^2 \leq 2 d(x, \mu)^2 + 2 d(x, Q)^2.
\]

Summing across all \(x \in X\), we obtain
\[
d(\mu, Q)^2 \leq \frac{2}{|X|} \sum_{x' \in X} d(x', \mu)^2 + \frac{2}{|X|} \sum_{x' \in X} d(x', Q)^2.
\]

This implies that for all \(x \in X\) and \(Q \subset \mathbb{R}^d\) of cardinality \(k\)
\[
d(x, Q)^2 \leq 2 d(x, \mu)^2 + 2 d(\mu, Q)^2
\]
\[
\leq 2 d(x, \mu)^2 + \frac{4}{|X|} \sum_{x' \in X} d(x', \mu)^2
\]
\[
+ \frac{4}{|X|} \sum_{x' \in X} d(x', Q)^2.
\]

5. Analysis

Theorem 2 is our main result and guarantees that Algorithm 1 produces valid lightweight coresets if sufficiently many points are sampled. The sample complexity \(m\) is independent of the number of data points, linear in the dimensionality and near-linear in the number of centers.
Scalable and Distributed Clustering via Lightweight Coresets

We divide by
\[ \tilde{f}(Q) = \frac{1}{2|X|} \sum_{x' \in X} d(x', Q)^2 + \frac{1}{2|X|} \sum_{x' \in X} d(x', \mu)^2 \]
and obtain for \( \mathcal{L} = \frac{d(x, Q)^2}{\tilde{f}(Q)} \) that
\[
\mathcal{L} \leq \frac{2d(x, \mu)^2}{2|X|} \sum_{x' \in X} d(x', \mu)^2 + \frac{1}{2|X|} \sum_{x' \in X} d(x', Q)^2 + \frac{1}{2|X|} \sum_{x' \in X} d(x', Q)^2 \leq \frac{16d(x, \mu)^2}{|X|} + 16,
\]
for all \( x \in X \) and \( Q \subset \mathbb{R}^d \) of cardinality \( k \).

Lemma 1 implies that the ratio between the cost contribution of a single point \( x \in X \) and \( \tilde{f}(Q) \) is bounded for all \( Q \subset \mathbb{R}^d \) of cardinality \( k \) by
\[
s(x) = \frac{16d(x, \mu)^2}{|X| \sum_{x' \in X} d(x', \mu)^2} + 16.
\]

We define \( S = \frac{1}{|X|} \sum_{x' \in X} s(x') \) and note that \( S = 32 \) for any data set \( X \). We define the probability measure \( q(x) = s(x)/(|X| \cdot S) \) and note that it matches the importance sampling distribution in Algorithm 1. For any \( Q \subset \mathbb{R}^d \) of cardinality \( k \) we obtain that
\[
\phi_X(Q) = \sum_{x \in X} d(x, Q)^2 = |X| \cdot S \cdot \tilde{f}(Q) \sum_{x \in X} s(x) \frac{d(x, Q)^2}{\tilde{f}(Q) s(x)} := \phi_Q(x)
\]
\[
= 32 \cdot |X| \cdot \tilde{f}(Q) \cdot \mathbb{E}_q[g_Q(x)]
\]
where \( \mathbb{E}_q[g_Q(x)] = \sum_{x \in X} q(x)g_Q(x) \).

As is standard in recent coreset constructions (Feldman & Langberg, 2011; Balcan et al., 2013; Lucic et al., 2016), we would like to apply the following seminal result of Li et al. (2001).

Definition 2 (Haussler (1992); Li et al. (2001)). Fix a countably infinite domain \( X \). The pseudo-dimension of a set \( \mathcal{F} \) of functions from \( X \) to \( [0, 1] \), denoted by \( \text{Pdim} (\mathcal{F}) \), is the largest \( d' \) such there is a sequence \( x_1, \ldots, x_{d'} \) of domain elements from \( X \) and a sequence \( r_1, \ldots, r_{d'} \) of reals such that for each \( b_1, \ldots, b_{d'} \in \{\text{above}, \text{below}\} \), there is an \( f \in \mathcal{F} \) such that for all \( i = 1, \ldots, d' \), we have \( f(x_i) \geq r_i \iff b_i = \text{above} \).

Theorem 3 (Li et al. (2001)). Let \( \alpha > 0 \), \( \nu > 0 \) and \( \delta > 0 \). Fix a countably infinite domain \( X \) and let \( P \) be any probability distribution over \( X \). Let \( \mathcal{F} \) be a set of functions from \( X \) to \( [0, 1] \) with \( \text{Pdim} (\mathcal{F}) = d' \). Denote by \( C \) a sample of \( m \) points from \( X \) independently drawn according to \( P \). Then, for \( m \in \Omega\left(\frac{1}{\alpha^2 \nu^2} (d' \log \frac{1}{\nu} + \log \frac{1}{\delta})\right) \), we have with probability at least \( 1 - \delta \)
\[
\forall f \in \mathcal{F} \quad \mathbb{E}_P[f] \left( 1 - \frac{1}{|S|} \sum_{x \in S} f(x) \right) \leq \alpha
\]
where \( \mathbb{E}_P(a, b) = \frac{|a - b|}{a + b + \nu} \). Furthermore, over all choices of \( \mathcal{F} \) with \( \text{Pdim} (\mathcal{F}) = d \), this bound is tight.

To obtain a uniform guarantee over all possible clusterings \( Q \), we would like to apply Theorem 3 to approximate \( \mathbb{E}_q[g_Q(x)] \) uniformly for the function family
\[
\mathcal{G} = \{ g_Q(x) : Q \subset \mathbb{R}^d, |Q| = k \}.
\]

For this, we require a bound on the pseudo-dimension of the function family \( \mathcal{G} \) which measures the richness of the function family and may be viewed as a generalization of the Vapnik-Chervonenkis (VC) dimension. Previous work (Feldman & Langberg, 2011; Balcan et al., 2013; Lucic et al., 2016) has used that the pseudo-dimension of \( k \)-Means (or equivalently the function family \( \mathcal{G} \)) is essentially bounded by the VC dimension of \( k \)-fold intersections of halfspaces in \( \mathcal{O}(d) \)-dimensional Euclidean space.\(^4\)

However, Feldman & Langberg (2011), Balcan et al. (2013) as well as Lucic et al. (2016) all use a different definition of pseudo-dimension than the underlying theorem by Li et al. (2001): they define it as the smallest integer \( d \) that bounds the number of dichotomies induced by \( \mathcal{G} \) on a sample of \( m \) points by \( m^d \). Such bound on the growth function of the number of dichotomies may be regarded as a generalization of the primal shattering dimension in classical VC theory (Har-Peled, 2011; Matoušek, 2009). The aforementioned papers bound the primal shattering dimension for \( k \)-Means by \( \mathcal{O}(dk) \), for example in Theorem 6 of Lucic et al. (2016), and then proceed to (incorrectly) apply Theorem 3.

While both notions are closely related, one has to be careful: A primal shattering dimension of \( d' \) only implies a VC dimension of at most \( \mathcal{O}(d' \log d') \) (Har-Peled, 2011). For the function family \( \mathcal{G} \), this would imply that the pseudo-dimension is bounded by \( \mathcal{O}(dk \log dk) \) and not \( \mathcal{O}(dk) \). In fact, it not known whether for \( d > 3 \) \( k \)-fold intersections of halfspaces are VC-linear, i.e., the VC dimension is bounded by \( \mathcal{O}(dk) \) (Johnson, 2008). The currently best bound on the VC dimension of \( k \)-fold intersections of halfspaces for

\(^4\)This can be shown by the use of a lifting map as in Theorem 6 of Lucic et al. (2016).
Scalable and Distributed Clustering via Lightweight Coresets

general $d$ is $O(dk \log k)$ (Eisenstat & Angluin, 2007). This implies that the coreset constructions in Feldman & Langberg (2011), Balcan et al. (2013), Lucic et al. (2016) as well as this paper require an additional $\log k$ factor in the coreset size compared to the bounds obtained with the primal shattering dimension of $O(dk)$.

We note that the function $g_Q(x)$ is bounded in $[0, 1]$ for all $x \in \mathcal{X}$ and $Q \subset \mathbb{R}^d$ of cardinality $k$. This allows us to apply Theorem 3 to approximate $E_q[g_Q(x)]$ in (4). Moreover, for any $\epsilon, \delta > 0$, we now instantiate Theorem 3 with $\alpha = \epsilon / 96$ and $\nu = 1/2$ to the function family $\mathcal{G}$. It follows that, $m \in \Omega\left(\frac{dk \log k + \log \frac{1}{\delta}}{\epsilon^2}\right)$ implies that with probability at least $1 - \delta$ and for all sets $Q \subset \mathbb{R}^d$ of cardinality $k$:

$$d_{\nu}\left(E_q[g_Q(x)], \frac{1}{|C|} \sum_{x \in C} g_Q(x)\right) \leq \frac{\epsilon}{96}.$$  

We note that both arguments to $d_{\nu}(\cdot, \cdot)$ are bounded in $[0, 1]$. As a result the denominator in $d_{\nu}(\cdot, \cdot)$ is bounded by 3 which implies

$$\left|E_q[g_Q(x)] - \frac{1}{|C|} \sum_{x \in C} g_Q(x)\right| \leq \frac{\epsilon}{32}$$

for all sets $Q \subset \mathbb{R}^d$ of cardinality $k$. We multiply both sides by $|\mathcal{X}| \tilde{f}(Q)$ to obtain

$$32 \tilde{f}(Q) \left|\mathcal{X}| \tilde{f}(Q) - \frac{|\mathcal{X}|}{|C|} \sum_{x \in C} g_Q(x)\right| \leq \epsilon |\mathcal{X}| \tilde{f}(Q).$$

Let $(C, u)$ be a weighted set that contains all $x \in C$ with weight $u(x) = \frac{|\mathcal{X}|}{|C|} g_Q(x)$. From the definition of $g_Q(x)$ we have

$$\frac{|\mathcal{X}|}{|C|} \sum_{x \in C} 32 \tilde{f}(Q) g_Q(x) = \sum_{x \in C} \tilde{f}(Q) \left|\mathcal{X}| \tilde{f}(Q) - \frac{|\mathcal{X}|}{|C|} g_Q(x)\right| d(x, Q)^2$$

$$= \sum_{x \in C} u(x) d(x, Q)^2$$

$$= \phi_C(Q).$$

By (4) and the definition of $\tilde{f}(Q)$, we directly obtain the desired lightweight coreset property, i.e., for all sets $Q \subset \mathbb{R}^d$ of cardinality $k$ we have

$$|\phi_X(Q) - \phi_C(Q)| \leq \frac{\epsilon}{2} \phi_X(Q) + \frac{\epsilon}{2} \phi_X(|\mu(\mathcal{X})|).$$

\section{6. Extension to $\mu$-similar Bregman divergences}

Building on the results of Lucic et al. (2016), our results can be extended to hard and soft clustering with $\mu$-similar Bregman divergences, a broad class of divergence measures that includes the squared Mahalanobis distance, the KL-divergence and the Itakura-Saito distance. Let $d_{\phi}(\cdot, \cdot)$ denote a $\mu$-similar Bregman divergence and $d_A(\cdot, \cdot)$ the corresponding squared Mahalanobis distance implied by $\mu$-similarity. The lightweight coreset property of Definition 1 can then be modified as follows. For hard clustering, we simply replace all occurrences of the squared Euclidean distance $d(\cdot, \cdot)^2$ by the Bregman divergence $d_{\phi}(\cdot, \cdot)$. For soft clustering, the hard-min is further replaced by a soft-min. In Algorithm 1, the squared Euclidean distance between the points and the mean of the data set is replaced by the squared Mahalanobis distance $d_A(\cdot, \cdot)$. The required coreset size is $\Omega\left(\frac{dk \log k + \log \frac{1}{\delta}}{\mu^2 \epsilon^2}\right)$ for hard clustering and $\Omega\left(\frac{d^2 k^2 \log k}{\mu^2 \epsilon^2}\right)$ for soft clustering. The analysis in Section 5 is adapted as follows: For hard clustering, one needs to add an additional factor of $\frac{1}{\mu}$ on the RHS of Lemma 1 due to $\mu$-similarity and scale $S$ accordingly. For soft clustering, one further needs to apply Lemma 3 of Lucic et al. (2016) to account for the soft-min. The pseudo dimension is bounded by $O(dk)$ for hard and $O(d^2 k^2)$ for soft clustering (Lucic et al., 2016).

\section{7. Experimental results}

Experimental setup.\footnote{All experiments were run on an Intel Xeon machine with 36 $\times$ 2.3GHz processors and 1.5TB memory. The experimental code will be released after publication on the author’s web page.} We compare the lightweight coresets constructed with Algorithm 1 and denoted by LWCS with two different subsampling methods: UNIFORM, the “naive” strategy of uniformly subsampling the data points, and CS, the state-of-the-art coreset construction by Lucic et al. (2016).

For each of these methods, we generate subsamples of size $m \in \{1000, 2000, 5000, 10000, 20000\}$. We then use both steps of the state-of-the-art algorithm $k$-means++ (Arthur & Vassilvitskii, 2007) to solve on the subsample. We measure the elapsed time and then evaluate the clustering by computing the quantization error on the full data set.

In addition, we run $k$-means++ on the full data set (denoted by FULL) and again measure the time and the solution quality as evaluated on the full data set. We then compute the relative error $\eta$ for each method and subsample size compared to the full solution. We further report the relative speedup compared to the full method.

Since the experiments are randomized, we run them 50 times with different random seeds and compute sample averages with corresponding 95% confidence intervals based on the standard error of the mean.

Data sets. We consider the $k$-Means clustering problem on four different data sets for both $k = 100$ and $k = 500$: All experiments were run on an Intel Xeon machine with 36 $\times$ 2.3GHz processors and 1.5TB memory. The experimental code will be released after publication on the author’s web page.
Scalable and Distributed Clustering via Lightweight Coresets

Figure 1. Relative error in relation to subsample size for Uniform, LWCS and CS. LWCS captures most of the benefits of CS over Uniform. Results are averaged across 50 iterations and shaded areas denote 95% confidence intervals.

Figure 2. Relative error vs. time required for Uniform, LWCS and CS. LWCS outperforms CS substantially. Results are averaged across 50 iterations and shaded areas denote 95% confidence intervals. Note that computing the solution on the full data set takes up to 8604 seconds (SONG, k = 500).
Table 1. Relative error and speedup of different methods vs. FULL.

| $k$ | Data | Method | Relative error vs. FULL | Speedup vs. FULL |
|-----|------|--------|-------------------------|-----------------|
|     |      |        | $m = 1000$  | $m = 2000$  | $m = 5000$  | $m = 1000$  | $m = 2000$  | $m = 5000$  |
| 100 | KDD  | UNIFORM| 195.1% ± 20.7  | 105.9% ± 12.9  | 33.8% ± 3.4  | 2244.0×  | 809.1×  | 183.0×  |
|    |      | LWCS   | 18.5% ± 0.2   | 12.1% ± 0.2   | 6.8% ± 0.2   | 828.1×  | 506.0×  | 190.2×  |
|    |      | CS     | 16.0% ± 0.3   | 10.1% ± 0.2   | 5.1% ± 0.1   | 124.8×  | 113.3×  | 81.1×   |
|    | CSN  | UNIFORM| 190.5% ± 6.2  | 123.8% ± 4.2  | 75.2% ± 4.0  | 557.7×  | 210.9×  | 48.7×   |
|    |      | LWCS   | 24.6% ± 0.5   | 16.2% ± 0.3   | 8.4% ± 0.3   | 293.5×  | 174.0×  | 62.2×   |
|    |      | CS     | 18.0% ± 0.4   | 10.5% ± 0.3   | 5.0% ± 0.3   | 61.4×   | 55.6×   | 35.2×   |
|    | SONG | UNIFORM| 22.4% ± 0.3   | 16.0% ± 0.2   | 10.0% ± 0.1  | 8027.1× | 2912.1× | 639.8×  |
|    |      | LWCS   | 14.9% ± 0.1   | 9.9% ± 0.1    | 5.2% ± 0.0   | 1168.2× | 957.5×  | 509.3×  |
|    |      | CS     | 14.6% ± 0.1   | 9.3% ± 0.1    | 4.9% ± 0.0   | 144.9×  | 139.1×  | 127.0×  |
| 500 | KDD  | UNIFORM| 231.0% ± 26.6 | 200.2% ± 27.2 | 64.5% ± 6.1  | 979.8×  | 648.8×  | 240.6×  |
|    |      | LWCS   | 33.1% ± 0.2   | 24.6% ± 0.2   | 15.9% ± 0.1  | 820.0×  | 655.5×  | 260.7×  |
|    |      | CS     | 32.9% ± 0.4   | 23.4% ± 0.2   | 14.3% ± 0.1  | 101.7×  | 97.1×   | 83.3×   |
|    | CSN  | UNIFORM| 521.5% ± 18.3 | 361.7% ± 9.7  | 212.3% ± 8.0 | 79.3×   | 60.9×   | 35.9×   |
|    |      | LWCS   | 77.5% ± 0.9   | 46.5% ± 0.4   | 24.5% ± 0.2  | 74.6×   | 69.1×   | 39.8×   |
|    |      | CS     | 57.8% ± 0.8   | 32.4% ± 0.3   | 15.8% ± 0.2  | 31.8×   | 31.2×   | 26.7×   |
|    | SONG | UNIFORM| 43.0% ± 0.2   | 32.3% ± 0.2   | 21.4% ± 0.1  | 4951.6× | 2866.3× | 992.2×  |
|    |      | LWCS   | 31.4% ± 0.1   | 22.7% ± 0.1   | 14.2% ± 0.0  | 2740.6× | 2051.8× | 914.1×  |
|    |      | CS     | 33.0% ± 0.1   | 23.9% ± 0.1   | 14.7% ± 0.0  | 137.8×  | 134.1×  | 128.4×  |
|    | RNA  | UNIFORM| 786.5% ± 75.3 | 312.1% ± 19.3 | 163.4% ± 9.2 | 58.2×   | 52.4×   | 48.4×   |
|    |      | LWCS   | 189.2% ± 8.7  | 88.0% ± 2.7   | 39.5% ± 2.0  | 49.8×   | 48.7×   | 39.0×   |
|    |      | CS     | 68.8% ± 1.0   | 36.4% ± 0.4   | 17.8% ± 0.2  | 8.0×    | 7.8×    | 7.5×    |

(1) KDD — 145'751 samples with 74 features measuring the match between a protein and a native sequence (KDD Cup, 2004).

(2) CSN — 7GB of cellphone accelerometer data processed into 80,000 observations and 17 features (Faulkner et al., 2011).

(3) MSYP — 90 features from 515'345 songs of the Million Song datasets used for predicting the year of songs (Bertin-Mahieux et al., 2011).

(4) CODRNA — 8 features from 488'565 RNA input sequence pairs (Uzilov et al., 2006).

Discussion of results. Figure 1 shows the relative error of UNIFORM, LWCS and CS for different subsample sizes $m$. The approximation error decreases for all methods as the sample size is decreased. CS provides substantial improvements compared to UNIFORM on all the data sets considered and for both $k = 100$ and $k = 500$. LWCS retains most of these improvements as it performs roughly as good as CS (on KDD and SONG) or slightly worse (on CSN and RNA). Figure 2 displays the relative error in relation to the time required to construct the coreset and then solve on the coreset. As lightweight coresets (LWCS) are much cheaper to construct, they strongly outperform the “traditional” construction (CS) across all data sets. Furthermore, they also produce better solutions than UNIFORM except for the smaller subsample sizes on MSYP and CODRNA.

The practical impact may be seen in Tables 1. For KDD with $k = 100$ and $m = 1000$, UNIFORM leads to a speedup of 2366× compared to solving on the full data set but also incurs a high relative error of 195.1%. CS reduces the relative error to 16.0% but only obtains a speedup of 166×. Lightweight coresets capture the best of both worlds — a speedup of 990× at a relative error of only 18.5%. In absolute terms, one may compute 100 cluster centers on a 145,751 point data set in 0.58 seconds compared to 566 seconds if one naively uses the full data set.

8. Conclusion

We introduced and motivated lightweight coresets — a novel notion of coresets that allows for both multiplicative and additive errors. We proposed a simple and practical algorithm.
Scalable and Distributed Clustering via Lightweight Coresets

for lightweight coreset construction with corresponding theoretical guarantees on the solution quality. Empirically, the produced coresets match the quality of traditional constructions while they are computed at a fraction of the cost.

References

Arthur, David and Vassilvitskii, Sergei. k-means++: The advantages of careful seeding. In Symposium on Discrete Algorithms (SODA), pp. 1027–1047. SIAM, 2007.

Bahmani, Bahman, Moseley, Benjamin, Vattani, Andrea, Kumar, Ravi, and Vassilvitskii, Sergei. Scalable K-Means++. Very Large Data Bases (VLDB), 5(7):622–633, 2012.

Balcan, Maria-Florina, Ehrlich, Steven, and Liang, Yingyu. Distributed k-means and k-median clustering on general topologies. In Advances in Neural Information Processing Systems (NIPS), pp. 1995–2003, 2013.

Bertin-Mahieux, Thierry, Ellis, Daniel P.W., Whitman, Brian, and Lamere, Paul. The million song dataset. In Proceedings of the 12th International Conference on Music Information Retrieval, 2011.

Chen, Ke. On coresets for k-median and k-median clustering in metric and Euclidean spaces and their applications. SIAM Journal on Computing, 39(3):923–947, 2009.

Eisenstat, David and Angluin, Dana. The vc dimension of k-fold union. Information Processing Letters, 101(5):181–184, 2007.

Faulkner, Matthew, Olson, Michael, Chandy, Rishi, Krause, Jonathan, Chandy, K. Mani, and Krause, Andreas. The next big one: Detecting earthquakes and other rare events from community-based sensors. In ACM/IEEE International Conference on Information Processing in Sensor Networks, 2011.

Feldman, Dan and Langberg, Michael. A unified framework for approximating and clustering data. In Symposium on Theory of Computing (STOC), pp. 569–578. ACM, 2011.

Feldman, Dan, Monemizadeh, Morteza, and Sohler, Christian. A PTAS for k-means clustering based on weak coresets. In Symposium on Computational Geometry, pp. 11–18. ACM, 2007.

Feldman, Dan, Faulkner, Matthew, and Krause, Andreas. Scalable training of mixture models via coresets. In Advances in Neural Information Processing Systems (NIPS), pp. 2142–2150, 2011.

Har-Peled, Sariel. Geometric approximation algorithms, volume 173. American mathematical society Boston, 2011.

Har-Peled, Sariel and Kushal, Akash. Smaller coresets for k-median and k-means clustering. In SOCG, pp. 126–134. ACM, 2005.

Har-Peled, Sariel and Mazumdar, Soham. On coresets for k-means and k-median clustering. In Symposium on Theory of Computing (STOC), pp. 291–300. ACM, 2004.

Haussler, David. Decision theoretic generalizations of the PAC model for neural net and other learning applications. Information and Computation, 100(1):78–150, 1992.

Huggins, Jonathan, Campbell, Trevor, and Broderick, Tamara. Coresets for scalable bayesian logistic regression. In Advances In Neural Information Processing Systems, pp. 4080–4088, 2016.

Johnson, Hunter R. Definable families of finite Vapnik Chervonenkis dimension. ProQuest, 2008.

KDD Cup. Protein Homology Dataset. Available at http://osmot.cs.cornell.edu/kddcup/datasets.html, 2004.

Langberg, Michael and Schulman, Leonard J. Universal ε-approximators for integrals. In SODA, pp. 598–607. SIAM, 2010.

Li, Yi, Long, Philip M, and Srinivasan, Aravind. Improved bounds on the sample complexity of learning. Journal of Computer and System Sciences, 2011.

Lucic, Mario, Bachem, Olivier, and Krause, Andreas. Strong coresets for hard and soft Bregman clustering with applications to exponential family mixtures. In Proc. International Conference on Artificial Intelligence and Statistics (AISTATS), May 2016.

Matousek, Jiri. Geometric discrepancy: An illustrated guide, volume 18. Springer Science & Business Media, 2009.

Reddi, Sashank J, Poczos, Barnabás, and Smola, Alex. Communication efficient coresets for empirical loss minimization. In Conference on Uncertainty in Artificial Intelligence (UAI), 2015.

Rosman, Guy, Volkov, Mikhail, Feldman, Dan, Fisher III, John W, and Rus, Daniela. Coresets for k-segmentation of streaming data. In Advances in Neural Information Processing Systems (NIPS), pp. 559–567, 2014.

Telgarsky, Matus J and Dasgupta, Sanjoy. Moment-based uniform deviation bounds for k-means and friends. In Advances in Neural Information Processing Systems, pp. 2940–2948, 2013.

Uzilov, Andrew V, Keegan, Joshua M, and Mathews, David H. Detection of non-coding rnas on the basis of predicted secondary structure formation free energy change. BMC bioinformatics, 7 (1):1, 2006.

Uzilov, Andrew V, Keegan, Joshua M, and Mathews, David H. Detection of non-coding rnas on the basis of predicted secondary structure formation free energy change. BMC bioinformatics, 7 (1):1, 2006.