Layered Sampling for Robust Optimization Problems

Hu Ding 1  Zixiu Wang 1

Abstract
In real world, our datasets often contain outliers. Moreover, the outliers can seriously affect the final machine learning result. The most existing algorithms for handling outliers take high time complexities (e.g., quadratic or cubic complexity). Coreset is a popular approach for compressing data so as to speed up the optimization algorithms. However, the current coreset methods cannot be easily extended to handle the case with outliers. In this paper, we propose a new variant of coreset technique, layered sampling, to deal with two fundamental robust optimization problems: \textit{k}-median/means clustering with outliers and linear regression with outliers. This new coreset method is in particular suitable to speed up the iterative algorithms (which often improve the solution within a local range) for those robust optimization problems. Moreover, our method is easy to be implemented in practice. We expect that our framework of layered sampling will be applicable to other robust optimization problems.

1. Introduction
Coreset is a widely studied technique for solving many optimization problems (Phillips, 2016; Bachem et al., 2017; Munteanu et al., 2018; Feldman, 2020). The (informal) definition is as follows. Given an optimization problem with the objective function $\Delta$, denote by $\Delta(P, C)$ the objective value determined by a dataset $P$ and a solution $C$; a small set $S$ is called a coreset if

$$\Delta(P, C) \approx \Delta(S, C)$$

for any feasible solution $C$. Roughly speaking, the coreset is a small set of data approximately representing a much larger dataset, and therefore existing algorithm can run on the coreset (instead of the original dataset) so as to reduce the complexity measures like running time, space, and communication. In the past years, the coreset techniques have been successfully applied to solve many optimization problems, such as clustering (Chen, 2009; Feldman & Langberg, 2011; Huang et al., 2018), logistic regression (Huggins et al., 2016; Munteanu et al., 2018), linear regression (Dasgupta et al., 2009; Drineas et al., 2006), and Gaussian mixture model (Lucic et al., 2017; Karnin & Liberty, 2019).

A large part of existing coreset construction methods are based on the theory of sensitivity which was proposed by (Langberg & Schulman, 2010). Informally, each data point $p \in P$ has the sensitivity $\phi(p)$ (in fact, we just need to compute an appropriate upper bound of $\phi(p)$) to measure its importance to the whole instance $P$ over all possible solutions, and $\Phi(P) = \sum_{p \in P} \phi(p)$ is called the total sensitivity. The coreset construction is a simple sampling procedure where each point $p$ is drawn i.i.d. from $P$ proportional to $\frac{\phi(p)}{\Phi(P)}$; each sampled point $p$ is assigned a weight $w(p) = \frac{\Phi(P)}{m\phi(p)}$ where $m$ is the sample size depending on the “pseudo-dimension” of the objective function $\Delta$ (Feldman & Langberg, 2011; Li et al., 2001)); eventually, the set of weighted sampled points form the desired coreset $S$.

In real world, datasets are noisy and contain outliers. Moreover, outliers could seriously affect the final results in data analysis (Chandola et al., 2009; Goodfellow et al., 2018). However, the sensitivity based coreset approach is not appropriate to handle robust optimization problems involving outliers (e.g., $k$-means clustering with outliers). For example, it is not easy to compute the sensitivity $\phi(p)$ because the point $p$ could be inlier or outlier for different solutions; moreover, it is challenging to build the relation, such as (1), between the original instance $P$ and the coreset $S$ (e.g., how to determine the number of outliers for the instance $S'$).

1.1. Our Contributions
In this paper, we consider two important robust optimization problems: \textit{k}-median/means clustering with outliers and linear regression with outliers. Their quality guaranteed algorithms exist but often have high complexities that seriously limit their applications in real scenarios (see Section 1.2 for more details). We observe that these problems can be often efficiently solved by some heuristic algorithms in practice, though they only guarantee local optimums in theory. For
Figure 1. The red point represents the initial solution $\tilde{C}$; and our goal is to guarantee (2) for a local range around $\tilde{C}$.

example, (Chawla & Gionis, 2013b) proposed the algorithm $k$-means- to solve the problem of $k$-means clustering with outliers, where the main idea is an alternating minimization strategy. The algorithm is an iterative procedure, where it alternatively updates the outliers and the $k$ cluster centers in each iteration; eventually the solution converges to a local optimum. The alternating minimization strategy is also widely used for solving the problem of linear regression with outliers, e.g., (Shen & Sanghavi, 2019). A common feature of these methods is that they usually start from an initial solution and then locally improve the solution round by round. Therefore, a natural question is can we construct a “coreset” only for a local range in the solution space?

Using such a coreset, we can substantially speed up those iterative algorithms. Motivated by this question, we introduce a new variant of coreset method called layered sampling. Given an initial solution $\tilde{C}$, we partition the given data set $P$ into a consecutive sequence of “layers” surrounding $\tilde{C}$ and conduct the random sampling in each layer; the union of the samples, together with the points located in the outermost layer, form the coreset $S$. Actually, our method is partly inspired by the coreset construction method of $k$-median/means clustering (without outliers) proposed by (Chen, 2009). However, we need to develop significantly new idea in theory to prove its correctness for the case with outliers. The purpose of layered sampling is not to guarantee the approximation quality (as (1)) for any solution $C$, instead, it only guarantees the quality for the solutions in a local range $\mathcal{L}$ in the solution space (the formal definition is given in Section 1.3). Informally, we need to prove the following result to replace (1):

$$\forall C \in \mathcal{L}, \Delta(P, C) \approx \Delta(S, C)$$

See Figure 1 for an illustration. In other words, the new method can help us to find a local optimum faster. Our main results are shown in Theorem 1 and 2. The construction algorithms are easy to implement.

1.2. Related Works

$k$-median/means clustering (with outliers). $k$-median/means clustering are two popular center-based clustering problems (Awasthi & Balcan, 2014). It has been extensively studied for using coreset techniques to reduce the complexities of $k$-median/means clustering algorithms (Chen, 2009; Har-Peled & Kushal, 2007; Fichtenberger et al., 2013; Feldman et al., 2013); in particular, (Feldman & Langberg, 2011) proposed a unified coreset framework for a set of clustering problems. However, the research on using coreset to handle outliers is still quite limited. Recently, (Huang et al., 2018) showed that a uniform independent sample can serve as a coreset for clustering with outliers in Euclidean space; however, such uniform sampling based method often misses some important points and therefore introduces an unavoidable error on the number of outliers. (Gupta, 2018) also studied the uniform random sampling idea but under the assumption that each optimal cluster should be large enough. Partly inspired by the method of (Mettu & Plaxton, 2004), (Chen et al., 2018) proposed a novel summary construction algorithm to reduce input data size which guarantees an $O(1)$ factor of distortion on the clustering cost.

In theory, the algorithms with provable guarantees for $k$-median/means clustering with outliers (Chen, 2008; Krishnaswamy et al., 2018; Friggstad et al., 2018) have high complexities and are difficult to be implemented in practice. The heuristic but practical algorithms have also been studied before (Chawla & Gionis, 2013b; Ott et al., 2014). By using the local search method, (Gupta et al., 2017b) provided a 27.4-approximation algorithm of $k$-means clustering with outliers but needing to discard more than the desired number of outliers; to improve the running time, they also used $k$-means++ (Arthur & Vassilvitskii, 2007b) to seed the “coreset” that yields an $O(1)$ factor approximation. Based on the idea of $k$-means++, (Bhaskara et al., 2019) proposed an $O(\log k)$-approximation algorithm.

Linear regression (with outliers). Several coreset methods for ordinary linear regression (without outliers) have been proposed (Drineas et al., 2006; Dasgupta et al., 2009; Boutsidis et al., 2013). For the case with outliers, which is also called “Least Trimmed Squares linear estimator (LTS)”, a uniform sampling approach was studied by (Mount et al., 2014; Ding & Xu, 2014). But similar to the scenario of clustering with outliers, such uniform sampling approach introduces an unavoidable error on the number of outliers. (Mount et al., 2014) also proved that it is impossible to achieve even an approximate solution for LTS within polynomial time under the conjecture of the hardness of affine degeneracy (Erickson & Seidel, 1995), if the dimensionality $d$ is not fixed. Despite of its high complexity, several practical algorithms were proposed before and most of them are based on the idea of alternating minimization that improves the solution within a local range, such as (Rousseeuw, 1984; Rousseeuw & van Driessen, 2006; Hawkins, 1994; Mount et al., 2016; Bhatia et al., 2015; Shen & Sanghavi, 2019). (Klivans et al., 2018) provided another approach based on the sum-of-squares method.
1.3. Preliminaries

Below, we introduce several important definitions.

i. k-Median/Means Clustering with Outliers. Suppose $P$ is a set of $n$ points in $\mathbb{R}^d$. Given two integers $1 \leq z, k < n$, the problem of $k$-median clustering with $z$ outliers is to find a set of $k$ points $C = \{c_1, \ldots, c_k\} \subset \mathbb{R}^d$ and a subset $P' \subset P$ with $|P'| = n - z$, such that the following objective function

$$K^z_k(P, C) = \frac{1}{n - z} \sum_{p \in P'} \min_{1 \leq j \leq k} \|p - c_j\|$$

is minimized. Similarly, we have the objective function

$$K^z_k(P, C) = \frac{1}{n - z} \sum_{p \in P'} \min_{1 \leq j \leq k} \|p - c_j\|^2$$

for $k$-means clustering with outliers. The set $C$ is also called a solution of the instance $P$. Roughly speaking, given a solution $C$, the farthest $z$ points to $C$ are discarded, and the remaining subset $P'$ is partitioned into $k$ clusters where each point is assigned to its nearest neighbor of $C$.

ii. Linear Regression with Outliers. Given a vector $h = (h_1, h_2, \ldots, h_d) \in \mathbb{R}^d$, the linear function defined by $h$ is $y = \sum_{j=1}^{d-1} h_j x_j + h_d$ for $d - 1$ real variables $x_1, x_2, \ldots, x_{d-1}$. Thus the linear function can be represented by the vector $h$. From geometric perspective, the linear function can be viewed as a $(d-1)$-dimensional hyperplane in the space. Let $z$ be an integer between 1 and $n$, and $P = \{p_1, p_2, \ldots, p_n\}$ be a set of $n$ points in $\mathbb{R}^d$, where each $p_i = (x_{i1}, x_{i2}, \ldots, x_{i,d-1}, y_i)$ for $1 \leq i \leq n$; the objective is to find a subset $P' \subset P$ with $|P'| = n - z$ and a $(d-1)$-dimensional hyperplane, represented as a coefficient vector $h = (h_1, h_2, \ldots, h_d) \in \mathbb{R}^d$, such that

$$\mathcal{L}_{R^z_k}(P', h) = \frac{1}{n - z} \sum_{p_i \in P'} |\text{Res}(p_i, h)|$$

or

$$\mathcal{L}_{R^z_k}(P', h) = \frac{1}{n - z} \sum_{p_i \in P'} (\text{Res}(p_i, h))^2$$

is minimized. $\text{Res}(p_i, h) = y_i - \sum_{j=1}^{d-1} h_j x_{ij} - h_d$ is the “residual” of $p_i$ to $h$. The objective functions (5) and (6) are called the “least absolute error” and “least squared error”, respectively.

Remark 1. All the above problems can be extended to weighted case. Suppose each point $p$ has a non-negative weight $w(p)$, then the (weighted) distance $\|p - c_j\| (\|p - c_j\|^2)$ is replaced by $w(p) \cdot \|p - c_j\| (w(p) \cdot \|p - c_j\|^2)$; we can perform the similar modification on $|\text{Res}(p_i, h)|$ and $(\text{Res}(p_i, h))^2$ for the problem of linear regression with outliers. Moreover, the total weights of the outliers should be equal to $z$. Namely, we can view each point $p$ as $w(p)$ unit-weight overlapping points.

Solution range. To analyze the performance of our layered sampling method, we also need to define the “solution range” for the clustering and linear regression problems. Consider the clustering problems first. Given a clustering solution $C = \{c_1, \ldots, c_k\} \subset \mathbb{R}^d$ and $L > 0$, we use “$C \pm L$” to denote the range of solutions $L = \\{c = \{c_1, \ldots, c_k\} | ||c_j - c_j|| \leq L, \forall 1 \leq j \leq k\}$. (7)

Next, we define the solution range for linear regression with outliers. Given an instance $P$, we often normalize the values in each of the first $d - 1$ dimensions as the preprocessing step; without loss of generality, we can assume that $x_{ij} \in [0, D]$ with some $D > 0$ for any $1 \leq i \leq n$ and $1 \leq j \leq d - 1$. For convenience, denote by $R_D$ the region \{(s_1, s_2, \ldots, s_d) | 0 \leq s_j \leq D, \forall 1 \leq j \leq d - 1\} and thus $P \subset R_D$ after the normalization. It is easy to see that the region $R_D$ actually is a vertical square cylinder in the space. Given a coefficient vector (hyperplane) $\tilde{h} = (\tilde{h}_1, \tilde{h}_2, \ldots, \tilde{h}_d) \in \mathbb{R}^d$ and $L > 0$, we use “$\tilde{h} \pm L$” to denote the range of hyperplanes $L = \{h = (h_1, h_2, \ldots, h_d) | ||\text{Res}(p, \tilde{h}) - \text{Res}(p, h)|| \leq L, \forall p \in R_D\}$. (8)

To understand the range defined in (8), we can imagine two linear functions $\tilde{h}^+ = (\tilde{h}_1, \tilde{h}_2, \ldots, \tilde{h}_d + L)$ and $\tilde{h}^- = (\tilde{h}_1, \tilde{h}_2, \ldots, \tilde{h}_d - L)$; if we only consider the region $R_D$, the range (8) contains all the linear functions “sandwiched” by $\tilde{h}^+$ and $\tilde{h}^-$. For both the clustering and regression problems, we also say that the size of the solution range $L$ is $|L| = L$.

2. The Layered Sampling Framework

We present the overview of our layered sampling framework. For the sake of completeness, we first introduce the core-set construction method for the ordinary $k$-median/means clustering proposed by (Chen, 2009).

Suppose $\alpha$ and $\beta \geq 1$. A “bi-criteria $(\alpha, \beta)$-approximation” means that it contains $\alpha k$ cluster centers, and the induced clustering cost is at most $\beta$ times the optimum. Usually, finding a bi-criteria approximation is much easier than achieving a single-criterion approximation. For example, one can obtain a bi-criteria approximation for $k$-median/means clustering in linear time with $\alpha = O(1)$ and $\beta = O(1)$ (Chen, 2009). Let $T = \{t_1, t_2, \ldots, t_{\alpha k}\} \subset \mathbb{R}^d$ be the obtained $(\alpha, \beta)$-approximate solution of the input instance $P$. For convenience, we use $B(c, r)$ to denote the ball centered at a point $c$ with radius $r > 0$. At the beginning of Chen’s core-set construction algorithm, it takes two carefully designed values $r > 0$ and $N = O(\log n)$, and partitions the space into $N + 1$ layers $H_0, H_1, \ldots, H_N$, where $H_0 = \bigcup_{j=1}^{\alpha k} B(t_j, r)$ and $H_i = (\bigcup_{j=1}^{\alpha k} B(t_j, 2^i r)) \setminus (\bigcup_{j=1}^{\alpha k} B(t_j, 2^{i-1} r))$ for $1 \leq i \leq N$. It can be proved that $P$ is
Layered Sampling for Robust Optimization Problems

covered by \( \bigcup_{i=0}^{N} H_i \); then the algorithm takes a random sample \( S_i \) from each layer \( P \cap H_i \), and the union \( \bigcup_{i=0}^{N} S_i \) forms the desired coreset \( S \) satisfying the condition (1).

However, this approach cannot directly solve the case with outliers. First, it is not easy to obtain a bi-criteria approximation for the problem of \( k \)-median/means clustering with outliers (e.g., in linear time). Moreover, it is challenging to guarantee the condition (1) for any feasible solution \( C \), because the set of outliers could change when \( C \) changes (this is also the major challenge for proving the correctness of our method later on). We propose a modified version of Chen’s coreset construction method and aim to guarantee (2) for a local range of solutions. We take the \( k \)-median clustering with outliers problem as an example. Let \( \tilde{C} = \{ \tilde{c}_1, \cdots, \tilde{c}_k \} \subset \mathbb{R}^d \) be a given solution. Assume \( \epsilon > 0 \) and \( N \in \mathbb{Z}^+ \) are two pre-specified parameters. With a slight abuse of notations, we still use \( H_0, H_1, \cdots, H_N \) to denote the layers surrounding \( \tilde{C} \), i.e.,

\[
H_0 = \bigcup_{j=1}^{k} B(\tilde{c}_j, r); \quad H_i = (\bigcup_{j=1}^{k} B(\tilde{c}_j, 2^i r)) \setminus (\bigcup_{j=1}^{k} B(\tilde{c}_j, 2^{i-1} r)) \quad \text{for } 1 \leq i \leq N. \tag{9}
\]

In addition, let

\[
H_{\text{out}} = \mathbb{R}^d \setminus \bigcup_{j=1}^{k} B(\tilde{c}_j, 2^N r). \tag{10}
\]

Here, we set the value \( r \) to satisfy the following condition:

\[
|P \cap H_{\text{out}}| = (1 + \frac{1}{\epsilon})z. \tag{12}
\]

That is, the union of the layers \( \bigcup_{i=0}^{N} H_i \) covers \( n - (1 + \frac{1}{\epsilon})z \) points of \( P \) and excludes the farthest \( (1 + \frac{1}{\epsilon})z \). Obviously, such a value \( r \) always exists. Suppose \( P' \) is the set of \( n - z \) inliers induced by \( \tilde{C} \), and then we have

\[
2^N r \leq \frac{\epsilon}{z} \sum_{p \in P'} \min_{1 \leq j \leq k} ||p - \tilde{c}_j|| = \frac{\epsilon}{z} (n - z) K_{\tilde{C}}^{-}\mathbb{E}(P, \tilde{C}) \tag{13}
\]

via the Markov’s inequality. Our new coreset contains the following \( N + 2 \) parts:

\[
S = S_0 \cup S_1 \cup \cdots \cup S_N \cup S_{\text{out}}, \tag{14}
\]

where \( S_i \) is still a random sample from \( P \cap H_i \) for \( 0 \leq i \leq N \), and \( S_{\text{out}} \) contains all the \( (1 + \frac{1}{\epsilon})z \) points in \( H_{\text{out}} \). In Section 3, we will show that the coreset \( S \) of (14) satisfies (2) for the \( k \)-median clustering with outliers problem (and similarly for the \( k \)-means clustering with outliers problem).

For the linear regression with outliers problem, we apply the similar layered sampling framework. Define \( \mathbb{S}(h, r) \) to be the slab centered at a \( (d - 1) \)-dimensional hyperplane \( h \) with \( r > 0 \), i.e., \( \mathbb{S}(h, r) = \{ p \in \mathbb{R}^d \mid -r \leq R_{\text{es}}(p, h) \leq r \} \). Let \( P \) be an instance, and \( \bar{h} = (\bar{h}_1, \cdots, \bar{h}_d) \in \mathbb{R}^d \) be a given hyperplane. We divide the space into \( N + 2 \) layers \( H_0, H_1, \cdots, H_N, H_{\text{out}} \), where

\[
H_0 = \mathbb{S}(\bar{h}, r); \quad H_i = \mathbb{S}(\bar{h}, 2^i r) \setminus \mathbb{S}(\bar{h}, 2^{i-1} r) \quad \text{for } 1 \leq i \leq N; \tag{16}
\]

\[
H_{\text{out}} = \mathbb{R}^d \setminus \mathbb{S}(\bar{h}, 2^N r). \tag{17}
\]

Similar to (12), we also require the value \( r \) to satisfy the following condition:

\[
|P \cap H_{\text{out}}| = |P \setminus \mathbb{S}(\bar{h}_N, 2^N r)| = (1 + \frac{1}{\epsilon})z. \tag{18}
\]

And consequently, we have

\[
2^N r \leq \frac{\epsilon}{z} (n - z) K_{\bar{C}}^{-}\mathbb{E}(P, \bar{C}). \tag{19}
\]

Then, we construct the coreset for linear regression with outliers by the same manner of (14).

3. \( k \)-Median/Means Clustering with Outliers

In this section, we provide the details on applying our layered sampling framework to the problem of \( k \)-median clustering with outliers. See Algorithm 1. The algorithm and analysis can be easily modified to handle \( k \)-means clustering with outliers, where the only difference is that we need to replace (13) by “ \( 2^N r \leq \sqrt{\frac{\epsilon}{z} (n - z) K_{\bar{C}}^{-}\mathbb{E}(P, \bar{C})} \) ”.

**Theorem 1.** Algorithm 1 returns a point set \( S \) having the size \( |S| = \tilde{O}(k d (\frac{1}{\epsilon}) |d| + (1 + \frac{1}{\epsilon})z) \). Moreover, with probability

\[
1 \text{ The asymptotic notation } \tilde{O}(f) = O(f \cdot \text{polylog}(\frac{1}{\epsilon/\delta})).
\]
at least $1 - \eta$, for any $L > 0$ and any solution $C \in \hat{C} \pm L$, we have

$$K^{-z}(S, C) \in K^{-z}(P, C) \pm \epsilon(K^{-z}(P, \hat{C}) + L). \quad (20)$$

Here, $S$ is a weighted instance of $k$-median clustering with outliers, and the total weight of outliers is $z$ (see Remark 1).

**Remark 2.** (1) The running time of Algorithm 1 is $O(knd)$. For each point $p \in P$, we compute its shortest distance to $\hat{C}$, $\min_{1 \leq j \leq k} ||p - \hat{c}_j||$; then select the farthest $(1 + 1/\epsilon)z$ points and compute the value $r$ by running the linear time selection algorithm (Blum et al., 1973); finally, we obtain the $N + 1$ layers $H_i$, with $0 \leq i \leq N$ and take the samples $S_0, S_1, \cdots, S_N$ from them.

(2) Comparing with the standard_coreset (1), our result contains an additive error $\epsilon(K^{-z}(P, \hat{C}) + L)$ in (20) that depends on the initial objective value $K^{-z}(P, \hat{C})$ and the size $L$ of the solution range. In particular, the smaller the range size $L$, the lower the error of our coreset.

(3) The algorithm of (Chen et al., 2018) also returns a summary for compressing the input data. But there are two major differences comparing with our result. First, their summary guarantees a constant factor of distortion on the clustering cost, while our error approaches $0$ if $\epsilon$ is small enough. Second, their construction algorithm (called “successive sampling” from (Metti & Plaxton, 2004)) needs to scan the data multiple passes, while our Algorithm 1 is much simpler and only needs to read the data in one-pass. We also compare these two methods in our experiments.

To prove Theorem 1, we first show that $S_{H_i}$ is a good approximation of $P \setminus H_{out}$. Fixing a solution $C \in \hat{C} \pm L$, we view the distance from each point $p \in P$ to $C$, i.e., $\min_{1 \leq j \leq k} ||p - c_j||$, as a random variable $x_p$. For any point $p \in P \cap H_i$, with $0 \leq i \leq N$, we have the following bounds for $x_p$. Suppose $p$ is covered by $B(\hat{c}_j, 2r)$. Let the nearest neighbor of $p$ in $C$ be $c_{j_p}$. Then, we have the upper bound

$$x_p = ||p - c_{j_p}|| \leq ||p - c_j|| \leq ||p - \hat{c}_j|| + ||\hat{c}_j - c_j|| \leq 2r + L. \quad (21)$$

Similarly, we have the lower bound

$$x_p \geq \max\{2^{-1}r - L, 0\} \quad \text{if } i \geq 1; \quad x_p = 0 \quad \text{if } i = 0. \quad (22)$$

Therefore, we can take a sufficiently large random sample $\bar{S}_i$ from $P \cap H_i$, such that $\frac{1}{|S_i|} \sum_{p \in S_i} x_p \approx \frac{1}{|P \cap H_i|} \sum_{p \in P \cap H_i} x_p$ with certain probability. Specifically, combining (21) and (22), we have the following lemma through the Hoeffding’s inequality.

**Lemma 1.** Let $\eta \in (0, 1)$. If we randomly sample $O(\frac{1}{\epsilon} \log \frac{1}{\eta})$ points, denote by $\bar{S}_i$, from $P \cap H_i$, then with probability $1 - \eta$,

$$\frac{1}{|S_i|} \sum_{p \in S_i} x_p - \frac{1}{|P \cap H_i|} \sum_{p \in P \cap H_i} x_p \leq \epsilon(2r + 2L).$$

Lemma 1 is only for a fixed solution $C$. To guarantee the result for any $C \in \hat{C} \pm L$, we discretize the range $\hat{C} \pm L$. Imagine that we build a grid inside each $B(\hat{c}_j, L)$ for $1 \leq j \leq k$, where the grid side length is $\frac{L}{\sqrt{k}}$. Denote by $G_j$ the set of grid points inside each $B(\hat{c}_j, L)$, and then $G = G_1 \times G_2 \times \cdots \times G_k$ contains $O\left(\left(\frac{2rL}{\epsilon^2} + 1\right)^k\right)$ $k$-tuple points of $\hat{C} \pm L$ in total. We increase the sample size in Lemma 1 via replacing $\eta$ by $\frac{9}{N|S|}$ in the sample size “$O\left(\frac{1}{\epsilon} \log \frac{1}{\eta}\right)$”. As a consequence, through taking the union bound for the success probability, we have the following result.

**Lemma 2.** $S_j$ is the sample obtained from $P \cap H_i$ in Step 3 of Algorithm 1 for $0 \leq i \leq N$. Then with probability $1 - \eta$,

$$\frac{1}{|S_j|} \sum_{p \in S_j} x_p - \frac{1}{|P \cap H_i|} \sum_{p \in P \cap H_i} x_p \leq \epsilon(2r + 2L),$$

for each $i \in \{0, 1, \cdots, N\}$ and any $C \in G$.

Next, we show that for any $C \in \hat{C} \pm L$ (in particular the solutions in $(\hat{C} \pm L) \setminus G$), Lemma 2 is true. For any solution $C = \{c_1, \cdots, c_k\} \in \hat{C} \pm L$, let $C' = \{c'_1, \cdots, c'_k\}$ be its nearest neighbor in $G$, i.e., $c'_j$ is the grid point of the cell containing $c_j$ in $G_j$, for $1 \leq j \leq k$. Also, denote by $x'_p$ the distance $\min_{1 \leq j \leq k} ||p - c'_j||$. Then we consider to bound the error $\left|\frac{1}{|S_j|} \sum_{p \in S_j} x_p - \frac{1}{|P \cap H_i|} \sum_{p \in P \cap H_i} x'_p\right|$ through $C'$. By using the triangle inequality, we have

$$\left|\frac{1}{|S_j|} \sum_{p \in S_j} x_p - \frac{1}{|P \cap H_i|} \sum_{p \in P \cap H_i} x'_p\right| \leq \left|\frac{1}{|S_j|} \sum_{p \in S_j} x_p - \frac{1}{|S_j|} \sum_{p \in S_j} x'_p\right| + \left|\frac{1}{|S_j|} \sum_{p \in S_j} x'_p - \frac{1}{|P \cap H_i|} \sum_{p \in P \cap H_i} x'_p\right|$$

In (23), the term (a) is bounded by Lemma 2 since $C' \in G$. To bound the terms (a) and (c), we study the difference $|x_p - x'_p|$ for each point $p$. Suppose the nearest neighbor of $p$ in $C$ (resp., $C'$) is $c_j$ (resp., $c'_j$). Then

$$x_p = ||p - c_j|| \leq ||p - c_{j_p}|| \leq ||p - c_{j_p}|| + ||c_j - c_{j_p}|| \leq ||p - c'_{j_p}|| + \epsilon L = x'_p + \epsilon L, \quad (24)$$

Therefore, we have the desired result.
where the last inequity comes from the fact that $c_2'$ and $c_2$ are in the same grid cell with side length $\frac{c_2'}{d}L$. Similarly, we have $x'_p \leq x_p + L$. Overall, $|x_p - x'_p| \leq \epsilon L$. As a consequence, the terms (a) and (c) in (23) are both bounded by $\epsilon L$. Overall, (23) becomes

$$
\frac{1}{|S_i|} \sum_{p \in S_i} x_p - \frac{1}{|P \cap H_i|} \sum_{p \in P \cap H_i} x_p \leq O(\epsilon)(2^r + L).
$$

(25)

For convenience, we use $P_H$ to denote the set $\bigcup_{i=0}^{N} (P \cap H_i)$.

**Lemma 3.** Let $S_0, S_1, \cdots, S_N$ be the samples obtained in Algorithm 1. Then, with probability $1 - \eta$,

$$
\frac{1}{n - z} \sum_{i=0}^{N} \frac{|P \cap H_i|}{|S_i|} \sum_{p \in S_i} x_p - \sum_{p \in P_H} x_p \leq O(\epsilon)\left( K_{1}^{-z}(P, \tilde{C}) + L \right)
$$

(26)

for any $C \in \tilde{C} \pm L$.

**Proof.** For convenience, let $Err_i = | \frac{1}{|S_i|} \sum_{p \in S_i} x_p - \frac{1}{|P \cap H_i|} \sum_{p \in P \cap H_i} x_p |$ for $0 \leq i \leq N$. We directly have $Err_i \leq O(\epsilon)(2^r + L)$ from (25). Moreover, the left hand-side of (26) is

$$
\leq O(\epsilon) \sum_{i=0}^{N} \frac{|P \cap H_i|}{n - z} \cdot (2^r + L)
$$

(27)

It is easy to know that the term $\sum_{i=0}^{N} \frac{|P \cap H_i|}{n - z}(2^r)$ is at most $\frac{1}{n - z}(|P \cap H_0|2^r + 2 \sum_{p \in P_H \setminus H_0} x_p)$ $\leq r + 2K_1^{-z}(P, \tilde{C})$. Note we set $N = \lceil \log \frac{1}{\eta} \rceil$ in Algorithm 1. Together with (13), we know $r \leq \epsilon K_1^{-z}(P, \tilde{C})$ and thus $\sum_{i=0}^{N} \frac{|P \cap H_i|}{n - z}2^r \leq O(1)K_1^{-z}(P, \tilde{C})$. So (26) is true. \hfill \Box

Below, we always assume that (26) is true and consider to prove (20) of Theorem 1. The set $P$ is partitioned into two parts: $P_{in}^C$ and $P_{out}^C$, by $C$, where $P_{out}^C$ is the $z$ farthest points to $C$ (i.e., the outliers) and $P_{in}^C = P \setminus P_{out}^C$. Similarly, the core set $S$ is also partitioned into two parts $S_{in}^C$ and $S_{out}^C$ by $C$, where $S_{out}^C$ is the set of outliers with total weights $z$. In other words, we need to prove

$$
\sum_{p \in S_{in}^C} w(p)x_p = \sum_{p \in P_{in}^C} x_p.
$$

(28)

Consider two cases: (i) $P_H \setminus P_{in}^C = \emptyset$ and (ii) $P_H \setminus P_{in}^C \neq \emptyset$. Intuitively, the case (i) indicates that the set $P_{in}^C$ occupies the whole region $\bigcup_{i=0}^{N} H_i$; the case (ii) indicates that the region $\bigcup_{i=0}^{N} H_i$ contains some outliers from $P_{out}^C$. In the following subsections, we prove that (20) holds for both cases. For ease of presentation, we use $w(U)$ to denote the total weight of a weighted point set $U$ (please be not confused with $|U|$, which is the number of points in $U$).

### 3.1. Case (i): $P_H \setminus P_{in}^C = \emptyset$

We prove the following key lemma first.

**Lemma 4.** If $P_H \setminus P_{in}^C = \emptyset$, $S_{in}^C = S_H \cup (P_{in}^C \setminus P_H)$ and $S_{out}^C = P_{out}^C$ (recall $S_H = \bigcup_{i=0}^{N} S_i$ from Algorithm 1).

**Proof.** First, the assumption $P_H \setminus P_{in}^C = \emptyset$ implies

$$
P_H \subset P_{in}^C
$$

(29)

$$
|P_{in}^C \setminus P_H| = |P_{in}^C| - |P_H|
$$

(30)

In addition, since $S_H \subset P_H$, we have $S_H \subset P_{in}^C$ from (29). Consequently, the set $S_H \cup (P_{in}^C \setminus P_H) \subset P_{in}^C$. Therefore, for any $p \in S_H \cup (P_{in}^C \setminus P_H)$ and any $q \in P_{out}^C$, $x_p \leq x_q$.

Moreover, the set $S \setminus \left( S_H \cup (P_{in}^C \setminus P_H) \right)$

$$
\left( S_H \cup (P_{in}^C \setminus P_H) \right)
$$

$$
\left( S_H \cup (P_{in}^C \setminus P_H) \right)
$$

$$
P \setminus P_{in}^C = P_{out}^C
$$

(31)

It is easy to know that the term $\sum_{i=0}^{N} \frac{|P \cap H_i|}{n - z}(2^r)$ is at most $\frac{1}{n - z}(\sum_{i=0}^{N} |P \cap H_i|2^r) = \frac{1}{n - z} \left( \sum_{i=0}^{N} |P \cap H_i| \right) \leq O(1)K_1^{-z}(P, \tilde{C})$. So (26) is true. \hfill \Box

**Lemma 5.** If $P_H \setminus P_{in}^C = \emptyset$, (20) is true.

**Proof.** Because the set $S_{in}^C$ is equal to $S_H \cup (P_{in}^C \setminus P_H)$ from Lemma 4, the objective value $K_1^{-z}(S, C) = \frac{1}{n - z} \left( \sum_{p \in S_H} w(p)x_p + \sum_{p \in P_{in}^C \setminus P_H} x_p \right)$

$$
\frac{1}{n - z} \left( \sum_{i=0}^{N} \frac{|P \cap H_i|}{|S_i|} \sum_{p \in S_i} x_p + \sum_{p \in P_{in}^C \setminus P_H} x_p \right)
$$

(32)

From Lemma 3, the value of (32) is no larger than

$$
\leq \frac{1}{n - z} \left( \sum_{p \in P_H} x_p + O(\epsilon)(n - z)(K_1^{-z}(P, \tilde{C}) + L) \right)
$$

$$
+ \sum_{p \in P_{in}^C \setminus P_H} x_p
$$

(33)

Note that $P_H \setminus P_{in}^C = \emptyset$, and thus the sum of the two terms $\sum_{p \in P_H} x_p$ and $\sum_{p \in P_{in}^C \setminus P_H} x_p$ in (33) is $\sum_{p \in P_{in}^C} x_p$. Therefore, $K_1^{-z}(S, C) \leq

$$
\frac{1}{n - z} \sum_{p \in P_{in}^C} x_p + O(\epsilon)(K_1^{-z}(P, \tilde{C}) + L)
$$

(34)
Similarly, we have \( K_{1}^{-z}(S, C) \geq K_{1}^{-z}(P, C) - O(\varepsilon)(K_{1}^{-z}(P, \hat{C}) + L) \). Thus, (20) is true. \( \square \)

3.2. Case (ii): \( P_{H} \setminus P_{in}^{C} \neq \emptyset \)

Since \( S \setminus P_{H} = P \setminus P_{H} \) are the outermost \((1 + 1/\varepsilon)z\) points to \( \hat{C} \), we have the following claim first (due to the space limit, please refer to our supplement for the detailed proof).

**Claim 1.** Either \( S_{in}^{C}_1 \setminus P_{H} \subseteq P_{in}^{C} \setminus P_{H} \) or \( P_{in}^{C} \setminus P_{H} \subseteq S_{in}^{C}_1 \setminus P_{H} \) is true.

**Lemma 6.** If \( P_{H} \setminus P_{in}^{C} \neq \emptyset \), we have \( x_{p} \leq 2N_{r} + L \) for any \( p \in S_{in}^{C} \cup P_{in}^{C} \cup P_{H} \).

**Proof.** We consider the points in the three parts \( P_{H} \), \( P_{in}^{C} \), and \( S_{in}^{C} \) separately.

1. Due to (21), we have \( x_{p} \leq 2N_{r} + L \) for any \( p \in P_{H} \).

2. Arbitrarily select one point \( p_{0} \) from \( P_{H} \setminus P_{in}^{C} \). By (21) again, we have \( x_{p_{0}} \leq 2N_{r} + L \). Also, because \( P_{H} \setminus P_{in}^{C} \subseteq P_{out}^{C} \), we directly have \( x_{p} \leq x_{p_{0}} \) for any \( p \in P_{in}^{C} \). Namely, \( x_{p} \leq 2N_{r} + L \) for any \( p \in P_{in}^{C} \).

3. Below, we consider the points in \( S_{in}^{C} \). If \( w(S_{in}^{C} \cap P_{H}) > |P_{in}^{C} \setminus P_{H}| \), i.e., \( P_{H} \) contains more inliers of \( S \) than that of \( P \), then the outer region \( H_{out} \) should contain less inliers of \( S \) than that of \( P \). Thus, from Claim 1, we have \( S_{in}^{C} \setminus P_{H} \subseteq P_{in}^{C} \setminus P_{H} \). Hence, \( S_{in}^{C} = (S_{in}^{C} \setminus P_{H}) \cup (S_{in}^{C} \cap P_{H}) \subseteq (P_{in}^{C} \setminus P_{H}) \cup P_{in}^{C} \cup P_{H} \). From (1) and (2), we know \( x_{p} \leq 2N_{r} + L \) for any \( p \in S_{in}^{C} \).

Else, \( w(S_{in}^{C} \cap P_{H}) \leq |P_{in}^{C} \cap P_{H}| \). Then \( w(S_{in}^{C} \cap S_{H}) \leq |P_{in}^{C} \cap P_{H}| \) since \( S_{in}^{C} \cap P_{H} = S_{in}^{C} \cap S_{H} \). Because \( w(S_{H}) = |P_{H}| \), we have

\[
\sum_{p \in S_{in}^{C} \setminus S_{H}} w(p)x_{p} \geq |P_{H}| - 2L.
\]

Also, the assumption \( P_{H} \setminus P_{in}^{C} \neq \emptyset \) implies \( w(S_{H} \setminus S_{in}^{C}) \geq |P_{H} \setminus P_{in}^{C}| > 0 \), i.e.,

\[
S_{H} \setminus S_{in}^{C} \neq \emptyset.
\]

Arbitrarily select one point \( p_{0} \) from \( S_{H} \setminus S_{in}^{C} \). We know \( x_{p_{0}} \leq 2N_{r} + L \) since \( p_{0} \in S_{H} \setminus S_{in}^{C} \subseteq P_{H} \). Also, for any point \( p \in S_{in}^{C} \), we have \( x_{p} \leq x_{p_{0}} \) because \( p_{0} \in S_{H} \setminus S_{in}^{C} \subseteq S_{out} \). Therefore \( x_{p} \leq 2N_{r} + L \). \( \square \)

**Lemma 7.** If \( P_{H} \setminus P_{in}^{C} \neq \emptyset \), (20) is true.

**Proof.** We prove the upper bound of \( K_{1}^{-z}(S, C) \) first. We analyze the clustering costs of the two parts \( S_{in}^{C} \cap S_{H} \) and \( S_{in}^{C} \setminus S_{H} \) separately.

\[
K_{1}^{-z}(S, C) = \frac{1}{n - z} \left( \sum_{p \in S_{in}^{C} \cap S_{H}} w(p)x_{p} + \sum_{p \in S_{in}^{C} \setminus S_{H}} x_{p} \right).
\]

Note the points of \( S_{in}^{C} \setminus S_{H} \) have unit-weight (since \( S_{in}^{C} \setminus S_{H} \subseteq P \setminus P_{H} \) are the points from the outermost \((1 + 1/\varepsilon)z\) points of \( P \)). Obviously, the part (a) is no larger than

\[
\sum_{p \in S_{in}^{C} \cap S_{H}} w(p)x_{p} = \sum_{i=0}^{N} \frac{|P \cap H_{i}|}{|S_{H}|} \sum_{p \in \tilde{S}_{i}} x_{p} \leq \sum_{p \in \tilde{S}_{i}} x_{p} + O(\varepsilon)(n - z)(K_{1}^{-z}(P, \hat{C}) + L)
\]

from Lemma 3. The set \( P_{H} \) consists of two parts \( P_{H} \cap P_{in}^{C} \) and \( P_{H} \setminus P_{in}^{C} \). From Lemma 6 and the fact \( |P_{H} \setminus P_{in}^{C}| \leq |P_{out}^{C}| = z \), we know \( \sum_{p \in P_{H} \setminus P_{in}^{C}} x_{p} \leq z(2N_{r} + L) \). Thus, the upper bound of the part (a) becomes

\[
\sum_{p \in P_{H} \setminus P_{in}^{C}} x_{p} + z(2N_{r} + L) + O(\varepsilon)(n - z)(K_{1}^{-z}(P, \hat{C}) + L).
\]

To bound the part (b), we consider the size \( |S_{in}^{C} \setminus S_{H}| \). Since the total weight of outliers is \( z \), \( w(S_{H} \cap S_{in}^{C}) \).

\[
w(S_{H}) - w(S_{H} \cap S_{in}^{C}) \geq w(S_{H}) - z
\]

Together with the fact \( w(S_{H} \cap S_{in}^{C}) + |S_{in}^{C} \setminus S_{H}| = |P_{H} \cap P_{in}^{C}| + |P_{in}^{C} \setminus P_{H}| = n - z \), we have

\[
|S_{in}^{C} \setminus S_{H}| \leq |P_{in}^{C} \setminus P_{H}| + z.
\]

Therefore \( (S_{in}^{C} \setminus S_{H}) \setminus P_{in}^{C} \setminus P_{H} \) \( \leq z \) from Claim 1. Through Lemma 6 again, we know that the part (b) is no larger than \( \sum_{p \in P_{in}^{C} \setminus P_{H}} x_{p} + \left| S_{in}^{C} \setminus S_{H} \right| \cdot \left| P_{in}^{C} \setminus P_{H} \right| \cdot (2N_{r} + L) \)

\[
\leq \sum_{p \in P_{in}^{C} \setminus P_{H}} x_{p} + z(2N_{r} + L).
\]

Putting (38) and (41) together, we have

\[
K_{1}^{-z}(S, C) \leq K_{1}^{-z}(P, C) + O(\varepsilon)(K_{1}^{-z}(P, \hat{C}) + L) + \frac{2z}{n - z}(2N_{r} + L).
\]

Recall \( \gamma = z/(n - z) \) in Algorithm 1. If \( \gamma \geq \varepsilon \), the size of our coreset \( S \) is at least \((1 + 1/\varepsilon)z \geq n \); that is, \( \hat{C} \) contains all the points of \( P \). For the other case \( \varepsilon > \gamma \), together with (13), the term \( \frac{2z}{n - z}(2N_{r} + L) \) in (42) is at most

\[
O(\varepsilon)(K_{1}^{-z}(P, \hat{C}) + L).
\]

Overall, \( \hat{K}_{1}^{-z}(S, C) \leq \hat{K}_{1}^{-z}(P, C) + O(\varepsilon)(K_{1}^{-z}(P, \hat{C}) + L) \) via (42). So we complete the proof for the upper bound.
Algorithm 2 Layered Sampling for Lin1-Outlier

Input: An instance $P \subset \mathbb{R}^d$ of linear regression with $z$ outliers, a solution $\hat{h} = (\hat{h}_1, \ldots, \hat{h}_k)$, and two parameters $\epsilon, \eta \in (0, 1)$.

1. Let $\gamma = z/(n - z)$ and $N = \lceil \log \frac{1}{\gamma} \rceil$. Compute the value $r$ satisfying (18).

2. As described in (15), (16), and (17), the space is partitioned into $N + 2$ layers $H_0, H_1, \ldots, H_N$ and $H_{out}$.

3. Randomly sample $\min \{O(\frac{1}{\epsilon^2} d \log \frac{\delta}{\gamma}) | P \cap H_i|, \lceil N \rceil \}$ points, denoted by $S_i$, from $P \cap H_i$ for $0 \leq i \leq N$.

4. For each point $p \in S_i$, set its weight to be $w(p)$. Output $S = S_H \cup (P \cap H_{out})$.

Now we consider the lower bound of $K_{1}^{-z}(S, C)$. Denote by $X = S_H \cup (P^c \cap P_H)$ and $Y \subseteq S_{in}^c \setminus P^c$. Obviously,

$$K_{1}^{-z}(S, C) \geq \frac{1}{n - z} \left( \sum_{p \in X} w(p) x_p - \sum_{p \in Y} w(p) x_p \right) \quad \text{(c)}$$

From Lemma 3, the part (c) is at least

$$\sum_{p \in P_H} x_p - O(\epsilon(K_{1}^{-z}(P, \hat{C}) + L)) + \sum_{p \in P^c \cap P_H} x_p \geq \sum_{p \in P^c} x_p - O(\epsilon(K_{1}^{-z}(P, \hat{C}) + L)) \quad \text{(d)}$$

Further, since $w(Y) \leq z$ and $Y \subseteq X \subseteq P_{in}^c \cup P_H$, the part (d) is no larger than $z(2^{N}r + L)$ from Lemma 6. Using the similar manner for proving the upper bound, we know that $K_{1}^{-z}(S, C) \geq K_{1}^{-z}(P, \hat{C}) - O(\epsilon(K_{1}^{-z}(P, \hat{C}) + L)) \quad \square$

4. Linear Regression with Outliers

In this section, we consider the problem of linear regression with outliers. Our algorithm and analysis are for the objective function $LR^{-z}_{1}$, and the ideas can be extended to handle the objective function $LR^{-z}_{2}$.

Theorem 2. Algorithm 2 returns a point set $S$ having the size $|S| = O(\frac{1}{\epsilon^2} d) + (1 + \frac{1}{\epsilon})z$. Moreover, with probability at least $1 - \eta$, for any $L > 0$ and any solution $h \in \hat{h} \pm L$, we have

$$LR^{-z}_{1}(S, h) \in LR^{-z}_{1}(P, h) \pm \epsilon(LR^{-z}_{1}(P, \hat{h}) + L) \quad \text{(45)}$$

Here, $S$ is a weighted instance of linear regression with outliers, and the total weight of outliers is $z$ (see Remark 1). We still use $P_H$ to denote the set $\bigcup_{i=0}^{N} (P \cap H_i)$. First, we need to prove that $S_H$ is a good approximation of $P_H$. Given a hyperplane $h$, we define a random variable $x_p = \lfloor Res(p, h) \rfloor$ for each $p \in P$. If $p \in P_H$ for $0 \leq i \leq N$, similar to (21) and (22), we have the following bounds for $x_p$: $x_p \leq 2^r + L$; $x_p \geq \max \{2^r - r - L, 0 \}$ if $i \geq 1$ and $x_p \geq 0$ if $i = 0$.

Then, we can apply the similar idea of Lemma 3 to obtain the following lemma, where the only difference is about the discretization on $h \in \mathbb{R}$. Recall that $h$ is defined by the coefficients $\hat{h}_1, \ldots, \hat{h}_d$ and the input set $P$ is normalized within the region $\mathcal{R}_D$. We build a grid inside each vertical segment $\mathcal{G}_j$ for $0 \leq j \leq d-1$, where $l_0 = (0, \ldots, 0, \hat{h}_d - L)$, $u_0 = (0, \ldots, 0, \hat{h}_d + L)$, and

$$l_j = (0, \ldots, 0, D_j, 0, \ldots, 0, \hat{h}_j D + \hat{h}_d - L), \quad u_j = (0, \ldots, 0, D_j, 0, \ldots, 0, \hat{h}_j D + \hat{h}_d + L) \quad \text{(46)}$$

for $j \neq 0$; the grid length is $\frac{2^r}{2^k} L$. Denote by $G$ the set of grid points inside the segment $\mathcal{G}_j$. Obviously, $G = G_0 \times G_1 \times \cdots \times G_{d-1}$ contains $(2^k)^d d$-tuple points, and each tuple determines a $(d - 1)$-dimensional hyperplane in $\hat{h} \pm L$; moreover, we have the following claim (see the proof in our supplement).

Claim 2. For each $h \in \hat{h} \pm L$, there exist a hyperplane $h'$ determined by a $d$-tuple points from $G$, such that $|Res(p, h') - Res(p, h)| \leq \epsilon L$ for any $p \in P$.

Lemma 8. Let $S_0, S_1, \ldots, S_N$ be the samples obtained in Algorithm 2. Then, with probability $1 - \eta$,

$$\frac{1}{n - z} \left| \sum_{i=0}^{N} |P \cap H_i| \sum_{p \in S_i} x_p - \sum_{p \in P_H} x_p \right| \leq O(\epsilon(LR^{-z}_{1}(P, \hat{h}) + L) \quad \text{(48)}$$

for any $h \in \hat{h} \pm L$.

We fix a solution $h \in \hat{h} \pm L$, Similar to the proof of Theorem 1 in Section 3, we also consider the two parts $P^h_{in}$ and $P^h_{out}$ of $P$ partitioned by $h$, where $P^h_{out}$ is the $z$ farthest points to the hyperplane $h$ (i.e., the outliers) and $P^h_{in} = P \setminus P^h_{out}$. Similarly, $S$ is also partitioned into two parts $S^h_{in}$ and $S^h_{out}$ by $h$, where $S^h_{out}$ is the set of outliers with total weights $z$. For case (i) $P_H \setminus P^h_{in} = \emptyset$ and case (ii) $P_H \setminus P^h_{in} \neq \emptyset$, we can apply almost the identical ideas in Section 3.1 and 3.2 respectively to prove (45).

5. Experiments

For both Algorithm 1 and 2, we need to compute an initial solution $\hat{C}$ or $\hat{h}$ first. For $k$-median/means clustering, we
run the algorithm of Local Search with Outliers from (Gupta et al., 2017a) on a small sample of size \(O(k)\) to obtain the \(k\) initial centers. We do not directly use the \(k\)-means ++ method (Arthur & Vassilvitskii, 2007a) to seed the \(k\) initial centers because it is sensitive to outliers. For linear regression, we run the standard linear regression algorithm on a small random sample of size \(O(z)\) to compute an initial solution.

**Different coreset methods** Each of the following methods returns a weighted set as the coreset, and then we run the alternating minimization algorithm \(k\)-means-- (Chawla & Gionis, 2013a) (or (Shen & Sanghavi, 2019) for linear regression) on it to obtain the solution. For fairness, we keep the coresets from different methods to have the same coreset size for each instance.

- **Layered Sampling (LaySam).** *i.e.*, Algorithm 1 and 2 proposed in this paper.
- **Uniform Sampling (UniSam).** The most natural and simple method is to take a sample \(S\) uniformly at random from the input data set \(P\), where each sampled point has the weight \(|P|/|S|\).
- **Uniform Sampling + Nearest Neighbor Weight (NN)** (Gupta et al., 2017a; Chen et al., 2018). Similar to UniSam, we also take a random sample \(S\) from the input data set \(P\). For each \(p \in P\), we assign it to its nearest neighbor in \(S\); for each \(q \in S\), we set its weight to be the number of points assigned to it.
- **Summary (Chen et al., 2018).** It is a method to construct the coreset for \(k\)-median/means clustering with outliers by successively sampling and removing points from the original data until the number of the remaining points is small enough.

The above LaySam, UniSam and NN are also used for linear regression in our experiments. We run 10 trials for each case and take the average. All the experimental results were obtained on a Ubuntu server with 2.4GHz E5-2680V4 and 256GB main memory; the algorithms were implemented in Matlab R2018b.

**Performance Measures** The following measures will be taken into account in the experiment.

- \(\ell_1\)-loss: \(K_1^{-2}\) or \(LR_1^{-2}\).
- \(\ell_2\)-loss: \(K_2^{-2}\) or \(LR_2^{-2}\).
- \text{recall/precision. Let } O^* \text{ and } O \text{ be the sets of outliers with respect to the optimal solution and our obtained solution, respectively. recall } = \frac{|O \cap O^*|}{|O^*|} \text{ and precision } = \frac{|O \cap O^*|}{|O|}. \text{ Since } |O^*| = |O| = z, \text{ recall } = \text{ precision } = \frac{|O \cap O^*|}{z}.
- \text{pre-recall. It indicates the proportion of } O^* \text{ that are included in the coreset. Let } S \text{ be the coreset and pre-recall } = \frac{|S \cap O^*|}{|O^*|}. \text{ We pay attention in particular to this measure, because the outliers could be quite important and may reveal some useful information (e.g., anomaly detection). For example, as for clustering, if we do not have any prior knowledge of a given biological data, the outliers could be from an unknown tiny species. Consequently it is more preferable to keep such information when compressing the data. More detailed discussion on the significance of outliers can be found in (Beyer & Sendhoff, 2007; Zimek et al., 2012; Moitra, 2018; Goodfellow et al., 2018).}

**Datasets** We consider the following datasets in our experiments.

- **syncluster** We generate the synthetic data as follows: Firstly we create \(k\) centers with each dimension randomly located in \([0, 100]\). Then we generate the points following standard Gaussian distributions around the centers.
- **synregression** Firstly, we randomly set the \(d\) coefficients of hyperplane \(h\) in \([-5, +5]\) and construct \(x_i\) in \([0, 10]^{d-1}\) by uniform sampling. Then let \(y_i\) be the inner product of \((x_i, 1)\) and \(h\). Finally we randomly perturb each \(y_i\) by \(N(0, 1)\).
- **3DSpatial** \((n = 434874, d = 4)\). This dataset was constructed by adding the elevation information to a 2D road network in North Jutland, Denmark (Kaul et al., 2013).
- **covertype** \((n = 581012, d = 10)\). It is a forest cover type dataset from Jock A. Blackard (UCI Machine Learning Repository), and we select its first 10 attributes.
- **skin** \((n = 245057, d = 3)\). The skin dataset is collected by randomly sampling B, G, R values from face images of various age groups and we select its first three dimension (Bhatt & Dhall).
- **SGEMM** \((n = 241600, d = 15)\). It contains the running times for multiplying two 2048 x 2048 matrices using a GPU OpenCL SGEMM kernel with varying parameters (Ballester-Ripoll et al., 2017).
- **PM2.5** \((n = 41757, d = 11)\). It is a data set containing the PM2.5 data of US Embassy in Beijing (Liang et al., 2015).
For each dataset, we randomly pick \( z \) points to be outliers by perturbing their locations in each dimension. We use a parameter \( \sigma \) to measure the extent of perturbation. For example, we consider the Gaussian distribution \( \mathcal{N}(0, \sigma) \) and uniform distribution \([-\sigma, +\sigma]\). So the larger the parameter \( \sigma \) is, the more diffused the outliers will be. For simplicity, we use the notations in the form of [dataset]-[distribution]-\( \sigma \) to indicate the datasets, e.g., syncluster-gauss-\( \sigma \).

5.1. Coreset Construction Time

We fix the coreset size and vary the data size \( n \) of the synthetic datasets, and show the coreset construction times in Figure 2(a) and 2(b). It is easy to see that the construction time of NN is larger than other construction times by several orders of magnitude. It is not out of expectation that UniSam is the fastest (because it does not need any operation except uniform random sampling). Our LaySam lies in between UniSam and Summary.

![Figure 2. Coreset construction time w.r.t. data size. (a) Clustering: coreset size=10^4, d = 5 and k = 10; (b) Linear Regression: coreset size=10^4 and d = 20.](image)

5.2. Performance

Figure 4(a)-4(e) show the performances of clustering on \( \ell_2 \)-loss with different \( \sigma \)s. The results on \( \ell_1 \)-loss are very similar (more results are summarized in Table 1 and 2). We can see that LaySam outperforms the other methods in terms of both synthetic and real-world datasets. Moreover, its performance remains quite stable (with small standard deviation) and is also robust when \( \sigma \) increases. UniSam works well when \( \sigma \) is small, but it becomes very unstable when \( \sigma \) rises to large. Both LaySam and UniSam outperform Summary on most datasets.

Similar comparison of the performance for linear regression are shown in Figure 5(a)-5(c).

The three coreset methods achieve very close values of recall and precision. But UniSam has much lower pre-recall than those of Summary and LaySam.

6. Conclusion

To reduce the time complexities of existing algorithms for clustering and linear regression with outliers, we propose a new variant of coreset method which can guarantee the quality for any solution in a local range surrounding the given initial solution. In future, it is worth considering to apply our framework to a broader range of robust optimization problems, such as logistic regression with outliers and Gaussian mixture model with outliers.

![Figure 3. Construction time w.r.t. k. (a) syncluster with data size n = 10^6, d = 20; (b) covertype.](image)

We also study the influence of \( k \) (for clustering) on the construction time by testing the synthetic datasets and the real-world dataset covertype (see Figure 3(a) and 3(b)).
Layered Sampling for Robust Optimization Problems

Figure 4. Clustering: $\ell_2$-loss and stability w.r.t. $\sigma$.

(a) syncluster-gauss-$\sigma$, with $d = 20$, $k = 10$, $z = 2 \cdot 10^4$ and coreset size $= 5 \cdot 10^3$.
(b) 3DSpatial-gauss-$\sigma$, with $k = 5$, $z = 4000$ and coreset size $= 10^4$.
(c) covertype-gauss-$\sigma$, with $k = 20$, $z = 10^4$ and coreset size $= 3 \cdot 10^4$.
(d) covertype-uniform-$\sigma$, with $k = 20$, $z = 10^4$ and coreset size $= 3 \cdot 10^4$.
(e) skin-uniform-$\sigma$, with $k = 40$, $z = 3000$ and coreset size $= 10^4$.

Figure 5. Linear Regression: $\ell_2$-loss and stability w.r.t. $\sigma$.

(a) synregression-gauss-$\sigma$, with $d = 20$, $z = 10^4$ and coreset size $= 2 \cdot 10^4$.
(b) SGEMM-gauss-$\sigma$, with $z = 4000$ and coreset size $= 10^4$.
(c) PM2.5-uniform-$\sigma$, with $z = 1000$ and coreset size $= 3000$. 
(a) syncluster-gauss-σ, with $d = 20$, $k = 10$, $z = 2 \cdot 10^4$ and coreset size $= 5 \cdot 10^4$.

| σ | 20   | 100   | 200   |
|---|------|-------|-------|
| Coreset | LaySam | UniSam | Summary | LaySam | UniSam | Summary | LaySam | UniSam | Summary |
| $\ell_1$-loss | 3.976 | 3.976 | 4.073 | 3.976 | 3.976 | 4.067 | 3.977 | 4.048 | 4.074 |
| $\ell_2$-loss | 18.01 | 18   | 18.9 | 18.01 | 18.01 | 18.84 | 18.01 | 18.14 | 18.91 |
| Prec | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Pre-Rec | 0.0506 | 1 | 0.0499 | 1 | 1 | 0.0503 | 1 |

(b) covertype-gauss-σ, with $k = 20$, $z = 10^4$ and coreset size $= 3 \cdot 10^4$.

| σ | 20   | 100   | 200   |
|---|------|-------|-------|
| Coreset | LaySam | UniSam | Summary | LaySam | UniSam | Summary | LaySam | UniSam | Summary |
| $\ell_1$-loss | 1.781 | 1.781 | 1.868 | 1.779 | 1.785 | 1.871 | 1.786 | 1.799 | 1.853 |
| $\ell_2$-loss | 3.501 | 3.501 | 3.818 | 3.505 | 3.523 | 3.874 | 3.515 | 3.576 | 3.767 |
| Prec | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Pre-Rec | 0.0524 | 1 | 0.0511 | 1 | 1 | 0.0547 | 1 |

(c) skin-uniform-σ, with $k = 40$, $z = 3000$ and coreset size $= 10^4$.

| σ | 20   | 100   | 200   |
|---|------|-------|-------|
| Coreset | LaySam | UniSam | Summary | LaySam | UniSam | Summary | LaySam | UniSam | Summary |
| $\ell_1$-loss | 0.1906 | 0.1906 | 0.1925 | 0.1883 | 0.1902 | 0.1914 | 0.1954 | 0.2032 | 0.1957 |
| $\ell_2$-loss (×10$^{-2}$) | 6.46  | 6.531 | 6.579 | 6.449 | 6.849 | 6.565 | 6.471 | 7.173 | 6.565 |
| Prec | 0.9993 | 0.9995 | 0.9993 | 1 | 1 | 1 | 1 | 1 | 1 |
| Pre-Rec | 0.9997 | 0.0403 | 1 | 1 | 0.0403 | 1 | 1 | 0.0437 | 1 |

Table 1. Performance on clustering with outliers.

(a) synregression-gauss-σ, with $d = 20$, $z = 10^4$ and coreset size $= 2 \cdot 10^4$.

| σ | 20   | 300   | 600   |
|---|------|-------|-------|
| Coreset | LaySam | UniSam | LaySam | UniSam | LaySam | UniSam |
| $\ell_1$-loss | 0.7996 | 0.7982 | 0.7989 | 0.8007 | 0.7987 | 0.7998 |
| $\ell_2$-loss | 1.003 | 0.9993 | 1.001 | 1.01 | 1.002 | 1.025 |
| Prec | 0.9305 | 0.931 | 0.9953 | 0.9953 | 0.9975 | 0.9978 |
| Pre-Rec | 0.9535 | 0.0108 | 0.9968 | 0.0093 | 0.9975 | 0.0098 |

(b) PM2.5-uniform-σ, with $z = 1000$ and coreset size $= 3000$.

| σ | 20   | 500   | 1000  |
|---|------|-------|-------|
| Coreset | LaySam | UniSam | LaySam | UniSam | LaySam | UniSam |
| $\ell_1$-loss | 0.6292 | 0.6244 | 0.637 | 0.6368 | 0.6349 | 0.6791 |
| $\ell_2$-loss | 0.7179 | 0.7075 | 0.744 | 0.7473 | 0.7456 | 0.8819 |
| Prec | 0.9188 | 0.921 | 0.99 | 0.9901 | 0.9918 | 0.9917 |
| Pre-Rec | 0.9714 | 0.0732 | 0.999 | 0.0725 | 1 | 0.0734 |

Table 2. Performance on linear regression with outliers.
References

Arthur, D. and Vassilvitskii, S. K-means++: The advantages of careful seeding. In Proceedings of the Eighteenth Annual ACM-SIAM Symposium on Discrete Algorithms, SODA ’07, pp. 1027–1035, Philadelphia, PA, USA, 2007a. Society for Industrial and Applied Mathematics. ISBN 978-0-898716-24-5.

Arthur, D. and Vassilvitskii, S. k-means++: The advantages of careful seeding. In Proceedings of the eighteenth annual ACM-SIAM symposium on Discrete algorithms, pp. 1027–1035. Society for Industrial and Applied Mathematics, 2007b.

Awasthi, P. and Balcan, M.-F. Center based clustering: A foundational perspective. 2014.

Bachem, O., Lucic, M., and Krause, A. Practical core-set constructions for machine learning. arXiv preprint arXiv:1703.06476, 2017.

Ballester-Ripoll, R., Paredes, E. G., and Pajarola, R. Sobol tensor trains for global sensitivity analysis. CoRR, abs/1712.00233, 2017.

Beyer, H.-G. and Sendhoff, B. Robust optimization–a comprehensive survey. Computer methods in applied mechanics and engineering, 196(33-34):3190–3218, 2007.

Bhaskara, A., Vadgama, S., and Xu, H. Greedy sampling for approximate clustering in the presence of outliers. In Advances in Neural Information Processing Systems, pp. 11146–11155, 2019.

Bhatia, K., Jain, P., and Kar, P. Robust regression via hard thresholding. In Advances in Neural Information Processing Systems 28: Annual Conference on Neural Information Processing Systems 2015, December 7-12, 2015, Montreal, Quebec, Canada, pp. 721–729, 2015.

Bhatt, R. and Dhall, A. Skin segmentation dataset. UCI Machine Learning Repository.

Blum, M., Floyd, R. W., Pratt, V., Rivest, R. L., and Tarjan, R. E. Time bounds for selection. Journal of Computer and System Sciences, 7(4):448–461, 1973.

Boutsidis, C., Drineas, P., and Magdon-Ismail, M. Near-optimal coresets for least-squares regression. IEEE Trans. Information Theory, 59(10):6880–6892, 2013. doi: 10.1109/TIT.2013.2272457.

Chandola, V., Banerjee, A., and Kumar, V. Anomaly detection: A survey. ACM Computing Surveys (CSUR), 41(3):15, 2009.

Chawla, S. and Gionis, A. k-means--: A unified approach to clustering and outlier detection. In Proceedings of the 2013 SIAM International Conference on Data Mining, pp. 189–197. SIAM, 2013b.

Chen, J., Azer, E. S., and Zhang, Q. A practical algorithm for distributed clustering and outlier detection. In Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, 3-8 December 2018, Montréal, Canada, pp. 2253–2262, 2018.

Chen, K. A constant factor approximation algorithm for k-median clustering with outliers. In Proceedings of the nineteenth annual ACM-SIAM symposium on Discrete algorithms, pp. 826–835. Society for Industrial and Applied Mathematics, 2008.

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

Dasgupta, A., Drineas, P., Harb, B., Kumar, R., and Mahoney, M. W. Sampling algorithms and coresets for \ell_p regression. SIAM Journal on Computing, 38(5):2060–2078, 2009.

Ding, H. and Xu, J. Sub-linear time hybrid approximations for least trimmed squares estimator and related problems. In 30th Annual Symposium on Computational Geometry, SOCG’14, Kyoto, Japan, June 08 - 11, 2014, pp. 110, 2014. doi: 10.1145/2582112.2582131.

Drineas, P., Mahoney, M. W., and Muthukrishnan, S. Sampling algorithms for \ell_2 regression and applications. In Proceedings of the seventeenth annual ACM-SIAM symposium on Discrete algorithms, pp. 1127–1136. Society for Industrial and Applied Mathematics, 2006.

Erickson, J. and Seidel, R. Better lower bounds on detecting affine and spherical degeneracies. Discrete & Computational Geometry, 13:41–57, 1995. doi: 10.1007/BF02574027.

Feldman, D. Core-sets: An updated survey. Wiley Interdiscip. Rev. Data Min. Knowl. Discov., 10(1), 2020.

Feldman, D. and Langberg, M. A unified framework for approximating and clustering data. In Proceedings of the 43rd ACM Symposium on Theory of Computing, STOC 2011, San Jose, CA, USA, 6-8 June 2011, pp. 569–578, 2011.

Feldman, D., Schmidt, M., and Sohler, C. Turning big data into tiny data: Constant-size coresets for k-means, PCA and projective clustering. In Proceedings of the Twenty-Fourth Annual ACM-SIAM Symposium on Discrete Algorithms, SODA 2013, New Orleans, Louisiana, USA, January 6-8, 2013, pp. 1434–1453, 2013.
Layered Sampling for Robust Optimization Problems

Fichtenberger, H., Gillé, M., Schmidt, M., Schwiegelshohn, C., and Sohler, C. Bico: Birch meets coresets for k-means clustering. In European Symposium on Algorithms, pp. 481–492. Springer, 2013.

Friggstad, Z., Khodamoradi, K., Rezapour, M., and Salavatipour, M. R. Approximation schemes for clustering with outliers. In Proceedings of the Twenty-Ninth Annual ACM-SIAM Symposium on Discrete Algorithms, pp. 481–492. SIAM, 2018.

Gupta, S. Approximation algorithms for clustering and facility location problems. PhD thesis, University of Illinois at Urbana-Champaign, 2018.

Hawkins, D. M. The feasible solution algorithm for least trimmed squares regression. Computational Statistics and Data Analysis, 17, 1994. doi: 10.1016/0167-9473(92)00070-8.

Huang, L., Jiang, S., Li, J., and Wu, X. Epsilon-coresets for clustering (with outliers) in doubling metrics. In 2018 IEEE 59th Annual Symposium on Foundations of Computer Science (FOCS), pp. 814–825. IEEE, 2018.

Klivans, A. R., Kothari, P. K., and Meka, R. Efficient algorithms for outlier-robust regression. In Conference On Learning Theory, COLT 2018, Stockholm, Sweden, 6-9 July 2018, pp. 1420–1430, 2018.

Krishnaswamy, R., Li, S., and Sandeep, S. Constant approximation for k-median and k-means with outliers via iterative rounding. In Proceedings of the 50th Annual ACM SIGACT Symposium on Theory of Computing, pp. 646–659. ACM, 2018.

Mettu, R. R. and Plaxton, C. G. Optimal time bounds for approximate clustering. Machine Learning, 56(1-3):35–60, 2004.

Moitra, A. Robustness meets algorithms (invited talk). In 16th Scandinavian Symposium and Workshops on Algorithm Theory, SWAT 2018, June 18-20, 2018, Malmö, Sweden, pp. 3:1–3:1, 2018.

Mount, D. M., Netanyahu, N. S., Piatko, C. D., Silverman, R., and Wu, A. Y. On the least trimmed squares estimator. Algorithmica, 69(1):148–183, 2014. doi: 10.1007/s00453-012-9721-8.

Mount, D. M., Netanyahu, N. S., Piatko, C. D., Wu, A. Y., and Silverman, R. A practical approximation algorithm for the LTS estimator. Computational Statistics and Data Analysis, 99:148–170, 2016. doi: 10.1016/j.csda.2016.01.016.

Munteanu, A., Schwiegelshohn, C., Sohler, C., and Woodruff, D. On coresets for logistic regression. In Advances in Neural Information Processing Systems, pp. 6561–6570, 2018.

Moitra, A. Robustness meets algorithms (invited talk). In 16th Scandinavian Symposium and Workshops on Algorithm Theory, SWAT 2018, June 18-20, 2018, Malmö, Sweden, pp. 3:1–3:1, 2018.

Mount, D. M., Netanyahu, N. S., Piatko, C. D., Silverman, R., and Wu, A. Y. On the least trimmed squares estimator. Algorithmica, 69(1):148–183, 2014. doi: 10.1007/s00453-012-9721-8.

Mount, D. M., Netanyahu, N. S., Piatko, C. D., Wu, A. Y., and Silverman, R. A practical approximation algorithm for the LTS estimator. Computational Statistics and Data Analysis, 99:148–170, 2016. doi: 10.1016/j.csda.2016.01.016.

Munteanu, A., Schwiegelshohn, C., Sohler, C., and Woodruff, D. On coresets for logistic regression. In Advances in Neural Information Processing Systems, pp. 6561–6570, 2018.
Layered Sampling for Robust Optimization Problems

Ott, L., Pang, L., Ramos, F. T., and Chawla, S. On integrated clustering and outlier detection. In Advances in neural information processing systems, pp. 1359–1367, 2014.

Phillips, J. M. Coresets and sketches. Computing Research Repository, 2016.

Rousseeuw, P. and van Driessen, K. Computing LTS regression for large data sets. Data Min. Knowl. Discov., 12(1): 29–45, 2006. doi: 10.1007/s10618-005-0024-4.

Rousseeuw, P. J. Least median of squares regression. Journal of the American Statistical Association, 79, 12 1984. doi: 10.1080/01621459.1984.10477105.

Shen, Y. and Sanghavi, S. Iterative least trimmed squares for mixed linear regression. In Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, 8-14 December 2019, Vancouver, BC, Canada, pp. 6076–6086, 2019.

Zimek, A., Schubert, E., and Kriegel, H.-P. A survey on unsupervised outlier detection in high-dimensional numerical data. Statistical Analysis and Data Mining: The ASA Data Science Journal, 5(5):363–387, 2012.

7. Proof of Claim 1

Since $S^C_{in}$ is the set of inliers to $C$, there must exist some value $r_S > 0$ such that

$$S^C_{in} = \{ p \mid p \in S, \min_{1 \leq j \leq k} \| p - c_j \| \leq r_S \}. \quad (49)$$

And therefore

$$S^C_{in} \setminus P_H = \{ p \mid p \in S \setminus P_H, \min_{1 \leq j \leq k} \| p - c_j \| \leq r_S \}. \quad (50)$$

Similarly, there exists some value $r_P > 0$ such that

$$P^C_{in} \setminus P_H = \{ p \mid p \in P \setminus P_H, \min_{1 \leq j \leq k} \| p - c_j \| \leq r_P \}. \quad (51)$$

Note $S \setminus P_H = P \setminus P_H$. So, if $r_S \leq r_P$, we have $S^C_{in} \setminus P_H \subseteq P^C_{in} \setminus P_H$. Otherwise, $P^C_{in} \setminus P_H \subseteq S^C_{in} \setminus P_H$.

8. Proof of Claim 2

Let $h = (h_1, \cdots, h_d)$, and suppose $h' = (h'_1, \cdots, h'_d)$ is $h$'s nearest neighbor in $G$, i.e., $\| h'_j - h_d \| \leq \frac{\epsilon}{2d} L$ and $|Dh'_j + h'_d - Dh_j - h_d| \leq \frac{\epsilon}{2d} L$ for $1 \leq j \leq d - 1$. Then,

$$|h'_j - h_j| \leq \frac{1}{D} \left( \frac{\epsilon}{2d} L + |h'_d - h_d| \right)$$

$$\leq \frac{\epsilon}{Dd} L \quad (52)$$

for $1 \leq j \leq d - 1$. For any $p = (x_1, \cdots, x_d) \in \mathcal{R}_D$,

$$|Res(p, h) - Res(p, h')|$$

$$\leq \sum_{j=1}^{d-1} |h'_j - h_j| \cdot |x_j| + |h'_d - h_d|$$

$$\leq \sum_{j=1}^{d-1} |h'_j - h_j| \cdot D + |h'_d - h_d|$$

$$\leq \epsilon L. \quad (53)$$