Relational Algorithms for k-means Clustering

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Abstract

This paper gives a $k$-means approximation algorithm that is efficient in the relational algorithms model. This is an algorithm that operates directly on a relational database without performing a join to convert it to a matrix whose rows represent the data points. The running time is potentially exponentially smaller than $N$, the number of data points to be clustered that the relational database represents.

Few relational algorithms are known and this paper offers techniques for designing relational algorithms as well as characterizing their limitations. We show that given two data points as cluster centers, if we cluster points according to their closest centers, it is NP-Hard to approximate the number of points in the clusters on a general relational input. This is trivial for conventional data inputs and this result exemplifies that standard algorithmic techniques may not be directly applied when designing an efficient relational algorithm. This paper then introduces a new method that leverages rejection sampling and the $k$-means++ algorithm to construct a $O(1)$-approximate $k$-means solution.

1 Introduction

Kaggle surveys [2] show that the majority of learning tasks faced by data scientists involve relational data. Conventional formats usually represent data with multi-dimensional points where each dimension corresponds to a feature of the data. In contrast, a relational database consists of tables $T_1, T_2, \ldots, T_m$ where the features could be stored partially in the tables. The columns in each table are a subset of features and the rows are data records for these features. The underlying data is represented by the design matrix $J = T_1 \Join \cdots \Join T_m$ where each row in $J$ can be interpreted as a data point. Here the join ($\Join$) is a binary operator on two tables $T_i$ and $T_j$. The result of the join is the set of all possible concatenations of two rows from $T_i$ and $T_j$ such that they are equal in their common columns/features. If $T_i$ and $T_j$ have no common columns their join is the cross product of all rows. See Table 1 for an example of join operation on two tables.

Almost all learning tasks are designed for data in matrix format. The current standard practice for a data scientist is the following.

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1In relational database context the columns are also referred to as attributes but here we call them features per the tradition of broader communities.
Table 1: A join of tables $T_1$ and $T_2$. Each has 5 rows and 2 features, sharing $f_2$. The join has all features from both tables. The rows with $f_2 = x$ in the join is the cross product of all rows with $f_2 = x$ from $T_1$ and $T_2$. For example, for $f_2 = 1$, the four rows in $T_1 \bowtie T_2$ has $(f_1, f_3)$ values $\{(1, 1), (1, 2), (2, 1), (2, 2)\}$, this is the cross product of $f_1 \in \{1, 2\}$ from $T_1$ and $f_3 \in \{1, 2\}$ from $T_2$.

| $T_1$   | $T_2$   | $T_1 \bowtie T_2$ |
|---------|---------|-------------------|
| $f_1$   | $f_2$   | $f_1$ $f_2$ $f_3$|
| 1       | 1       | 1 1 1             |
| 2       | 1       | 1 1 2             |
| 3       | 2       | 2 3 3             |
| 4       | 3       | 2 1 1             |
| 5       | 4       | 3 2 3             |

**Standard Practice:**

1. Extract the data points from the relational database by taking the join of all tables to find the design matrix $J = T_1 \bowtie \cdots \bowtie T_m$.
2. Then interpret each row of $J$ as a point in a Euclidean space and the columns as the dimensions, corresponding to the features of data.
3. Import this design matrix $J$ into a standard algorithm.

A relational database is a highly compact data representation format. The size of $J$ can be exponentially larger than the input size of the relational database [10]. Extracting $J$ makes the standard practice inefficient. Theoretically, there is a potential for exponential speed-up by running algorithms directly on the tables in relational data. We call such algorithms relational algorithms if their running time is polynomial in the size of tables when the database is acyclic. Acyclic databases will be defined shortly. This leads to the following exciting algorithmic question.

**The Relational Algorithm Question:**

A. Which standard algorithms can be implemented as relational algorithms?

B. For standard algorithms that are not implementable by relational algorithms, is there an alternative efficient relational algorithm that has similar performance?

This question has recently been of interest to the community. However, few algorithmic techniques are known. Moreover, we do not have a good understanding of which problems can be solved on relational data and which cannot. Relational algorithm design has a interesting combinatorial structure that requires a deeper understanding.

We design a relational algorithm for $k$-means. It has a polynomial time complexity for acyclic relational databases. The relational database is acyclic if there exists a tree with the following properties. There is exactly one node in the tree for each table. Moreover, for any feature (i.e. column) $f$, let $V(f)$ be the set of nodes whose corresponding tables contain feature $f$. The subgraph induced on $V(f)$ must be a connected component. Acyclicity can be easily checked, as the tree can be found in polynomial time if it exists [27].

Luckily, most of the natural database schema are acyclic or nearly acyclic. Answering seemingly simple questions on general (cyclic) databases, such as if the join is empty or not is NP-Hard. For general databases, efficiency is measured in terms of the fractional hypertree width of the database (denoted by “fhtw”[1]). This measures how close the database structure is to being acyclic. This parameter is 1 for acyclic databases and larger as the database is farther from being acyclic.

State-of-the-art algorithms for queries as simple as counting the number of rows in the design matrix have linear dependency on $n^{fhtw}$ where $n$ is the maximum number of rows in all input tables [2]. Running in time linear in $n^{fhtw}$ is [2]See Appendix E for a formal definition.
the goal, as fundamental barriers need to be broken to be faster. Notice that this is polynomial time when fhtw is a fixed constant (i.e. nearly acyclic). Our algorithm has linear dependency on \( n^{\text{fw}} \), matching the state-of-the-art.

**Relational Algorithm for \( k \)-means:** \( k \)-means is perhaps the most widely used data mining algorithm (e.g. \( k \)-means is one of the few models in Google’s BigQuery ML package [1]). The input to the \( k \)-means problem consists of a collection \( S \) of points in a Euclidean space and a positive integer \( k \). A feasible output is \( k \) points \( c_1, \ldots, c_k \), which we call centers. The objective is to choose the centers to minimize the aggregate squared distance from each original point to its nearest center.

Recall extracting all data points could take time exponential in the size of a relational database. Thus, the problem is to find the cluster centers without fully realizing all data points the relational data represents.

[15] was the first paper to give a non-trivial \( k \)-means algorithm that works on relational inputs. The paper gives an \( O(1) \)-approximation. The algorithm’s running time has a superlinear dependency on \( k^d \) when the tables are acyclic and thus is not polynomial. Here \( k \) is the number of cluster centers and \( d \) is the dimension (a.k.a number of features) of the points. This is equivalently the number of distinct columns in the relational database. For a small number of dimensions, this algorithm is a large improvement over the standard practice and they showed the algorithm gives up to 350x speed up on real data versus performing the query to extract the data points (not even including the time to cluster the output points).

Several questions remain. Is there a relational algorithm for \( k \)-means? What algorithmic techniques can we use as building blocks to design relational algorithms? Moreover, how can we show some problems are hard to solve using a relational algorithm?

**Overview of Results:** The main result of the paper is the following.

**Theorem 1.1.** Given an acyclic relational database with tables \( T_1, T_2, \ldots, T_m \) where the design matrix \( J \) has \( N \) rows and \( d \) columns. Let \( n \) be the maximum number of rows in any table. Then there is a randomized algorithm running in time polynomial in \( d, n \) and \( k \) that computes an \( O(1) \) approximate \( k \)-means clustering solution with high probability.

In appendix [E] we discuss the algorithm’s time complexity for cyclic databases. To illustrate the challenges for finding such an algorithm as described in the prior theorem, even when the database is acyclic, consider the following theorem.

**Theorem 1.2.** Given an acyclic relational database with tables \( T_1, T_2, \ldots, T_m \) where the design matrix \( J \) has \( N \) rows and \( d \) columns. Given \( k \) centers \( c_1, \ldots, c_k \), let \( J_i \) be the set of points in \( J \) that are closest to \( c_i \) for \( i \in [k] \). It is \( \#P \)-Hard to compute \(|J_i|\) for \( k \geq 2 \) and \( N \#P \)-Hard to approximate \(|J_i|\) to any factor for \( k \geq 3 \).

You may find the proof in Section [2]. We show it by reducing a \( N \#P \)-Hard problem to the problem of determining if \( J_i \) is empty or not. Counting the points closest to a center is a fundamental building block in almost all \( k \)-means algorithms. Moreover, we show even performing one iteration of the classic Lloyd’s algorithm is \( \#P \)-Hard in Appendix [E]. Together this necessitates the design of new techniques to address the main theorem, shows that seemingly trivial algorithms are difficult relationally, and suggests computing a coreset is the right approach for the problem as it is difficult to cluster the data directly.

**Overview of Techniques:** We first compute a coreset of all points in \( J \). That is, a collection of points with weights such that if we run an \( O(1) \) approximation algorithm on this weighted set, we will get a \( O(1) \) approximate solution for all of \( J \). To do so, we sample points according to the principle in \( k \)-means++ algorithm and assign weights to the points sampled. The number of points chosen will be \( \Theta(k \log N) \). Any \( O(1) \)-approximate weighted \( k \)-means algorithm can be used on the coreset to give Theorem 1.1.

**\( k \)-means++:** \( k \)-means++ is a well-known \( k \)-means algorithm [2][8]. The algorithm iteratively chooses centers \( c_1, c_2, \ldots \). The first center \( c_1 \) is picked uniformly from \( J \). Given that \( c_1, \ldots, c_{i-1} \) are picked, a point \( x \) is picked as \( c_i \) with probability \( P(x) = \frac{L(x)}{Y} \) where \( L(x) = \min_{i \in \{1, \ldots, i-1\}} \| x - c_i \|^2 \) and \( Y = \sum_{x \in J} L(x) \). Here \([i-1] \) denotes \( \{1, 2, \ldots, i-1\} \).

Say we sample \( \Theta(k \log N) \) centers according to this distribution, which we call the \( k \)-means++ distribution. It was shown in [8] that if we cluster the points by assigning them to their closest centers, the total squared distance between points and their cluster centers is at most \( O(1) \) times the optimal \( k \)-means cost with high probability. Note that this is not a feasible \( k \)-means solution because more than \( k \) centers are used. However, leveraging this, the work showed
that we can construct a coreset by weighting these centers according to the number of points in their corresponding clusters.

We seek to mimic this approach with a relational algorithm. Let’s focus on one iteration where we want to sample the center $c_i$ given $c_1, \ldots, c_{i-1}$ according to the $k$-means++ distribution. Consider the assignment of every point to its closest center in $c_1, \ldots, c_{i-1}$. Notice that the $k$-means++ probability is determined by this assignment. Indeed, the probability of a point being sampled is the cost of assigning this point to its closest center $\left(\min_{j \in [i-1]} \|x - c_j\|_2^2\right)$ normalized by $Y$. $Y$ is the summation of this cost over all points.

The relational format makes this distribution difficult to compute without the design matrix $J$. It is hard to efficiently characterize which points are closest to which centers. The assignment partitions the data points according to their closest centers, where each partition may not be easily represented by a compact relational database (unlike $J$).

**A Relational $k$-means++ Implementation:** Our approach will sample every point according to the $k$-means++ distribution without computing this distribution directly. Instead, we use rejection sampling [13], which allows one to sample from a “hard” distribution $P$ using an “easy” distribution $Q$. Rejection sampling works by sampling from $Q$ first, then reject the sample with another probability used to bridge the gap between $Q$ and $P$. The process is repeated until a sample is accepted. In our setting, $P$ is the $k$-means++ distribution, and we need to find a $Q$ which could be sampled efficiently with a relational algorithm (without computing $J$). Rejection sampling theory shows that for the sampling to be efficient, $Q$ should be close to $P$ point-wise to avoid high rejection frequency. In the end, we will perfectly simulate the $k$-means++ algorithm.

We now describe the intuition for designing such a $Q$. Recall that $P$ is determined by the assignment of points to their closest centers. We will approximate this assignment up to a factor of $O(i^2d)$ when sampling the $i^{th}$ center $c_i$, where $d$ is the number of columns in $J$. Intuitively, the approximate assignment makes things easier since for any center we can easily find the points assigned to it using an efficient relational algorithm. Then $Q$ is found by normalizing the squared distance between each point and its assigned center.

The approximate assignment is designed as follows. Consider the $d$-dimensional Euclidean space where the data points in $J$ are located. The algorithm divides space into a laminar collection of hyper-rectangles (i.e., $\{x \in \mathbb{R}^d : v_j \leq x_j \leq w_j, j = 1, \ldots, d\}$, here $x_j$ is the value for feature $f_j$). We assign each hyper-rectangle to a center. A point assigns itself to the center that corresponds to the smallest hyper-rectangle containing the point.

The key property of hyper-rectangles that benefits our relational algorithm is: we can efficiently represent all points from $J$ inside any hyper-rectangle by removing some entries in each table from the original database and taking the join of all tables. For example, if a hyper-rectangle has constraint $v_j \leq x_j \leq w_j$, we just remove all the rows with value outside of range $[v_j, w_j]$ for column $f_j$ from the tables containing column $f_j$. The set of points assigned to a given center can be found by adding and subtracting a laminar set of hyper-rectangles, where each hyper-rectangle can be represented by a relational database.

**Weighting the Centers:** We have sampled a good set of cluster centers. To get a coreset, we need to assign weights to them. As we have already mentioned, assuming $P \neq \#P$, the weights cannot be computed relationally. In fact, they cannot be approximated up to any factor in polynomial time unless $P = \#P$. Rather, we design an alternative relational algorithm for computing the weights. Each weight will not be an approximate individually, but we prove that the weighted centers form an $O(1)$-approximate coreset in aggregate.

The main algorithmic idea is that for each center $c_i$ we generate a collection of hyperspheres around $c_i$ containing geometrically increasing numbers of points. The space is then partitioned using these hyperspheres where each partition contains a portion of points in $J$. Using the algorithm from [13], we then sample a poly-log sized collection of points from each partition, and use this subsample to estimate the fraction of the points in this partition which are closer to $c_i$ than any other center. The estimated weight of $c_i$ is aggregated accordingly.

**Paper Organization:** As relational algorithms are relatively new, we begin with some special cases which help the reader build intuition. In Section 2 we give a warm-up by showing how to implement 1-means++ and 2-means++ (i.e. initialization steps of $k$-means++). In this section, we also prove Theorem 1.2 as an example of the limits of relational algorithms. In Section 3 we go over background on relational algorithms that our overall algorithm will leverage. In Section 4 we give the $k$-means++ algorithm via rejection sampling. Section 5 shows an algorithm to construct the weights and then analyze this algorithm. Many of the technical proofs appear in the appendix due to space.

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[1] A laminar set of hyper-rectangles means any two hyper-rectangles from the set either have no intersection, or one of them contains the other.
2 Warm-up: Efficiently Implementing 1-means++ and 2-means++

This section is a warm-up to understand the combinatorial structure of relational data. We will show how to do k-means++ for k ∈ {1, 2} (referred to as 1- and 2-means++) on a simple join structure. We will also show the proof of Theorem 1.2 which states that counting the number of points in a cluster is a hard problem on relational data.

First, let us consider relationally implementing 1-means++ and 2-means++. For better illustration, we consider a special type of acyclic table structure named path join. The relational algorithm used will be generalized to work on more general join structures when we move to the full algorithm in Section 4.

In a path join each table $T_i$ has two features/columns $f_i$ and $f_{i+1}$. Table $T_i$ and $T_{i+1}$ then share a common column $f_{i+1}$. Assume for simplicity that each table $T_i$ contains $n$ rows. The design matrix $J = T_1 \Join T_2 \Join \ldots \Join T_m$ has $d = m + 1$ features, one for each feature (i.e., column) in the tables.

Even with this simple structure, the size of the design matrix $J$ could still be exponential in the size of database - $J$ could contain up to $n^{m/2}$ rows, and $d n^{m/2}$ entries. Thus the standard practice could require time and space $\Omega(m n^{m/2})$ in the worst case.

| $T_1$ | $T_2$ | $J = T_1 \Join T_2$ |
|-------|-------|---------------------|
| $f_1$ | $f_2$ | $f_1$ |
| $f_2$ | $f_3$ | $f_2$ |
| 1     | 1     | 1                   |
| 2     | 1     | 1                   |
| 3     | 2     | 2                   |
| 4     | 3     | 3                   |
| 5     | 4     | 5                   |

Table 2: A path join instance where the two tables $T_1$ and $T_2$ have $m = 2$ and $n = 5$. This shows $T_1, T_2$, the design matrix $J$, and the resulting layered directed graph $G$. Every path from the left most layer to the right most layer of this graph $G$ corresponds to one data point for the clustering problem (i.e. a row of the design matrix).

Graph Illustration of the Design Matrix: Conceptually consider a directed acyclic graph $G$, where there is one layer of nodes corresponding to each feature $f_i (i = 1, \ldots, d)$, and edges only point from nodes in layer $f_i$ to layer $f_{i+1}$.

The nodes in $G$ correspond to feature values, and edges in $G$ correspond to rows in tables. There is one vertex $v$ in layer $f_i$ for each value that appears in column $f_i$ in table $T_i$ or $T_{i-1}$, and one edge pointing from $u$ in layer $f_i$ to $v$ in layer $f_{i+1}$, if $(u, v)$ is a row in table $T_i$. Then, there is a one-to-one correspondence between full paths in $G$ (paths from layer $f_1$ to layer $f_d$) and rows in the design matrix.

A Relational Implementation of 1-means++: Implementing the 1-means++ algorithm is equivalent to generating a full path uniformly at random from $G$. We generate this path by iteratively picking a row from table $T_1, \ldots, T_m$, corresponding to picking an arc pointing from layer $f_1$ to $f_2$, $f_2$ to $f_3$, ..., such that concatenating all picked rows (arcs) will give a point in $J$ (full path in $G$).

To sample a row from $T_1$, for every row $r \in T_1$, consider $r \propto J$, which is all rows in $J$ whose values in columns $(f_1, f_2)$ are equivalent to $r$. Let the function $F_1(r)$ denote the total number of rows in $r \propto J$. This is also the number of full paths passing arc $r$. Then, every $r \in T_1$ is sampled with probability $\frac{F_1(r)}{\sum_{r' \in T_1} F_1(r')}$, notice $\sum_{r' \in T_1} F_1(r')$ is the total number of full paths. Let the picked row be $r_1$.

After sampling $r_1$, we can conceptually throw away all other rows in $T_1$ and focus only on the rows in $J$ that uses $r_1$ to concatenate with rows from other tables (i.e., $r_1 \propto J$). For any row $r \in T_2$, let the function $F_2(r)$ denote the number of rows in $r \propto r_1 \propto J$, also equivalent to the total number of full paths passing arc $r_1$ and $r$. We sample every $r$ with probability $\frac{F_2(r)}{\sum_{r' \in T_2} F_2(r')}$. Notice that $\sum_{r' \in T_2} F_2(r') = F_1(r_1)$, the number of full paths passing arc $r_1$. Repeat this procedure until we have sampled a row in the last table $T_m$: for table $T_i$ and $r \in T_i$, assuming we have sampled $r_1, \ldots, r_{i-1}$ from $T_1, \ldots, T_{i-1}$ respectively, throw away all the other rows in previous tables and focus on $r_1 \propto \ldots \propto r_{i-1} \propto J$. $F_i(r)$ is the number of rows in $r \propto r_1 \propto \ldots \propto r_{i-1} \propto J$ and $r$ is sampled with probability proportional to $F_i(r)$. It is easy to verify that every full path is sampled uniformly.

For every table $T_i$, we need to find the function $F_i(\cdot)$ which is defined on all its rows. There are $m$ such functions. For each $F_i(\cdot)$, we can find all $F_i(r)$ values for $r \in T_i$ using a one-pass dynamic programming and then sample
A Relational Implementation for 2-means++: Assume \( x = (x_1, \ldots, x_d) \) is the first center sampled and now we want to sample the second center. By k-means++ principles, any row \( r \in J \) is sampled with probability \( \frac{\|x-r\|^2}{\sum_{r' \in J} \|r'-x\|^2} \). For a full path in \( G \) corresponding to a row \( r \in J \) we refer to \( \|r-x\|^2 \) as the aggregated cost over all \( d \) nodes/features.

Similar to 1-means++, we pick one row in each table from \( T_1 \) to \( T_m \) and putting all the rows together gives us the sampled point. Assume we have sampled the rows \( r_1, r_2, \ldots, r_i-1 \) from the first \( i-1 \) tables and we focus on all full paths passing \( r_1, \ldots, r_i-1 \) (i.e., the new design matrix \( r_1 \times \ldots \times r_i-1 \times J \)). In 1-means++, we compute \( F_i(r) \) which is the total number of full paths passing \( r_1, \ldots, r_i-1, r \) (i.e., \( r \times r_1 \times \ldots \times r_i-1 \times J \)) and sample \( r \in T_i \) from a distribution normalized using \( F_i(r) \) values. In 2-means++, we define \( F_i(r) \) to be the summation of aggregated costs over all full paths which pass arcs \( r_1, \ldots, r_i-1, r \). We sample \( r \in T_i \) from a distribution normalized using \( F_i(r) \) values.

It is easy to verify the correctness. Again, each \( F_i(\cdot) \) could be computed using a one-pass dynamic programming which gives the values for all rows in \( T_i \) when we sample from \( T_i \). This would involve \( m \) rounds of such computations and give a polynomial algorithm.

2.1 Hardness of Relationally Computing the Weights:

Here we prove Theorem 1.2. We will focus on showing that given a set of centers, counting the number of points in \( J \) that is closest to any of them is \#P-hard. Due to space, see Appendix C for a proof of the other part of the theorem that it is hard to approximate the center weights for three centers. We prove \#P-Hardness by a reduction from the well known \#P-hard Knapsack Counting problem. The input to the Knapsack Counting problem consists of a set \( W = \{w_1, \ldots, w_h\} \) of nonnegative integer weights, and a nonnegative integer \( L \). The output is the number of subsets of \( W \) with aggregate weight at most \( L \). To construct the relational instance, for each \( i \in [h] \), we define the tables \( T_{2i-1} \) and \( T_{2i} \) as follows:

\[
\begin{array}{c|c|c}
\hline
& T_{2i-1} & T_{2i} \\
\hline
f_{2i-1} & 0 & 0 \\
0 & w_i & 0 \\
\hline
\end{array}
\]

Let centers \( c_1 \) and \( c_2 \) be arbitrary points such that points closer to \( c_1 \) than \( c_2 \) are those points \( p \) for which \( \sum_{i=1}^d p_i \leq L \). Then there are \( 2^h \) rows in \( J \), since \( w_i \) can either be selected or not selected in feature \( 2i \). The weight of \( c_1 \) is the number of points in \( J \) closer to \( c_1 \) than \( c_2 \), which is in turn exactly the number of subsets of \( W \) with total weight at most \( L \).

3 Related Work and Background

Related Work on K-means: Constant approximations are known for the \( k \)-means problem in the standard computational setting [21][13]. Although the most commonly used algorithm in practice is a local search algorithm called Lloyd’s algorithm, or sometimes confusingly just called “the \( k \)-means algorithm”. The \( k \)-means++ algorithm from [19] is a \( \Theta(\log k) \) approximation algorithm, and is commonly used in practice to seed Lloyd’s algorithm. Some coreset construction methods have been used before to design algorithms for the \( k \)-means problem in other restricted access computational models, including streaming [17][12], and the MPC model [16][11], as well as speeding up sequential methods [22][25].

Relational Algorithms for Learning Problem: Training different machine learning models on relational data has been studied; however, many of the proposed algorithms are not efficient under our definition of a relational algorithm. It has been shown that using repeated patterns in the design matrix, linear regression, and factorization machines can be implemented [23] more efficiently. [20][24][5] has improved the relational linear regression and factorization machines for different scenarios. A unified relational algorithm for problems such as linear regression, singular value
decomposition and factorization machines proposed in [6]. Algorithms for training support vector machine is studied in [26, 4]. In [14], a relational algorithm is introduced for Independent Gaussian Mixture Models, and they have shown experimentally that this method is faster than materializing the design matrix.

Relational Algorithm Building Blocks: In the path join scenario, the 1- and 2-means+ sampling methods introduced in subsection 2 have similar procedures: starting with the first table \( T_1 \), iteratively evaluate some function \( F_i(\cdot) \) defined on all rows in the table \( T_i \), sample one row \( r_i \) according to the distribution normalized from \( F_i(\cdot) \). The function \( F_i(\cdot) \) for table \( T_i \) is defined on the matrix \( r_1 \times \ldots \times r_{i-1} \times J \) where \( J \) is the design matrix. This matrix is also the design matrix of a new relational database, constructed by throwing away all rows in previous tables apart from the sampled \( r_1, \ldots, r_{i-1} \).

We can generalize the computation of \( F_i(\cdot) \) functions into a broader class of queries that we know could be implemented efficiently on any acyclic relational databases, namely **SumProd queries**. See [7] for more details. In the following lemmas assume the relational database has tables \( T_1, \ldots, T_m \) and their design matrix is \( J \), let \( n \) be the maximum number of rows in each table \( T_i \), \( m \) be the number of tables and \( d \) be the number of columns in \( J \).

**Definition 3.1.** For the \( j \)th feature \((j \in [d]) \) let \( q_j : \mathbb{R} \rightarrow S \) be an efficiently computable function that maps feature values to some set \( S \). Let the binary operations \( \oplus \) and \( \otimes \) be any operators such that \((S, \oplus, \otimes)\) forms a commutative semiring. The value of \( \bigoplus_{x \in J} \bigotimes_{j \in [d]} q_j(x_j) \) is a SumProd query.

**Lemma 3.2 ([7]).** Any SumProd query can be computed efficiently in time \( O(md^2 \log \log(n)) \) where \( fhtw \) is the fractional hypertree width of the database. For acyclic databases \( fhtw=1 \) so the running time is polynomial.

Despite the cumbersome formal definition of SumProd queries, below we list their key applications used in this paper. With a little abuse of notation, throughout this paper we use \( \Psi(n, d, m) \) to denote the worst-case time bound on any SumProd queries.

**Lemma 3.3.** Given a point \( y \in \mathbb{R}^d \) and a hyper-rectangle \( b = \{x \in \mathbb{R}^d : v_i \leq x_i \leq w_i, i = 1, \ldots, d \} \) where \( v \) and \( w \) are constant vectors, we let \( J \cap b \) denote the data points represented by rows of \( J \) that also fall into \( b \). Pick any table \( T_j \). Using one single SumProd query we can compute for all \( r \in T_j \) the value \( \sum_{p \in J \cap b} \|p - y\|_2^2 \). The time required is at most that required by one SumProd query, \( \Psi(n, d, m) \).

**Lemma 3.3** is an immediate result of Theorem 9 which you may find in Appendix F and the fact that we can efficiently represent all points from \( J \) inside any hyper-rectangle by removing some entries in each table from the original database and taking the join of all tables. The following lemma follows by an application of the main result in [3]. In Appendix F we formally show to apply their result to give the following lemma.

**Lemma 3.4 ([3]).** Given a hypersphere \( \{x \in \mathbb{R}^d : \|x - y_0\|_2^2 \leq z_0^2 \} \) where \( y_0 \) is a given point and \( z_0 \) is the radius, a \((1+\epsilon)\)-approximation of the number of points in \( J \) that lie inside this hypersphere could be computed in \( O \left( \frac{m^n \log n}{\epsilon^2} \Psi(n, d, m) \right) \) time.

Notice that a SumProd query could be used to output either a scalar (similar to Lemma 3.4) or a vector whose entries are function values for every row \( r \) in a chosen table \( T_j \) (in Lemma 3.3). We say the SumProd query is grouped by \( T_j \) in the latter case.

### 4 The \( k \)-means++ Algorithm

In this section, we describe a relational implementation of the \( k \)-means++ algorithm. It is sufficient to explain how center \( c_i \) is picked given the previous centers \( c_1, \ldots, c_{i-1} \). Recall that the \( k \)-means++ algorithm picks a point \( x \) to be \( c_i \) with probability \( P(x) = \frac{L(x)}{Y} \) where \( L(x) = \min_{j \in [i-1]} \|x - c_j\|_2^2 \) and \( Y = \sum_{x \in J} L(x) \) is a normalizing constant.

The implementation consists of two parts. The first part, described in Section 4.1 shows how to partition the \( d \)-dimensional Euclidean space into a laminar set of hyper-rectangles (referred to as boxes hereafter) that are generated around the previous centers. The second part, described in Section 4.2 samples according to the “hard” distribution \( P \) using rejection sampling and an “easy” distribution \( Q \).
Conceptually, we assign every point in the design matrix \( J \) to an *approximately* nearest center among \( c_1, \ldots, c_{i-1} \). This is done by assigning every point in \( J \) to one of the centers contained in the *smallest* box this point belongs to. Then \( Q \) is derived using the squared distance between the points in \( J \) and their assigned centers.

For illustration, we show the special case of when \( k = 3 \) in Appendix A. We refer the reader to this section as a warm-up before reading the general algorithm below.

### 4.1 Box Construction

Here we explain the algorithm for constructing a set of laminar boxes given the centers sampled previously. The construction is completely combinatorial. It only uses the given centers and we don’t need any relational operation for the construction.

**Algorithm Description:** Assume we want to sample the \( i^{th} \) point in \( k\)-means++. The algorithm maintains two collections \( G_i \) and \( B_i \) of tuples. Each tuple consists of a box and a point in that box, called the **representative** of the box. This point is one of the previously sampled centers. One can think of the tuples in \( G_i \) as “active” ones that are subject to changes and those in \( B_i \) as “frozen” ones that are finalized, thus removed from \( G_i \) and added to \( B_i \). When the algorithm terminates, \( G_i \) will be empty, and the boxes in \( B_i \) will be a laminar collection of boxes that we use to define the “easy” probability distribution \( Q \).

The initial tuples in \( G_i \) consist of one unit hyper-cube (side length is 1) centered at each previous center \( c_j, j \in [i-1] \), with its representative point \( c_j \). Up to scaling of initial unit hyper-cubes, we can assume that initially no pair of boxes in \( G_i \) intersect. This property of \( G_i \) is maintained throughout the process. Initially \( B_i \) is empty. Over time, the implementation keeps growing the boxes in \( G_i \) in size and moves tuples from \( G_i \) to \( B_i \).

The algorithm repeats the following steps in rounds. At the beginning of each round, there is no intersection between any two boxes in \( G_i \). The algorithm performs a doubling step where it doubles every box in \( G_i \). Doubling a box means each of its \( d-1 \) dimensional face is moved twice as far away from its representative. Mathematically, a box whose representative point is \( y \in \mathbb{R}^d \) may be written as \( \{ x \in \mathbb{R}^d : y_i - v_i \leq x_i \leq y_i + w_i, i = 1, \ldots, d \} \) \((v_i, w_i > 0)\). This box becomes \( \{ x \in \mathbb{R}^d : y_i - 2w_i \leq x_i \leq y_i + 2w_i, i = 1, \ldots, d \} \) after doubling.

After doubling, the algorithm performs the following operations on intersecting boxes until there are none. The algorithm iteratively picks two arbitrary intersecting boxes from \( G_i \). Say the boxes are \( b_1 \) with representative \( y_1 \) and \( b_2 \) with representative \( y_2 \). The algorithm executes a **melding** step on \((b_1, y_1)\) and \((b_2, y_2)\), which has the following procedures:

- Compute the smallest box \( b_3 \) in the Euclidean space that contains both \( b_1 \) and \( b_2 \).
- Add \((b_3, y_1)\) to \( G_i \) and delete \((b_1, y_1)\) and \((b_2, y_2)\) from \( G_i \).
- Check if \( b_1 \) (or \( b_2 \)) is a box created by the doubling step at the beginning of the current round and hasn’t been melded with other boxes ever since. If so, the algorithm computes a box \( b'_1 \) (resp. \( b'_2 \)) from \( b_1 \) (resp. \( b_2 \)) by **halving** it. That is, each \( d-1 \) dimensional face is moved so that its distance to the box’s representative is halved. Mathematically, a box \( \{ x \in \mathbb{R}^d : y_i - v_i \leq x_i \leq y_i + w_i, i = 1, \ldots, d \} \) \((v_i, w_i > 0)\), where vector \( y \) is its representative, becomes \( \{ x \in \mathbb{R}^d : y_i - \frac{1}{2}v_i \leq x_i \leq y_i + \frac{1}{2}w_i, i = 1, \ldots, d \} \) after halving. Then \((b'_1, y_1)\) (or \((b'_2, y_2)\)) is added to \( B_i \). Otherwise do nothing.

Notice that melding decreases the size of \( G_i \).

The algorithm terminates when there is one tuple \((b_0, y_0)\) left in \( G_i \), at which point the algorithm adds a box that contains the whole space with representative \( y_0 \) to \( B_i \). Note that during each round of the doubling and melding, the boxes which are added to \( B_i \) are the ones that after doubling were melded with other boxes, and they are added at their shapes before the doubling step.

**Lemma 4.1.** The collection of boxes in \( B_i \) constructed by the above algorithm is laminar.

**Proof.** Note that right before each doubling step, the boxes in \( G_i \) are disjoint and that is because the algorithm in the previous iteration melds all the boxes that have intersection with each other. We prove by induction that at all time, for every box \( b \) in \( B_i \) there exist a box \( b' \) in \( G_i \) such that \( b \subseteq b' \). Since the boxes added to \( B_i \) in each iteration are a subset...
of the boxes in $\mathcal{G}_t$ before the doubling step and they do not intersect each other, laminarity of $B_t$ is a straight-forward consequence.

Initially $B_1$ is empty and therefore the claim holds. Assume in some arbitrary iteration $\ell$ this claim holds right before the doubling step, then after the doubling step since every box in $\mathcal{G}_t$ still covers all of the area it was covering before getting doubled, the claim holds. Furthermore, in the melding step every box $b_3$ that is resulted from melding of two boxes $b_1$ and $b_2$ covers both $b_1$ and $b_2$; therefore, $b_3$ will cover $b_1$ and $b_2$ if they are added to $B_1$, and if a box in $B_t$ was covered by either of $b_1$ or $b_2$, it will be still covered by $b_3$. 

The collection of boxes in $B_t$ can be thought of as a tree where every node corresponds to a box. The root node is the entire space. In this tree, for any box $b'$, among all boxes included by $b'$, we pick the inclusion-wise maximal boxes and let them be the children of $b'$. Thus the number of boxes in $B_t$ is $O(i)$ since the tree has $i$ leaves, one for each center.

### 4.2 Sampling

To define our easy distribution $Q$, for any point $x \in J$, let $b(x)$ be the minimal box in $B_t$ that contains $x$ and $y(x)$ be the representative of $b(x)$. Define $R(x) = \|x - y(x)\|_2^2$, and $Q(x) = \frac{R(x)}{Z}$ where $Z = \sum_{x \in J} R(x)$ normalizes the distribution. We call $R(x)$ the assignment cost for $x$. We will show how to sample from target distribution $P(\cdot)$ using $Q(\cdot)$ and rejection sampling, and how to implement the this designed sampling step relationally.

**Rejection Sampling:** The algorithm repeatedly samples a point $x$ with probability $Q(x)$, then either (A) rejects $x$ and resamples, or (B) accepts $x$ as the next center $c_i$ and finishes the sampling process. After sampling $x$, the probability of accepting $x$ is $\frac{L(x)}{R(x)}$, and that of rejecting $x$ is $1 - \frac{L(x)}{R(x)}$. Notice that here $\frac{L(x)}{R(x)} \leq 1$ since $R(x) = \|x - y(x)\|_2^2 \geq 2 \min_{j \in [i-1]} \|x - c_j\|_2^2$.

If $S(x)$ is the the event of initially sampling $x$ from distribution $Q$, and $A(x)$ is the event of subsequently accepting $x$, the probability of choosing $x$ to be $c_i$ in one given round is:

$$\Pr[S(x) \text{ and } A(x)] = \Pr[A(x) \mid S(x)] \Pr[S(x)] = \frac{L(x)}{R(x)} Q(x) = \frac{L(x)}{Z}$$

Thus the probability of $x$ being the accepted sample is proportional to $L(x)$, as desired.

We would like $Q(\cdot)$ to be close to $P(\cdot)$ point-wise so that the algorithm is efficient. Otherwise, the acceptance probability $\frac{L(x)}{R(x)}$ is low and it might keep rejecting samples.

**Relational Implementation of Sampling:** We now explain how to relationally sample a point $x$ with probability $Q(x)$. The implementation heavily leverages Lemma 3.3 which states for given box $b^*$ with representative $y^*$, the cost of assigning all points in $r \propto J \cap b^*$ to $y^*$ for each row $r \in T_\ell$ can be computed in polynomial time using a SumProd query grouped by $T_\ell$. Recall that we assign all points in $J$ to the representative of the smallest box they belong to. We show that the total assignment cost is computed by evaluating SumProd queries on the boxes and then adding/subtracting the query values for different boxes.

Following the intuition provided in Section 2, the implementation generates a single row from table $T_1, T_2, \ldots, T_m$ sequentially. The concatenation of these rows (or the join of them) gives the sampled point $x$. It is sufficient to explain assuming we have sampled $r_1, \ldots, r_{\ell-1}$ from the first $\ell - 1$ tables, how to implement the generation of a row from the next table $T_\ell$. Just like 1- and 2-means++ in subsection 2, the algorithm evaluates a function $F(\cdot)$ defined on rows in $T_\ell$ using SumProd queries, and samples $r$ with probability $\sum_{r' \in T_\ell} F(r')$. Again, we focus on $r_1 \propto \ldots \propto r_{\ell-1} \propto J$, denoting the points in $J$ that uses the previously sampled rows. The value of $F(r)$ is determined by points in $r \propto r_1 \propto \ldots \propto r_{\ell-1} \propto J$.

To ensure we generate a row according to the correct distribution $Q$, we define the function $F(r)$ as follows. Let $F(\cdot)$ be the total assignment cost of all points in $r \propto r_1 \propto \ldots \propto r_{\ell-1} \propto J$. That is, $F(r) = \sum_{x \in T_\ell} R(x)$ where $R(x)$ is the definition of function $F(\cdot)$ is very similar to 2-means++ apart from that each point is no longer assigned to a given center, but the representative of the smallest box containing it.

Let $G(r, b^*, y^*)$ denote the cost of assigning all points from $r \propto r_1 \propto \ldots \propto r_{\ell-1} \propto J$ that lies in box $b^*$ to a center $y^*$. By replacing the $J$ in Lemma 3.3 by $r_1 \propto \ldots \propto r_{\ell-1} \propto J$, we can compute all $G(r, b^*, y^*)$ values in polynomial
time using one SumProd query grouped by \( T_\ell \). The value \( F_\ell(r) \) can be expanded into subtraction and addition of 
\( G(r, b^*, y^*) \) terms. The expansion is recursive. For a box \( b_0 \), let 
\[ H(r, b_0) = \sum_{x \in r, \ell_1, \ldots, \ell_{r-1}, \ell \cap b_0} R(x). \]
Notice that 
\[ F_\ell(r) = H(r, b_0) \] if \( b_0 \) is the entire Euclidean space. Pick any row \( r \in T_\ell \). Assume we want to compute 
\( H(r, b_0) \) for some tuple \((b_0, y_0) \in B_1\).

Recall that the set of boxes in \( B_i \) forms a tree structure. If \( b_0 \) has no children this is the base case - 
\( H(r, b_0) = G(r, b_0, y_0) \) by definition since all points in \( b_0 \) must be assigned to \( y_0 \). Otherwise, let \((b_1, y_1), \ldots, (b_q, y_q)\) be the tuples in \( B_i \) where \( b_1, \ldots, b_q \) are children of \( b_0 \). Notice that, by definition all points in \( b_0 \setminus \bigcup_{j \in [q]} b_j \) is assigned to \( y_0 \). Then, one can check that the following equation holds for any \( r \):

\[
H(r, b_0) = G(r, b_0, y_0) - \sum_{j \in [q]} G(r, b_j, y_0) + \sum_{j \in [q]} H(r, b_j)
\]

Starting with setting \( b_0 \) as the entire Euclidean space, the equation above could be used to recursively expand 
\( H(\cdot, b_0) = F_\ell(\cdot) \) into addition and subtraction of \( O(|B_i|) \) number of \( G(\cdot, \cdot, \cdot) \) terms, where each term could be computed with one SumProd query by Lemma 3.3.

**Runtime Analysis of the Sampling:** We now discuss the running time of the sampling algorithm simulating \( k\)-means++. These lemmas show how close the probability distribution we compute is as compared to the \( k\)-means++ distribution. This will help bound the running time.

**Lemma 4.2.** Consider the box construction algorithm when sampling the \( i \)th point in the \( k\)-means++ simulation. Consider the end of the \( j \)th round where all melding is finished but the boxes have not been doubled yet. Let \( b \) be an arbitrary box in \( \mathcal{G}_i \) and \( h(b) \) be the number of centers in \( b \) at this time. Let \( c_a \) be an arbitrary one of these \( h(b) \) centers. Then:

A. The distance from \( c_a \) to any \( d \)−1 dimensional face of \( b \) is at least \( 2^j \).

B. The length of each side of \( b \) is at most \( h(b) \cdot 2^{j+1} \).

**Proof.** The first statement is a direct consequence of the definition of doubling and melding since at any point of time
the distance of all the centers in \( b \) is at least \( 2^j \). To prove the second statement, we define the assignment of the centers to the boxes as following. Consider the centers inside each box \( b \) right before the doubling step. We call these centers, the centers assigned to \( b \) and denote the number of them by \( h'(b) \). When two boxes \( b_1 \) and \( b_2 \) are melding into box \( b_3 \), we assign their assigned centers to \( b_3 \).

We prove each side length of \( b \) is at most \( h'(b)2^{j+1} \) by induction on the number \( j \) of executed doubling steps. Since
\( h'(b) = h(b) \) right before each doubling, this will prove the second statement. The statement is obvious in the base case, \( j = 0 \). The statement also obviously holds by induction after a doubling step as \( j \) is incremented and the side lengths double and the number of assigned boxes don’t change. It also holds during every meld step because each side length of the newly created larger box is at most the aggregate maximum side lengths of the smaller boxes that are moved to \( B_i \), and the number of assigned centers in the newly created larger box is the aggregate of the assigned centers in the two smaller boxes that are moved to \( B_i \). Note that since for any box \( b \) all the assigned centers to \( b \) are inside \( b \) at all times, \( h'(b) \) is the number of centers inside \( b \) before the next doubling.

This lemma bounds the difference of the two probability distributions.

**Lemma 4.3.** Consider the box generation algorithm when sampling the \( i \)th point in the \( k\)-means++ simulation. For all points \( x, R(x) \leq O(i^2d) \cdot L(x) \).

**Proof.** Consider an arbitrary point \( x \). Let \( c_\ell, \ell \in [i-1], \) be the center that is closest to \( x \) under the 2-norm distance. Assume \( j \) is minimal such that just before the \((j+1)\)th doubling round, \( x \) is contained in a box \( b \) in \( \mathcal{G}_i \). We argue about the state of the algorithm at two times, the time \( s \) just before doubling round \( j \) and the time \( t \) just before doubling round \( j + 1 \). Let \( b \) be a minimal box in \( \mathcal{G}_i \) that contains \( x \) at time \( t \), and let \( y \) be the representative for box \( b \). Notice that we assign \( x \) to the representative of the smallest box in \( B_i \) that contains it, so \( x \) will be assigned to \( y \). Indeed, none of the boxes added into \( B_i \) before time \( t \) contains \( x \) by the minimality of \( j \), and when box \( b \) gets added into \( B_i \) (potentially
after a few more doubling rounds) it still has the same representative $y$. By Lemma 4.2, the squared distance from from $x$ to $r$ is at most $(i - 1)^2 d 2^{2j-2}$. So it is sufficient to show that the squared distance from $x$ to $c_t$ is $\Omega(2^j)$.

Let $b'$ be the box in $G_t$ that contains $c_t$ at time $s$. Note that $x$ could not have been inside $b'$ at time $s$ by the definition of $t$ and $s$. Then by Lemma 4.2, the distance from $c_t$ to the edge of $b'$ at time $t$ is at least $2^{2j-2}$, and hence the distance from $c_t$ to $x$ is also at least $2^{2j-2}$ as $x$ is outside of $b'$.

The following theorem bounds the running time.

**Theorem 4.4.** The expected time complexity for running $k'$ iterations of this implementation of $k$-means++ is $O(k^4 dm \Psi(n, d, m)).$

**Proof.** When picking center $c_t$, a point $x$ can be sampled with probability $Q(x)$ in time $O(mi\Psi(n, m, d))$. This is because the implementation samples one row from each of the $m$ tables. To sample one row we evaluate $O(|B_i|)$ SumProd queries, each in $O(\Psi(n, m, d))$ time. As mentioned earlier $B_i$ can be thought of as a tree of boxes with $i - 1$ leaves, so $|B_i| = O(i)$.

By Lemma 4.3, the probability of accepting any sampled $x$ is $\frac{\ell(x)}{\ell(x)} = \frac{1}{O(\tau^d)}$. The expected number of sampling from $Q$ until getting accepted is $O(i^2 d)$. Thus the expected time of finding $c_t$ is $O(i^3 dm \Psi(n, m, d))$. Summing over $i \in [k']$, we get $O(k^4 dm \Psi(n, m, d))$. 

5 Weighting the Centers

Our algorithm samples a collection $C$ of $k' = \Theta(k \log N)$ centers using the $k$-means++ sampling described in the prior section. We give weights to the centers to get a coreset.

Ideally, we would compute the weights in the standard way. That is, let $w_i$ denote the number of points that are closest to point $c_i$ among all centers in $C$. These pairs of centers and weights $(c_i, w_i)$ are known to form a coreset. Unfortunately, as stated in Theorem 1.2 computing such $w_i$’s even approximately is NP hard. Instead, we will find a different set of weights which still form a coreset and are computable.

Next we describe a relational algorithm to compute a collection $W'$ of weights, one weight $w'_i \in W'$ for each center $c_i \in C$. The proof that the centers with these alternative weights $(c_i, w'_i)$ also form a coreset is postponed until the appendix.

**Algorithm for Computing Alternative Weights:** Initialize the weight $w'_i$ for each center $c_i \in C$ to zero. In the $d$-dimensional Euclidean space, for each center $c_i \in C$, we generate a collection of hyperspheres (also named balls) $\{B_{i,j}\}_{j \in [\log N]}$, where $B_{i,j}$ contains approximately $2^j$ points from $J$. The space is then partitioned into $\{B_{0,0}, B_{1,0} - B_{i,0}, B_{1,j} - B_{i,1}, \ldots\}$. For each partition, we will sample a small number of points and use this sample to estimate the number of points in this partition that are closer to $c_j$ than any other centers, and thus aggregating $w'_i$ by adding up the numbers. Fix small constants $\epsilon, \delta > 0$. The following steps are repeated for $j \in [\log N]$:

- Let $B_{i,j}$ be a ball of radius $r_{i,j}$ centered at $c_i$. Find a $r_{i,j}$ such that the number of points in $J \cap B_{i,j}$ lies in the range $|(1 - \delta)2^j, (1 + \delta)2^j|$. This is an application of Lemma 5.4.

- Let $\tau$ be a constant that is at least $30$. A collection $T_{i,j}$ of $\frac{\tau}{d^2 \log^2 N}$ “test” points are independently sampled following the same approximately uniform distribution with replacement from every ball $B_{i,j}$. Here an “approximately uniform” distribution means one where every point $p$ in $B_{i,j}$ is sampled with a probability $\gamma_{p,i,j} \in [(1 - \delta)/|B_{i,j}|, (1 + \delta)/|B_{i,j}|]$ on each draw. This can be accomplished efficiently similar to the techniques used in Lemma 4.4 from [3]. Further elaboration is given in the Appendix D.

- Among all sampled points $T_{i,j}$, find $S_{i,j}$, the set of points that lie in the “donut” $D_{i,j} = B_{i,j} - B_{i,j-1}$. Then the cardinality $s_{i,j} = |S_{i,j}|$ is computed.

- Find $t_{i,j}$, the number of points in $S_{i,j}$ that are closer to $c_i$ than any other center in $C$.

- Compute the ratio $f'_{i,j} = \frac{t_{i,j}}{s_{i,j}}$ (if $s_{i,j} = t_{i,j} = 0$ then $f'_{i,j} = 0$).
• If \( f'_{i,j} \geq \frac{1}{2k^{\frac{1}{2}}\log N} \) then \( w'_i \) is incremented by \( f'_{i,j} \cdot 2^{j-1} \), else \( w'_i \) stays the same.

At first glance, the algorithm appears naive: \( w'_i \) can be significantly underestimated if in some donuts only a small portion of points are closest to \( c_i \), making the estimation inaccurate based on sampling. However, in Section 6 we prove the following theorem which shows that the alternative weights computed by our algorithm actually form a coreset.

**Theorem 5.1.** The centers \( C \), along with the computed weights \( W' \), form an \( O(1) \)-approximate coreset with high probability.

The running time of a naive implementation of this algorithm would be dominated by sampling of the test points. Sampling a single test point can be accomplished with \( m \) applications of the algorithm from [3] and setting the approximation error to \( \delta = \epsilon/m \). Recall the running time of the algorithm from [3] is \( \mathcal{O}\left(\frac{m^2 \log n \Psi(n, d, m)}{\epsilon^2} \right) \). Thus, the time to sample all test points is \( \mathcal{O}\left(\frac{k^2 m^2 \log n \Psi(n, d, m)}{\epsilon^2} \right) \). Substituting for \( k' \) and noting that \( N \leq n^m \), we obtain a total time for a naive implementation of \( \mathcal{O}\left(\frac{k^2 m^{1+\log n} \Psi(n, d, m)}{\epsilon^2} \right) \).

6 Analysis of the Weighting Algorithm

The goal in this subsection is to prove Theorem 5.1 which states that the alternative weights form an \( O(1) \)-approximate coreset with high probability. Throughout our analysis, “with high probability” means that for any constant \( \rho > 0 \) the probability of the statement not being true can be made less than \( \frac{1}{N^\rho} \) asymptotically by appropriately setting the constants in the algorithm.

Intuitively if a decent fraction of the points in each donut are closer to center \( c_i \) than any other center, then Theorem 5.1 can be proven by using a straight-forward application of Chernoff bounds to show that each alternate weight \( w'_i \) is likely close to the true weight \( w_i \). The conceptual difficulty is if only a very small portion of points in a donut \( D_{i,j} \) are closer to \( c_i \) than any other points, in which case the estimated \( f'_{i,j} < \frac{1}{2k^{\frac{1}{2}}\log N} \) and thus the “uncounted” points in \( D_{i,j} \) would contribute no weight to the computed weight \( w'_i \). We call this the undersampled case. If many donuts around a center \( i \) are undersampled, the computed weight \( w'_i \) may well poorly approximate the actual weight \( w_i \).

To address this, we need to prove that omitting the weight from these uncounted points does not have a significant impact on the objective value. We break our proof into four parts. The first part, described in subsubsection 6.1 involves conceptually defining a fractional weight \( w'_i \) for each center \( c_i \in C \). Each point has a weight of 1, and instead of giving all this weight to its closest center, we allow fractionally assigning the weight to various “near” centers. \( w'_i \) is then the aggregated weight over all points for \( c_i \). The second part, described in subsubsection 6.2 establishes various properties of the fractional weight that we will need. The third part, described in subsubsection 6.3 shows that each fractional weight \( w'_i \) is likely to be closely approximated the computed weight \( w'_i \). The fourth part, described in subsubsection 6.4, shows that the fractional weights for the centers in \( C \) form a \( O(1) \)-approximate coreset. Subsubsection 6.4 also contains the proof of Theorem 5.1.

6.1 Defining the Fractional Weights

To define the fractional weights we first define an auxiliary directed acyclic graph \( G = (S, E) \) where there is one node in \( S \) corresponding to each row in \( J \). For the rest of this section, with a little abuse of notation we use \( S \) to denote both the nodes in graph \( G \), and the set of \( d \)-dimensional data points in the design matrix. Let \( p \) be an arbitrary point in \( S - C \). Let \( \alpha(p) \) denote the subscript of the center closest to \( p \), i.e., if \( c_i \in C \) is closest to \( p \) then \( \alpha(p) = i \). Let \( D_{i,j} \) be the donut around \( c_i \) that contains \( p \). If \( D_{i,j} \) is not undersampled then \( p \) will have one outgoing edge \( (p, c_i) \). So let us now assume that \( D_{i,j} \) is undersampled. Defining the outgoing edges from \( p \) in this case is a bit more complicated.

Let \( A_{i,j} \) be the points \( q \in D_{i,j} \) that are closer to \( c_i \) than any other center in \( C \) (i.e., \( \alpha(q) = i \)). If \( j = 1 \) then \( D_{i,1} \) contains only the point \( p \), and the only outgoing edge from \( p \) goes to \( c_i \). So let us now assume \( j > 1 \). Let \( c_h \) the center that is closest to the most points in \( D_{i,j-1} \), the next donut in toward \( c_i \) from \( D_{i,j} \). That is \( c_h = \arg \max_{j' \in E} \sum_{q \in D_{i,j-1}} 1_{\alpha(q) = c_{j'}} \). Let \( M_{i,j-1} \) be points in \( D_{i,j-1} \) that are closer to \( c_h \) than any other center. That is \( M_{i,j-1} \) is the collection of \( q \in D_{i,j-1} \) such that \( \alpha(q) = h \). Then there is a directed edge from \( p \) to each point in
We now break the proof into three cases, that cover the ways in which the statement of this lemma would not be true. More formally, the following flow step is repeated until it is no longer possible to do so:

Case 1: \( f_{i,j} \geq \frac{1}{2k^2 \log^2 N} \) and \( f_{i,j} \geq \frac{1}{2k^2 \log^2 N} \) and \( f_{i,j} \geq (1 + \epsilon) f_{i,j} \). We are going to prove the probability of this case happening is very low. If we set \( \lambda = \epsilon \mu \), then using Chernoff bound, we have

\[
\Pr[t_{i,j} \geq (1 + \epsilon) \mu] \leq \exp \left( -\frac{(\epsilon \mu)^2}{2\mu + \epsilon \mu} \right)
\]

[Upper Chernoff Bound]
Therefore, for $\delta \leq \varepsilon/2 \leq 1/10$ and $\tau \geq 30$ this case cannot happen with high probability.

**Case 2:** $f'_{i,j} \geq \frac{1}{2k^2 \log N}$ and $f_{i,j} > \frac{1-\varepsilon}{2k^2 \log N}$ and $f'_{i,j} < (1-\varepsilon)f_{i,j}$. We can use Lower Chernoff Bound with $\lambda = \varepsilon\mu$ to prove the probability of this event is very small.

\[
\Pr[t_{i,j} \leq (1-\varepsilon)\mu] \leq \exp \left( -\frac{(\varepsilon\mu)^2}{3}\right)
\]

\leq \exp \left( -\frac{\varepsilon^2(1-\delta)f_{i,j}s_{i,j}}{2} \right) \quad [\mu \geq (1-\delta)f_{i,j}s_{i,j}]

\leq \exp \left( -\frac{\varepsilon^2(1-\delta)(1-\varepsilon)s_{i,j}}{3(2k^2 \log N)} \right) \quad [f_{i,j} > \frac{1-\varepsilon}{2k^2 \log N}]

\leq \exp \left( -\frac{\varepsilon^2(1-\delta)(1-\varepsilon)\log 2 \log N}{3(2k^2 \log N)(3\varepsilon^2)} \right) \quad [s_{i,j} \geq \varepsilon \log 2 \log N]

= \exp \left( -\frac{(1-\delta)(1-\varepsilon)\log N}{18} \right)

Therefore, for $\delta \leq \varepsilon/2 \leq 1/10$ and $\tau \geq 30$ this case cannot happen with high probability.

**Case 3:** $f'_{i,j} \geq \frac{1}{2k^2 \log N}$ and $f_{i,j} \leq \frac{1-\varepsilon}{2k^2 \log N}$. Since $f'_{i,j} = \frac{t_{i,j}}{s_{i,j}}$, in this case:

\[
t_{i,j} \geq \frac{s_{i,j}}{2k^2 \log N}
\]

(1)

Since $\mu \leq f_{i,j}(1+\delta)s_{i,j}$, in this case:

\[
\mu \leq \frac{1-\varepsilon}{2k^2 \log N}(1+\delta)s_{i,j}
\]

(2)

Thus subtracting line [1] from line [2] we conclude that:

\[
t_{i,j} \geq \mu + \frac{(\varepsilon - \delta + \varepsilon\delta)s_{i,j}}{2k^2 \log N}
\]

(3)

Let $\lambda = \frac{(\varepsilon - \delta + \varepsilon\delta)s_{i,j}}{2k^2 \log N}$. We can conclude that

\[
\Pr[t_{i,j} \geq \mu + \lambda] \leq \exp \left( -\frac{\lambda^2}{2\mu + \lambda} \right) \quad \text{Upper Chernoff Bound}
\]

\leq \exp \left( -\frac{\lambda^2}{\frac{1-\varepsilon}{2k^2 \log N}(1+\delta)s_{i,j} + \lambda} \right) \quad \text{Using line [2]}

\]

\[
= \exp \left( -\frac{(\varepsilon - \delta + \varepsilon\delta)s_{i,j}^2}{\frac{1-\varepsilon}{2k^2 \log N}(1+\delta)s_{i,j} + \frac{(\varepsilon - \delta + \varepsilon\delta)s_{i,j}}{2k^2 \log N}} \right)
\]

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\[
\begin{align*}
  &= \exp \left( \frac{- (\epsilon - \delta + \epsilon \delta)^2 s_{i,j}}{k^2 \log N} \right) \\
  &\leq \exp \left( \frac{- (\epsilon - \delta + \epsilon \delta)^2}{12k^2 \log N} \right) \\
  &= \exp \left( \frac{- (\epsilon - \delta + \epsilon \delta)^2 \tau \log N}{12\epsilon^2} \right)
\end{align*}
\]

Substituting our lower bound on \( s_{i,j} \)

Therefore, for \( \delta \leq \epsilon/2 \leq 1/10 \) and \( \tau \geq 30 \) this case cannot happen with high probability.

The next case proves the how large \( f'_{i,j} \) is when we know that \( f_{i,j} \) is large.

**Lemma 6.4.** If \( f_{i,j} > \frac{1+\epsilon}{2k^2 \log N} \) then with high probability \( f'_{i,j} \geq \frac{1}{2k^2 \log N} \).

**Proof.** We can prove that the probability of \( f'_{i,j} < \frac{1}{2k^2 \log N} \) and \( f_{i,j} \geq \frac{1+\epsilon}{2k^2 \log N} \) is small. Multiplying the conditions for this case by \( s_{i,j} \) we can conclude that \( t_{i,j} < \frac{1}{2k^2 \log N} \) and \( \mu \geq (1-\delta) \frac{(1+\epsilon)s_{i,j}}{2k^2 \log N} \). And thus \( t_{i,j} \leq \mu - \lambda \) where \( \lambda = \frac{(\epsilon - \delta - \epsilon \delta)s_{i,j}}{2k^2 \log N} \). Then we can conclude that:

\[
\Pr[t_{i,j} \leq \mu - \lambda] \leq \exp \left( -\frac{\lambda^2}{3\mu} \right) \quad [\text{Lower Chernoff Bound}]
\]

\[
\begin{align*}
  &= \exp \left( -\frac{(\epsilon - \delta - \epsilon \delta)^2 s_{i,j}}{2k^2 \log N} \right) \\
  &\leq \exp \left( -\frac{(\epsilon - \delta - \epsilon \delta)^2}{3k^2 \log N} \cdot (1 + \delta)s_{i,j} \right) \\
  &= \exp \left( -\frac{(\epsilon - \delta - \epsilon \delta)^2}{3(1-\epsilon)(1+\delta)} \right) \\
  &\leq \exp \left( \frac{- (\epsilon - \delta)^2 s_{i,j}}{12k^2 \log N} \right) \quad [\delta < \epsilon \leq 1] \\
  &\leq \exp \left( \frac{- (\epsilon - \delta)^2 \left( \frac{3\tau k^2 \log^2 N}{3\tau k^2 \log^2 N} \right)}{12k^2 \log N} \right) \quad [\text{Using our lower bound on } s_{i,j}]
\end{align*}
\]

Therefore, for \( \delta \leq \epsilon/2 \leq 1/10 \) and \( \tau \geq 30 \) this case cannot happen with high probability.

We now seek to bound the fractional weights computed by the algorithm. Let \( \Delta_i(p) \) denote the total weight received by a point \( p \in S \setminus C \) from other nodes (including the initial weight one on \( p \)). Furthermore, let \( \Delta_i(p) \) denote the total weight sent by \( p \) to all other nodes. Notice that in the flow step \( \Delta_i(p) = \Delta_i(p) \) for all \( p \in S \setminus C \).

**Lemma 6.5.** Let \( \Delta_i(p) \) denote the total weight received by a point \( p \in S \setminus C \) from other nodes (including the initial weight one on \( p \)). Furthermore, let \( \Delta_i(p) \) denote the total weight sent by \( p \) to all other nodes. With high probability, for all \( q \in S \), \( \Delta_i(q) \leq 1 + \frac{1+\epsilon^2}{k^2 \log N} \max_{p:(p,q) \in E} \Delta_o(p) \).

**Proof.** Fix the point \( q \) that redirects its weight (has outgoing arcs in \( G \)). Consider its direct predecessors: \( P(q) = \{ p : (p,q) \in E \} \). Partition \( P(q) \) as follows: \( P(q) = \bigcup_{i=1,\ldots,k'} P_{e_i}(q) \), where \( P_{e_i}(q) \) is the set of points that have flowed
their weights into \( q \), but \( c_i \) is actually their closest center in \( C \). Observe the following. The point \( q \) can only belong to one donut around \( c_i \). Due to this, \( P_c_i(q) \) is either empty or contains a set of points in a single donut around \( c_i \) that redirect weight to \( q \).

Fix \( P_c_i(q) \) for some \( c_i \). If this set is non-empty suppose this set is in the \( j \)-th donut around \( c_i \). Conditioned on the events stated in Lemmas \( 6.2 \) and \( 6.4 \) since the points in \( P_c_i(q) \) are undersampled, we have \( |P_c_i(q)| \leq \frac{(1+\epsilon)2^{j-1}}{2k^2 \log N} \).

Consider any \( p \in P_c_i(q) \). Let \( \beta_p \) be the number of points that \( p \) charges its weight to (this is the same for all such points \( p \)). It is the case that \( \beta_p \) is at least \( \frac{(1-\delta)2^{j-1}}{2k^2} \) since \( p \) flows its weights to the points that are assigned to the center that has the most number of points assigned to it from \( c_i \)'s \((j-1)\)th donut.

Thus, \( q \) receives weight from \( |P_c_i(q)| \leq \frac{(1+\epsilon)2^{j-1}}{2k^2 \log N} \) points and each such point gives its weight to at least \( \frac{(1-\delta)2^{j-1}}{2k^2} \) points with equal split. The total weight that \( q \) receives from points in \( P_c_i(q) \) is at most the following.

\[
\frac{2k^2}{(1-\delta)2^{j-1}} \sum_{p \in P_c_i(q)} \Delta_o(p) \\
\leq \frac{2k^2}{(1-\delta)2^{j-1}} \sum_{p \in P_c_i(q)} \max_{p \in P_c_i(q)} \Delta_o(p) \\
\leq \frac{2k^2}{(1-\delta)2^{j-1}} \cdot \frac{(1+\epsilon)2^{j-1}}{2k^2 \log N} \max_{p \in P_c_i(q)} \Delta_o(p) \\
\leq 1 + \frac{2\epsilon}{k^2 \log N} \max_{p \in P_c_i(q)} \Delta_o(p)
\]

Switching the max to \( \max_{p \in P_c(q) \in E} \Delta_o(p) \), summing over all centers \( c_i \in C \) and adding the original unit weight on \( q \) gives the lemma.

The following crucial lemma bounds the maximum weight that a point can receive.

**Lemma 6.6.** Fix \( \eta \) to be a constant smaller than \( \frac{\log(N)}{10} \) and \( \epsilon < 1 \). Say that for all \( q \in S \setminus C \) it is the case that \( \Delta_o(q) = \eta \Delta_i(q) \). Then, with high probability for any \( p \in S \setminus C \) it is the case that \( \Delta_i(p) \leq 1 + \frac{2\eta}{\log N} \).

**Proof.** We can easily prove this by induction on nodes. The lemma is true for all nodes that have no incoming edges in \( G \). Now assume it is true for all nodes whose longest path that reaches them in \( G \) has length \( t-1 \). Now we prove it for nodes whose longest path that reaches then in \( G \) is \( t \). Fix such a node \( q \). For any node \( p \) such that \((p, q) \in E \), by induction we have \( \Delta_i(p) \leq 1 + \frac{2\eta}{\log N} \), so \( \Delta_o(p) \leq 2(1 + \frac{2\eta}{\log N}) \). By Lemma \( 6.5 \)

\[
\Delta_i(q) \leq 1 + \frac{2\eta}{\log N} \max_{(p, q) \in E} \Delta_o(p) \\
\leq 1 + \left( \frac{\eta(1+2\eta)}{\log N} \right) \left( 1 + \frac{2\eta}{\log N} \right) \\
= 1 + \frac{\eta}{\log N} + \frac{\eta}{\log N} + \frac{2(1+2\eta)\eta + 2\eta}{\log N} \\
\leq 1 + \frac{2\eta}{\log N}
\]

6.3 Comparing Alternative Weights to Fractional Weights

It only remains to bound the cost of mapping points to the centers they contribute weight to. This can be done by iteratively charging the total cost of reassigning each node with the flow. In particular, each point will only pass its weight to nodes that are closer to their center. We can charge the flow through each node to the assignment cost of that node to its closest center, and argue that the cumulative reassignment cost bounds the real fractional assignment cost. Further, each node only has \( 1 + \epsilon \) flow going through it. This will be sufficient to bound the overall cost in Lemma \( 6.8 \).

**Lemma 6.7.** With high probability, for every center \( c_i \), it is the case that the estimated weight \( w'_i \) computed by the weighting algorithm is \((1 \pm 2\epsilon)w_i^f \) where \( w_i^f \) is the fractional weight of \( i \).

**Proof.** Apply union of bounds to Lemma \( 6.2 \) and \( 6.4 \) over all \( i \) and \( j \).
Fix a center $c_i$. Consider all of the points that are closest to $c_i$ and are not undersampled. Let $w_i^p$ denote the number of these points. All the incoming edges to $c_i$ in $G$, are coming from these points; therefore based on Lemma 6.6, $w_i^p = |w_i^p| \leq \sqrt{1 + 2\log(\frac{N}{\epsilon})}$. On the other hand, $w_i^p$ is $(1 + \epsilon)$ approximation of $w_i^*$.

Therefore, $\frac{1 - \epsilon}{1 + \epsilon} w_i^p \leq w_i^p \leq (1 + \epsilon)w_i^p$. Assuming that $\log N$ is sufficiently larger than $\epsilon$, the lemma follows.

### 6.4 Comparing Fractional Weights to Optimal

Next we bound the total cost of the fractional assignment defined by the flow. According to the graph $G$, any point $p \in S$ and $c_i \in C$, we let $\omega(p, c_i)$ be the fraction of weights that got transferred from $p$ to $c_i$. Naturally we have $\sum_{c_i \in C} \omega(p, c_i) = 1$ for any $p \in S$ and the fractional weights $w_i^p = \sum_{p \in S} \omega(p, c_i)$ for any $c_i \in C$.

**Lemma 6.8.** Let $\phi_{opt}$ be the optimal $k$-means cost on the original set $S$. With high probability, it is the case that:

$$\sum_{p \in S} \sum_{c_i \in C} \omega(p, c_i) ||p - c_i||^2 \leq 160(1 + \epsilon)\phi_{opt}$$

**Proof.** Let $\phi^* = \sum_{p \in S} ||p - c_{\alpha(p)}||^2$. Consider any $p \in S$ and center $c_i$ such that $\omega(p, c_i) > 0$. Let $P$ be any path from $p$ to $c_i$ in $G$. If node $p$’s only outgoing arc is to its closest center $c_{\alpha(p)} = c_i$, then $P = p \rightarrow c_i$, we have $\sum_{c_i} \omega(p, c_i)||p - c_i||^2 = ||p - c_{\alpha(p)}||^2$. Otherwise assume $P = p \rightarrow q_1 \rightarrow q_2 \rightarrow \ldots \rightarrow q_k \rightarrow c_i$. Note that the closest center to $q_k$ is $c_i$. Let $\Delta(P)$ be the fraction of the original weight of 1 on $p$ that is given to $c_i$ along this path according to the flow of weights. As we observed in the proof of Lemma 6.1, we have $\Delta(p) \geq ||p - c_{\alpha(p)}||^2 \geq \Delta_1(p)$.

We make use of the relaxed triangle inequality for squared $\ell_2$ norms. For any three points $x, y, z$, we have $||x - z||^2 \leq 2(||x - y||^2 + ||y - z||^2)$. Thus, we bound $||p - c_i||^2$ by

$$||p - c_i||^2 = ||p - c_{\alpha(p)} + c_{\alpha(p)} - q_1 + q_1 - c_i||^2$$

$$\leq 2 ||p - c_{\alpha(p)} + c_{\alpha(p)} - q_1||^2 + 2 ||q_1 - c_i||^2$$

[relaxed triangle inequality]

$$\leq 2(||p - c_{\alpha(p)}|| + ||c_{\alpha(p)} - q_1||^2) + 2 ||q_1 - c_i||^2$$

[triangle inequality]

$$\leq 8 ||p - c_{\alpha(p)}||^2 + 2 ||q_1 - c_i||^2$$

Applying the prior steps to each $q_j$ gives the following.

$$||p - c_i||^2 \leq 8(||p - c_{\alpha(p)}||^2 + \sum_{j=1}^t 2^j ||q_j - c_{\alpha(q_j)}||^2)$$

Let $P_q(j)$ be the set of all paths $P$ that reach point $q$ using $j$ edges. If $j = 0$, it means $P$ starts with point $q$. We seek to bound $\sum_{j=0}^{\infty} 2^j \sum_{P \in P_q(j)} \Delta(P)||q - c_{\alpha(q_j)}||^2$. This will bound the charge on point $q$ above over all path $P$ that contains it.

Define a weight function $\Delta'(p)$ for each node $p \in S \setminus C$. This will be a new flow of weights like $\Delta$, except now the weight increases at each node. In particular, give each node initially a weight of 1. Let $\Delta'(p)$ be the total weight leaving $p$. This will be evenly divided among the nodes that have outgoing edges from $p$. Define $\Delta'(p)$ to be the weight incoming to $p$ from all other nodes plus one, the initial weight of $p$. Set $\Delta'(p)$ to be $2\Delta(p)$, twice the incoming weight.

Lemma 6.6 implies that the maximum weight of any point $p$ is $\Delta'(p) \leq 1 + \frac{4}{\log N}$. Further notice that for any $q$ it is the case that $\Delta'(q) = \sum_{j=0}^{\infty} 2^j \sum_{P \in P_q(j)} \Delta(P)$. Letting $P(p, c_i)$ be the set of all paths that start at $p$ to center $c_i$. Notice such paths correspond to how $p$’s unit weight goes to $c_i$. We have $\omega(p, c_i) = \sum_{P \in P(p,c_i)} \Delta(P)$. Let $P$ denote the set of all paths, $\ell(P)$ denote the length of path $P$ (number of edges on $P$), and let $P(j)$ denote the $j$th node on path $P$. Thus we have the following.
\[
\sum_{p \in S} \sum_{c_i \in C} \omega(p, c_i) ||p - c_i||^2
\]

\[
= \sum_{p \in S} \sum_{c_i \in C} \sum_{P \in P(p, c_i)} \Delta(P)||p - c_i||^2
\]

\[
\leq 8 \sum_{p \in S} \sum_{c_i \in C} \sum_{P \in P(p, c_i)} \Delta(P) \left( \sum_{j=0}^{\ell(p) - 1} 2^j ||P(j) - c_{\alpha(P(j))}||^2 \right)
\]

\[
= \sum_{P \in \mathcal{P}} 8 \sum_{q \in S} 2^j \Delta(P)||q - c_{\alpha(q)}||^2
\]

\[
= \sum_{q \in S} 8(1 + \frac{4}{\log N}) ||q - c_{\alpha(q)}||^2 = 8(1 + \frac{4}{\log N}) \phi^*
\]

Lemma 6.8 follows because if \( k' \geq 1067k \log N \), \( \phi^* \leq 20\phi_{\text{opt}} \) with high probability by Theorem 1 in [8].

Finally, we prove that finding any \( O(1) \)-approximation solution for optimal weighted \( k \)-means on the set \((C, W')\) gives a constant approximation for optimal \( k \)-means for the original set \( S \). Let \( W' = \{w'_1, \ldots, w'_k\} \) be the fractional weights for centers in \( C \). Let \( \phi'_{W'} \) denote the optimal weighted \( k \)-means cost on \((C, W')\), and \( \phi_{W'} \) denote the optimal weighted \( k \)-means cost on \((C, W')\). We first prove that \( \phi'_{W'} = O(1)\phi_{\text{opt}} \), where \( \phi_{\text{opt}} \) denote the optimal \( k \)-means cost on set \( S \).

**Lemma 6.9.** Let \((C, W')\) be the set of points sampled and the weights collected by fractional assignment \( \omega \). With high probability, we have \( \phi'_{W'} = O(1)\phi_{\text{opt}} \).

**Proof.** Consider the cost of the fractional assignment we’ve designed. For \( c_i \in C \), the weight is \( w'_i = \sum_{p \in S} \omega(p, c_i) \). Denote the \( k \)-means cost of \( \omega \) by \( \phi_{\omega} = \sum_{p \in S} \sum_{c \in C} \omega(p, c)||p - c||^2 \). By Lemma 6.8 we have that \( \phi_{\omega} \leq 160(1 + \epsilon)\phi_{\text{opt}} \).

Intuitively, in the following we show \( \phi'_{W'} \) is close to \( \phi_{\omega} \). As always, we let \( C_{\text{opt}} \) denote the optimal centers for \( k \)-means on set \( S \). For set of points \( X \) with weights \( Y : X \to \mathbb{R}^+ \) and a set of centers \( Z \), we let \( \phi(X, Y)(Z) = \sum_{x \in X} Y(x) \min_{z \in Z} \|x - z\|^2 \) denote the cost of assigning the weighted points in \( X \) to their closest centers in \( Z \). Note that \( \phi'_{W'} \leq \phi_{(C, W')}(C_{\text{opt}}) \) since \( C_{\text{opt}} \) is chosen with respect to \( S \).

\[
\phi'_{W'} \leq \phi_{(C, W')}(C_{\text{opt}})
\]

\[
= \sum_{c_i \in C} \left( \sum_{p \in S} \omega(p, c_i) \right) \min_{c \in C_{\text{opt}}} \|c_i - c\|^2
\]

\[
= \sum_{c_i \in C} \sum_{p \in S} \min_{c \in C_{\text{opt}}} \omega(p, c_i)||c_i - c||^2
\]

\[
\leq \sum_{c_i \in C} \sum_{p \in S} \min_{c \in C_{\text{opt}}} \omega(p, c_i) \cdot 2(||p - c_i||^2 + ||p - c||^2)
\]

[relaxed triangle inequality]

\[
= 2\phi_{\omega} + 2\phi_{\text{opt}} \leq 322(1 + \epsilon)\phi_{\text{opt}}
\]
Using the mentioned lemmas, we can prove the final approximation guarantee.

**Proof of Theorem 5.1.** Using Lemma 6.7, we know \(w_i' = (1 \pm 2\epsilon)w_i^f\) for any center \(c_i\). Let \(C_k'\) be \(k\) centers for \((C, W')\) that is a \(\gamma\)-approximate for optimal weighted \(k\)-means. Let \(C_{OPT}'\) be the optimal \(k\) centers for \((C, W')\), and \(C_{OPT}'\) optimal for \((C, W')\). We have \(\phi_{(C, W')}(C_{OPT}') \leq (1 + 2\epsilon)\phi_{(C, W')}(C_k')\) for the reason that the contribution of each point grows by at most \((1 + 2\epsilon)\) due to weight approximation. Using the same analysis, \(\phi_{(C, W')}(C_{OPT}') \leq (1 + 2\epsilon)\phi_{W'}\).

Combining the two inequalities, we have

\[
\phi_{(C, W')}(C_{OPT}') \leq (1 + 2\epsilon)^2\phi_{(C, W')}(C_{OPT}') \leq (1 + 2\epsilon)^2\gamma\phi_{W'} \tag{4}
\]

Let \(\phi_S(C_k') = \sum_{p \in S} \min_{c \in C_k'} \|p - c\|^2\). For every point \(p \in S\), to bound its cost \(\min_{c \in C_k'} \|p - c\|^2\), we use multiple relaxed triangle inequalities for every center \(c_i \in C\), and take the weighted average of them using \(\omega(p, c_i)\).

\[
\phi_S(C_k') = \sum_{p \in S} \min_{c \in C_k'} \|p - c\|^2 = \sum_{p \in S} \sum_{c \in C_k'} \omega(p, c_i) \min_{c \in C_k'} \|p - c\|^2 \tag{\[\sum_{c \in C} \omega(p, c_i) = 1\]}
\]

\[
\leq \sum_{p \in S} \sum_{c \in C_k'} \omega(p, c_i) \min_{c \in C_k'} 2\|p - c_i\|^2 + \|c_i - c\|^2 \tag{\text{relaxed triangle inequality}}
\]

\[
= 2\phi_\omega + 2\phi_{(C, W')}(C_k') \tag{\[\sum_{p \in S} \omega(p, c_i) = w_i^f\]}
\]

\[
\leq 2\phi_\omega + 2 \cdot 322\gamma(1 + 2\epsilon)^4\phi_{OPT} \tag{\text{inequality (4)}}
\]

\[
\leq 2 \cdot 160(1 + \epsilon)\phi_{OPT} + 2 \cdot 322\gamma(1 + 2\epsilon)^4\phi_{OPT} \tag{Lemma 6.8}
\]

\[
= O(\gamma)\phi_{OPT}
\]

\[\square\]

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A Relational Implementation of 3-means++

Recall that the 3-means++ algorithm picks a point \( x \) to be the third center \( c_3 \) with probability \( P(x) = \frac{L(x)}{Y} \) where \( L(x) = \min(\|x - c_1\|_2^2, \|x - c_2\|_2^2) \) and \( Y = \sum_{x \in J} L(x) \) is a normalizing constant. Conceptually think of \( P \) as being a 'hard' distribution to sample from.

**Description of the Implementation:** The implementation first constructs two identically-sized axis-parallel hypercubes/boxes \( b_1 \) and \( b_2 \) centered around \( c_1 \) and \( c_2 \) that are as large as possible subject to the constraints that the side lengths have to be non-negative integral powers of 2, and that \( b_1 \) and \( b_2 \) can not intersect. Such side lengths could be found since we may assume \( c_1 \) and \( c_2 \) have integer coordinates or they are sufficiently far away from each other that we can scale them and increase their distance. Conceptually the implementation also considers a box \( b_3 \) that is the whole Euclidean space.

![Figure 1: Boxes used for sampling the third center](image)

To define our “easy” distribution \( Q \), for each point \( x \) define \( R(x) \) to be

\[
R(x) = \begin{cases} 
\|x - c_1\|_2^2 & x \in b_1 \\
\|x - c_2\|_2^2 & x \in b_2 \\
\|x - c_1\|_2^2 & x \in b_3 \text{ and } x \notin b_1 \text{ and } x \notin b_2
\end{cases}
\]

In the above definition, note that when \( x \notin b_1 \) and \( x \notin b_2 \), the distance of \( x \) to both centers are relatively similar; therefore, we can assign \( x \) to either of the centers – here we have assigned it to \( c_1 \). Then \( Q(x) \) is defined to be \( \frac{R(x)}{Z} \), where \( Z = \sum_{x \in J} R(x) \) is normalizing constant. The implementation then repeatedly samples a point \( x \) with probability \( Q(x) \). After sampling \( x \), the implementation can either (A) reject \( x \), and then resample or (B) accept \( x \), which means setting the third center \( c_3 \) to be \( x \). The probability that \( x \) is accepted after it is sampled is \( \frac{L(x)}{R(x)} \), and thus the probability that \( x \) is rejected is \( 1 - \frac{L(x)}{R(x)} \).

It is straightforward to see how to compute \( b_1 \) and \( b_2 \) (note that \( b_1 \) and \( b_2 \) can be computed without any relational operations), and how to compute \( L(x) \) and \( R(x) \) for a particular point \( x \). Thus, the only non-straight-forward part is sampling a point \( x \) with probability \( Q(x) \), which we explain now:

- The implementation uses a SumProd query to compute the aggregate 2-norm squared distance from \( c_1 \) constrained to points in \( b_3 \) (all the points) and grouped by table \( T_1 \) using Lemma 3.3. Let the resulting vector be \( C \). So \( C_r \) is the aggregate 2-norm squared distance from \( c_1 \) of all rows in the design matrix that are extensions of row \( r \) in \( T_1 \).

- Then the implementation uses a SumProd query to compute the aggregated 2-norm squared distance from \( c_2 \), constrained to points in \( b_2 \), and grouped by \( T_1 \). Let the resulting vector be \( D \). Notice that an axis-parallel box constraint can be expressed as a collection of axis-parallel hyperplane constraints, and for every axis-parallel constraint it is easy to remove the points not satisfying it from the join by filtering one of the input tables having that dimension/feature. Then the sum product query is the same as the sum product query in the previous step.
• Then the implementation uses a SumProd query to compute the aggregated 2-norm squared distance from $c_1$, constrained to points in $b_2$, and grouped by $T_1$. Let the resulting vector be $E$.

• Then pick a row $r$ of $T_1$ with probability proportional to $C_r - E_r + D_r$.

• The implementation then replaces $T_1$ by a table consisting only of the picked row $r$.

• The implementation then repeats this process on table $T_2$, then table $T_3$ etc.

At the end $J$ will consist of one point/row $x$, where the probability that a particular point $x$ ends up as this final row is $Q(x)$. To see this note that in the iteration performed for $T_i$, $C - E$ is the aggregate 2-norm squared distances to $c_1$ for all points not in $b_2$ grouped by $T_i$, and $D$ is the aggregated squared distances of the points in $b_2$ to $c_2$ grouped by $T_i$.

We now claim that this implementation guarantees that $c_3 = x$ with probability $P(x)$. We can see this using the standard rejection sampling calculation. At each iteration of sampling from $Q$, let $S(x)$ be the event that point $x$ is sampled and $A(x)$ be the event that $x$ is accepted. Then,

$$\Pr[S(x) \text{ and } A(x)] = \Pr[A(x) \mid S(x)] \cdot \Pr[S(x)] = \frac{L(x)}{R(x)} Q(x) = \frac{L(x)}{Z},$$

Thus $x$ is accepted with probability proportional to $L(x)$, as desired.

As the number of times that the implementation has to sample from $Q$ is geometrically distributed, the expected number of times that it will have to sample is the inverse of the probability of success, which is $\max_x \frac{R(x)}{L(x)}$. It is not too difficult to see (we prove it formally in Lemma 4.3) that $\max_x \frac{R(x)}{L(x)} = O(d)$. It takes $3m$ SumProd queries to sample from $Q$. Therefore, the expected running time of our implementation of 3-means++ is $O(md\Psi(n, d, m))$.

### B Pseudo-code

In this section you may find the algorithms explained in Section 4 in pseudo-code format.

**Algorithm 1** Algorithm for creating axis-parallel hyperrectangles

1: procedure **CONSTRUCT BOXES**($C_{i-1}$)
2: Input: Current centers $C_{i-1} = \{c_1, \ldots, c_{i-1}\}$
3: Output: $B_i$, a set of boxes and their centers
4: $B_i \leftarrow \emptyset$
5: $G_i \leftarrow \{(b_j^*, c_j) \mid b_j^* \text{ is a unit size hyper-cube around } c_j, j \in [i-1]\}$ ◆ We assume there is no intersection between the boxes in $G$ initially, up to scaling
6: while $|G_i| > 1$ do
7: Double all the boxes in $G_i$.
8: $G_i' = \emptyset$ ◆ Keeps the boxes created in this iteration of doubling
9: while $\exists (b_1, y_1), (b_2, y_2) \in G_i$ that intersect with each other do
10: $b \leftarrow$ the smallest box in Euclidean space containing $b_1$ and $b_2$.
11: $G_i \leftarrow (G_i \setminus \{(b_1, y_1), (b_2, y_2)\}) \cup \{(b, y_1)\}$
12: $G_i' \leftarrow (G_i' \cup \{(b, y_1)\}$
13: if $(b_1, y_1) \notin G_i'$ then ◆ Check if box $b_1$ hasn’t been merged with other boxes in the current round
14: $b_1' \leftarrow$ halved $b_1$, add $(b_1', y_1)$ to $B_i$
15: if $(b_2, y_2) \notin G_i'$ then ◆ Check if box $b_2$ hasn’t been merged with other boxes in the current round
16: $b_2' \leftarrow$ halved $b_2$, add $(b_2', y_2)$ to $B_i$
17: There is only one box and its representative remaining in $G_i$, replace this box with the whole Euclidean space.
18: $B_i \leftarrow B_i \cup G_i'$
19: Return $B_i$. 

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## C Omitted Proofs

### NP-Hardness of Approximating Cluster Size

**Proof of [Theorem 1.2]**

We’ve proved the \#P-hardness in the main body. Here we prove the second part of Theorem 1.2 that given an acyclic database and a set of centers \(c_1, \ldots, c_k\), it is NP-Hard to approximate the number of points assigned to each center when \(k \geq 3\). We prove it by reduction from Subset Sum. In Subset Sum problem, the input is a set of integers \(A = w_1, \ldots, w_m\) and an integer \(L\), the output is true if there is a subset of \(A\) such that its summation is \(L\). We create the following acyclic schema. There are \(m\) tables. Each table \(T_i\) has a single unique column \(x_i\) with two rows \(w_i, 0\). Then the join of the tables has \(2^m\) rows, and it is a cross product of the rows in different tables in which each row represents one subset of \(A\).

Then consider the following three centers: \(c_1 = (\frac{L-1}{m}, \frac{L-1}{m}, \ldots, \frac{L-1}{m})\), \(c_2 = (\frac{L}{m}, \ldots, \frac{L}{m})\), and \(c_1 = (\frac{L+1}{m}, \frac{L+1}{m}, \ldots, \frac{L+1}{m})\). The Voronoi diagram that separates the points assigned to each of these centers consists of two parallel hyperplanes: \(\sum x_i = L - 1/2\) and \(\sum x_i = L + 1/2\) where the points between the two hyperplanes are the points assigned to \(c_2\). Since all the points in the design matrix have integer coordinates, the only points that are between these two hyperplanes are those points for which \(\sum x_i = L\). Therefore, the approximation for the number of points assigned to \(c_2\) is non-zero if and only if the answer to Subset Sum is True.

**Algorithm 2** Algorithm for sampling the next center

```plaintext
1: procedure KMMeans++Sample\((C_{i-1}, T_1, \ldots, T_m)\)
2:     Let \(p(b)\) be the box that is the parent of \(b\) in the tree structure of all boxes in \(B_i\).
3:     \(c_i \leftarrow \emptyset\)
4:     \(B_i \leftarrow \text{Construct Boxes}(C_{i-1})\)
5:     Let \((b_0, y_0)\) be the tuple where \(b_0\) is the entire Euclidean space in \(B_i\).
6:     \(\text{while } c_i = \emptyset \text{ do} \quad \triangleright \text{Sample one row from each table.}
7:         \text{for } 1 \leq \ell \leq m \text{ do}
8:             \(H_{r} \leftarrow \text{vector having an entry } H_{r} \text{ for each } r \in T_{\ell}.
9:         \) Focus on only the rows in \(J\) that uses all previously sampled rows from \(T_1, \ldots, T_{\ell-1}\) in the concatenation.
10: \(\forall r \in T_{\ell} \text{ evaluate } H_{r} \leftarrow \sum_{x \in \mathbb{R}^{n}, J \cap \emptyset} ||x - y_0||^2_2\)
11: \(\text{for } (b, y) \in B_i \setminus \{(b_0, y_0)\} \text{ do}
12:         \(H_{r} \leftarrow H_{r} - \sum_{x \in \mathbb{R}^{n}, J \cap \emptyset} ||x - y'||^2_2 + \sum_{x \in \mathbb{R}^{n}, J \cap \emptyset} ||x - y||^2_2\)
13:         \(\text{Sample a row } r_{\ell} \in T_{\ell} \text{ with probability proportional to } H_{r}.
14:         \) \(x \leftarrow r_{1} \times \cdots \times r_{m}\).
15:     \(\text{Let } (b^*, y^*) \text{ be the tuple where } b^* \text{ is the smallest box in } B_i \text{ containing } x.
16:     \(c_i \leftarrow x \text{ with probability } \frac{\min_{c \in C_{i-1}} ||x - c||^2_2}{||x - y^*||^2_2}. \triangleright \text{Rejection sampling.}
17: \) return \(c_i\).
```

### Uniform Sampling From a Hypersphere

In order to uniformly sample a point from inside a ball, it is enough to show how we can count the number of points located inside a ball grouped by a table \(T_i\). Because, if we can count the number of points grouped by input tables, then we can use similar technique to the one used in Section 4 to sample. Unfortunately, as we discussed in Section 2 it is \#P-Hard to count the number of points inside a ball; however, it is possible to obtain a \(1 \pm \delta\) approximation of
the number of points \[3\]. Bellow we briefly explain the algorithm in \[3\] for counting the number of points inside a hypersphere.

Given a center \(c\) and a radius \(R\), the goal is approximating the number of tuples \(x \in J\) for which \(\sum_{i}(c_i - x_i)^2 \leq R\). Consider the set \(S\) containing all the multisets of real numbers. We denote a multiset \(A\) by a set of pairs of \((v, f_A(v))\) where \(v\) is a real value and \(f(v)\) is the frequency of \(v\) in \(A\). For example, \(A = \{(2.3, 10), (3.5, 1)\}\) is a multiset that has 10 members with value 2.3 and 1 member with value 3.5. Then, let \(\oplus\) be the summation operator meaning \(C = A \oplus B\) if and only if for all \(x \in R\), \(f_C(x) = f_A(x) + f_B(x)\), and let \(\otimes\) be the convolution operator such that \(C = A \otimes B\) if and only if \(f_C(x) = \sum_{i \in R} f_A(i) + f_B(x - i)\). Then the claim is \((S, \oplus, \otimes)\) is a commutative semiring and the following SumProd query returns a multiset that has all the squared distances of the points in \(J\) from \(C\):

\[
\bigoplus_{x \in J} \otimes \{(x_i^2 - c_i^2, 1)\}
\]

Using the result of the multiset, it is possible to count exactly the number of tuples \(x \in J\) for which \(\|x - c\|_2^2 \leq R^2\). However, the size of the result is as large as \(\Omega(|J|)\).

In order to make the size of the partial results and time complexity of \(\oplus\) and \(\otimes\) operators polynomial, the algorithm uses \((1 + \delta)\) geometric bucketing. The algorithm returns an array where in \(j\)-th entry it has the smallest value \(r\) for which there are \((1 + \delta)\) tuples \(x \in J\) satisfying \(\|x - c\|_2^2 \leq r^2\).

The query can also be executed grouped by one of the input tables. Therefore, using this polynomial approximation scheme, we can calculate conditioned marginalized probability distribution with multiplicative \((1 + \delta)\). Therefore, using \(m\) queries, it is possible to sample a tuple from a ball with probability distribution \(\frac{n}{2}(1 \pm m\delta)\) where \(n\) is the number of points inside the ball. In order to get a sample with probability \(\frac{1}{n}(1 \pm \epsilon)\), all we need is to set \(\delta = \frac{\epsilon}{m}\); hence, on \(3\), the time complexity for sampling each tuple will be \(O\left(\frac{m^2 \log^2(n)}{\epsilon^2} \Psi(n, d, m)\right)\).

### E Hardness of Lloyd’s Algorithm

After choosing \(k\) initial centers, a type of local search algorithm, called Lloyd’s algorithm, is commonly used to iteratively find better centers. After associating each point with its closest center, and Lloyd’s algorithm updates the position of each center to the center of mass of its associated points. Meaning, if \(X_c\) is the set of points assigned to \(c\), its location is updated to \(\frac{\sum_{x \in X_c} x}{|X_c|}\). While this can be done easily when the data is given explicitly, we show in the following theorem that finding the center of mass for the points assigned to a center is \(\#P\)-hard when the data is relational, even in the special case of an acyclic join and two centers.

**Theorem E.1.** Given an acyclic join, and two centers, it is \(\#P\)-hard to compute the center of mass for the points assigned to each center.

**Proof.** We prove by a reduction from a decision version of the counting knapsack problem. The input to the counting knapsack problem consists of a the set \(W = \{w_1, \ldots, w_n\}\) of positive integer weights, a knapsack size \(L\), and a count \(D\). The problem is to determine whether there are at least \(D\) subsets of \(W\) with aggregate weight at most \(L\). The points in our instance of \(k\)-means will be given relationally. We construct a join query with \(n + 1\) columns/attributes, and \(n\) tables. All the tables have one column in common and one distinct column. The \(i\)-th table has 2 columns \((d_i, d_{n+i})\) and three rows \(\{(w_i, -1), (0, -1), (0, D)\}\). Note that the join has \(2^n\) rows with \(-1\) in dimension \(n + 1\), and one row with values \((0, 0, \ldots, 0, D)\). The rows with \(-1\) in dimension \(d + 1\) have all the subsets of \(\{w_1, \ldots, w_n\}\) in their first \(n\) dimensions. Let the two centers for \(k\)-means problem be any two centers \(c_1\) and \(c_2\) such that a point \(x\) is closer to \(c_1\) if it satisfies \(\sum_{d=1}^n x_d < L\) and closer to \(c_2\) if it satisfies \(\sum_{d=1}^n x_d > L\). Note that the row \((0, 0, \ldots, 0, D)\) is closer to \(c_1\). Therefore, the value of dimension \(n + 1\) of the center of mass for the tuples that are closer to \(c_1\) is \(Y = (D - C)/C\) where \(C\) is the actual number of subsets of \(W\) with aggregate weight at most \(L\). If \(Y\) is negative, then the number of solutions to the counting knapsack instance is at least \(D\). \(\square\)
F Background Information About Database Concepts

Given a tuple $x$, define $\Pi_F(x)$ to be projection of $x$ onto the set of features $F$ meaning $\Pi_F(x)$ is a tuple formed by keeping the entries in $x$ that are corresponding to the feature in $F$. For example let $T$ be a table with columns $(A, B, C)$ and let $x = (1, 2, 3)$ be a tuple of $T$, then $\Pi_{(A,C)}(x) = (1, 3)$.

**Definition F.1 (Join).** Let $T_1, \ldots, T_m$ be a set of tables with corresponding sets of columns/features $F_1, \ldots, F_m$ we define the join of them $J = T_1 \bowtie \cdots \bowtie T_m$ as a table such that the set of columns of $J$ is $\bigcup_i F_i$, and $x \in J$ if and only if $\Pi_{F_i}(x) \in T_i$.

Note that the above definition of join is consistent with the definition written in Section 1 but offers more intuition about what the join operation means geometrically.

**Definition F.2 (Join Hypergraph).** Given a join $J = T_1 \bowtie \cdots \bowtie T_m$, the hypergraph associated with the join is $H = (V, E)$ where $V$ is the set of vertices and for every column $a_i$ in $J$ there is a vertex $v_i$ in $V$, and for every table $T_i$ there is a hyper-edge $e_i$ in $E$ that has the vertices associated with the columns of $T_i$.

**Theorem F.3 (AGM Bound [10]).** Given a join $J = T_1 \bowtie \cdots \bowtie T_m$ with $d$ columns and its associated hypergraph $H = (V, E)$, and let $C$ be a subset of $\text{col}(J)$, let $X = (x_1, \ldots, x_m)$ be any feasible solution to the following Linear Programming:

\[
\begin{align*}
\text{minimize} & \quad \sum_{j=1}^m \log(|T_j|)x_j \\
\text{subject to} & \quad \sum_{j: v \in e_j} x_j \geq 1, \quad v \in C \\
& \quad 0 \leq x_j \leq 1, \quad j = 1, \ldots, t
\end{align*}
\]

Then $\prod_i |T_i|^{x_i}$ is an upper bound for the cardinality of $\Pi_C(J)$, this upperbound is tight if $X$ is the optimal answer.

We give another definition of acyclicity which is consistent with the definition in the main body.

**Definition F.4 (Acyclic Join).** We call a join query (or a relational database schema) **acyclic** if one can repeatedly apply one of the two operations and convert the set of tables to an empty set:

1. Remove a column that is only in one table.
2. Remove a table for which its columns are fully contained in another table.

**Definition F.5 (Hyptree Decomposition).** Let $H = (V, E)$ be a hypergraph and $T = (V', E')$ be a tree with a subset of $V$ associated to each vertex in $v' \in V'$ called bag of $v'$ and show it by $b(v') \subseteq V$. $T$ is called a hypertree decomposition of $H$ if the following holds:

1. For each hyperedge $e \in E$ there exists $v' \in V'$ such that $e \subseteq b(v')$
2. For each vertex $v \in E$ the set of vertices in $V'$ that have $v$ in their bag are all connected in $T$.

**Definition F.6.** Let $H = (V, E)$ be a join hypergraph and $T = (V', E')$ be its hypertree decomposition. For each $v' \in V'$, let $X_{v'} = (x_{v'}^1, x_{v'}^2, \ldots, x_{v'}^m)$ be the optimal solution to the following linear program: $\min \sum_{j=1}^m x_j$, subject to $\sum_{j:v \in e_j} x_j \geq 1, \forall v \in b(v')$ where $0 \leq x_j \leq 1$ for each $j \in [t]$. Then the width of $v'$ is $\sum_i x_i^{v'}$ denoted by $w(v')$ and the fractional width of $T$ is $\max_{v' \in V'} w(v')$.

**Definition F.7 (fhtw).** Given a join hypergraph $H = (V, E)$, the fractional hypertree width of $H$, denoted by fhtw, is the minimum fractional width of its hypertree decomposition. Here the minimum is taken over all possible hypertree decompositions.
Observation 1. The fractional hypertree width of an acyclic join is 1, and each bag in its hypertree decomposition is a subset of the columns in some input table.

Theorem F.8 (Inside-out [19]). There exists an algorithm to evaluate a SumProd query in time \(O(Tmd^{2n\text{fhtw}}\log(n))\) where fhtw is the fractional hypertree width of the query and \(T\) is the time needed to evaluate \(\oplus\) and \(\otimes\) for two operands. The same algorithm with the same time complexity can be used to evaluate SumProd queries grouped by one of the input tables.

Theorem F.9. Let \(Q_f\) be a function from domain of column \(f\) in \(J\) to \(\mathbb{R}\), and \(G\) be a vector that has a row for each tuple \(r \in T_i\). Then the query

\[
\sum_{X \in J} \sum_f Q_f(x_f)
\]

can be converted to a SumProd and the query returning \(G\) with definition

\[
G_r = \sum_{X \in Y \setminus J} \sum_f F_i(x_f)
\]

can be converted to a SumProd query grouped by \(T_i\).

Proof. Let \(S = \{(a, b) \mid a \in \mathbb{R}, b \in \mathbb{I}\}\), and for any two pairs of \((a, b), (c, d) \in S\) we define:

\[
(a, b) \oplus (c, d) = (a + c, b + d)
\]

and

\[
(a, b) \otimes (c, d) = (ad + cb, bd).
\]

Then the theorem can be proven by using the following two claims:

1. \((S, \oplus, \otimes)\) forms a commutative semiring with identity zero \(I_0 = (0, 0)\) and identity one \(I_1 = (0, 1)\).

2. The query \(\oplus_{X \in J} \otimes_f (Q_f(x_f), 1)\) is a SumProd FAQ where the first entry of the result is \(\sum_{X \in J} \sum_f Q_f(x_f)\) and the second entry is the number of rows in \(J\).

Proof of the first claim: Since arithmetic summation is commutative and associative, it is easy to see \(\oplus\) is also commutative and associative. Furthermore, based on the definition of \(\oplus\) we have \((a, b) \oplus I_0 = (a + 0, b + 0) = (a, b)\).

The operator \(\otimes\) is also commutative since arithmetic multiplication is commutative, the associativity of \(\otimes\) can be proved by

\[
(a_1, b_1) \otimes ((a_2, b_2) \otimes (a_3, b_3)) = (a_1, b_1) \otimes (a_2b_3 + a_3b_2, b_2b_3)
\]

\[
= (a_1b_2b_3 + b_1a_2b_3 + b_1b_2a_3, b_1b_2b_3)
\]

\[
= (a_1b_2 + b_1a_2, b_1b_2) \otimes (a_3, b_3)
\]

\[
= ((a_1, b_1) \otimes (a_2, b_2)) \otimes (a_3, b_3)
\]

Also note that based on the definition of \(\otimes\), \((a, b) \otimes I_0 = I_0\) and \((a, b) \otimes I_1 = (a, b)\). The only remaining property that we need to prove is the distribution of \(\otimes\) over \(\oplus\):

\[
(a, b) \otimes ((c_1, d_1) \oplus (c_2, d_2)) = (a, b) \otimes (c_1 + c_2, d_1 + d_2)
\]

\[
= (a, b) \oplus (c_1 + c_2, d_1 + d_2)
\]

\[
= (c_1b + c_2b + ad_1 + ad_2, bd_1 + bd_2)
\]

\[
= (c_1b + ad_1, bd_1) \oplus (c_2b + ad_2, bd_2)
\]

\[
= ((a, b) \otimes (c_1, d_1)) \oplus ((a, b) \otimes (c_2, d_2))
\]

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Now we can prove the second claim: To prove the second claim, since we have already shown the semiring properties of \((S, \oplus, \otimes)\) we only need to show what is the result of \(\oplus_{X \in J} \otimes_f (Q_f(x_f), 1)\). We have \(\otimes_f (Q_i(x_f), 1) = (\sum_f Q_i(x_f), 1)\), therefore

\[
\oplus_{X \in J} \otimes_f (Q_i(x_f), 1) = \oplus_{X \in J} (\sum_f Q_f(x_f), 1) = (\sum_{X \in J} \sum_f Q_f(x_f), \sum_{X \in J} 1)
\]

where the first entry is the result of the SumSum query and the second entry is the number of rows in \(J\).