ABSTRACT
We study the problem of efficiently estimating counts for queries involving complex filters, such as user-defined functions, or predicates involving self-joins and correlated subqueries. For such queries, traditional sampling techniques may not be applicable due to the complexity of the filter preventing sampling over joins, and sampling after the join may not be feasible due to the cost of computing the full join. The other natural approach of training and using an inexpensive classifier to estimate the count instead of the expensive predicate suffers from the difficulties in training a good classifier and giving meaningful confidence intervals. In this paper we propose a new method of learning to sample where we combine the best of both worlds by using sampling in two phases. First, we use samples to learn a probabilistic classifier, and then use the classifier to design a stratified sampling method to obtain the final estimates. We theoretically analyze algorithms for obtaining an optimal stratification, and compare our approach with a suite of natural alternatives like quantification learning, weighted and stratified sampling, and other techniques from the literature. We also provide extensive experiments in diverse use cases using multiple real and synthetic datasets to evaluate the quality, efficiency, and robustness of our approach.

1. INTRODUCTION
Counting is a fundamental problem in query processing. Counting queries can be expensive to evaluate, especially if it involves testing a complex predicate to decide whether an object should be counted towards the total. Consider the following example.

**Example 1** (Counting Points with Few Neighbors). Suppose table \( D(x, y) \) stores a set of 2d points, and we would like to count how many points have fewer than \( k \) points within distance \( d \) from them. We can write the following SQL query:

```sql
SELECT COUNT(*) FROM
(SELECT o1.id FROM D o1, D o2
WHERE SQRT(POWER(o1.x-o2.x,2)+POWER(o1.y-o2.y,2)) <= d
GROUP BY o1.id HAVING COUNT(*) <= k);
```

Here, the objects to be counted are produced by a self-join with a complex condition, followed by GROUP BY and HAVING. This “neighborhood” query has been well studied, with specialized index structures and processing algorithms. Still, there is a good chance that a typical database system will perform poorly, either because it has no specialized support for this query type, or it simply fails to recognize this query type from the way the query is written. Thus, making such queries run faster can require a lot of effort and expertise. There are even more complex cases involving expensive user-defined functions commonly found in machine learning workloads. The problem we tackle in this paper is how to evaluate counting queries efficiently, and in a general way.

Approximate answers are widely accepted for such expensive counting queries. Sampling is a powerful technique for producing approximate answers with statistical guarantees, with a long tradition and active research of its applications in databases. Yet sampling for complex queries remains a difficult problem. In general, not all query operators “commute” with sampling. For instance, in Example 1 if we only take a sample of \( D \) and evaluate the query on this sample, it would be difficult to make sense of the result because even the neighbor counts produced by the inner aggregation query would be off to begin with. Worse, if the predicate involves a black-box function with table inputs, we cannot expect sampling input tables to produce usable results.

Still, a viable approach is to conceptually treat the problem as counting the number of objects satisfying a predicate, where the objects can be enumerated or sampled efficiently, but the predicate is complex and expensive (e.g., involving user-defined functions or arbitrarily nested subqueries). We would sample some objects for which we evaluate the predicate “in full,” and then use these results to derive an estimate. For instance, in Example 1 given a point \( o1 \) from \( D \), the predicate would be a query over (full) \( D \) parameterized by the values of \( o1.x \) and \( o2.x \). Of course, evaluating the predicate in full for each sampled object can be expensive, but evaluating the original query as a whole can be much worse—there may be no better way for the database systems to process this query than a nested-loop join. While this sampling-based approach is simple and general, a question is whether we can make it more efficient.

Machine learning is another natural approach to this problem. It has the potential of being more “sample-efficient” because of its ability to generalize to unseen objects. One could draw some samples, pay the cost to “label” them (i.e., evaluate the expensive predicate), and use the labeled samples to learn a cheap classifier that approximates the result of the expensive predicate. The learned classifier can then be applied to objects to obtain an estimated count. Beyond this naive approach, we can apply ideas from quantification learning [6]. However, some difficulties remain: it is hard to offer meaningful statistical guarantees (such as confidence
intervals provided by sampling), and training a good classifier can be difficult and tricky itself (e.g., with challenges such as feature and model selection as well as overfitting).

A natural question is whether we can combine learning and sampling to get the “best of both worlds”: we want the ability to generalize by learning, but at the same time we want the statistical guarantees offered by sampling. This paper answers this question in positive. One idea is to use sampling to assess the errors produced by the learned classifier and correct its estimated count. We also provide a novel alternative that “learns to sample.” The key idea here is not to rely directly on the learned classifier’s predictions, but instead exploit the classifier’s knowledge in a more controlled manner by using it to design a sampling scheme. Then, we apply the sampling scheme to derive our estimates, complete with statistical guarantees. A good classifier leads to an efficient sampling scheme that uses few samples to get low-variance estimates; on the other hand, a poor classifier can lead to a less efficient sampling scheme that needs more samples to achieve the same accuracy, but we will always have unbiased estimates with confidence intervals.

Specifically, we make use of the scores produced by classifiers that reflect how confident they are in their predictions. Such scores are readily available for popular classification methods in standard libraries. A straightforward method is learned weighted sampling, which assigns higher sampling probabilities to objects that are more confidently predicted to contribute to the result count. This method is still sensitive to the scores produced by the classifiers, and tends to focus more on confidently positive objects instead of uncertain objects—but arguably, uncertain objects intuitively provide more information when labeled.

Hence, we further propose learned stratified sampling, which relies even less on the quality of the classifier. Instead of using the values of the scores, we use the scores only to induce an ordering among the objects. Based on this ordering, and with help from some additional samples, we find the optimal stratified sampling design that jointly considers the partitioning of objects into strata and the allocation of additional samples across strata. The score-induced ordering is useful because it brings together objects with similar levels of uncertainty, and in particular encourages putting the certainly positive objects and certainly negative objects into separate strata with low within-stratum variances. The sampling design problem is challenging because of joint consideration of stratification and allocation; we propose algorithms for this optimization problem with trade-offs between speed and optimality.

Our experiments show that our learn-to-sample approach generally outperforms approaches that are based on either sampling or learning alone, or those that apply sampling only to error assessment and correction. We achieve unbiased estimates with lower variances than other approaches, and in practice, the overhead of learning and sampling design is negligible compared with the total cost of evaluating expensive predicates on samples. Moreover, learned stratified sampling delivers robust performance even with poor classifiers. Finally, a key practical advantage of our learn-to-sample approach is that it is easy to implement: its constituent learning and sampling components are available off-the-shelf, so we readily benefit from both the classic sampling literature and a growing toolbox of classification algorithms. For example, for our experiments, we were able to apply standard classification algorithms out-of-box with very little tuning, thanks to the robustness of the learn-to-sample approach.

2. PROBLEM DEFINITION

Consider a set of objects \( O \), and a Boolean predicate \( q : O \rightarrow \{0, 1\} \), where 1 denotes true. We say an object \( o \) is positive if \( q(o) = 1 \), or negative if \( q(o) = 0 \). Our goal is to estimate \( C(O, q) \), the number of positive objects in \( O \); i.e., \( C(O, q) = \sum_{o \in O} q(o) \).

In general, each object \( o \) can have a complex structure (with multiple attributes including set-valued ones), and \( q(o) \) can be arbitrarily complex (e.g., accessing related information beyond the contents of \( o \), comparing \( o \) with other objects in \( O \), etc.).

We make two assumptions: 1) evaluation of \( q \) is costly; 2) members of \( O \) can be efficiently enumerated. The terms “costly” and “efficient,” of course, are relative. While the techniques in this paper do not depend on these assumptions for correctness, our proposed approach is intended for situations where these assumptions hold. For example, a costly \( q \) would make it attractive to use sampling to avoid evaluating \( q \) for all objects, or to use a learned model that predicts the outcome of \( q \) at a lower cost.

It should be obvious that the problem formulation above handles single-table selection queries whose conditions potentially involve expensive user-defined functions. The problem formulation is also general enough to capture more complex queries. The first example below illustrates the case where \( q \) is a complex SQL condition involving an aggregate subquery; the second illustrates the case where \( q \) involves a black-box function.

**Example 2 (k-skyband size).** Consider a set of 2d points in table \( D(id, x, y) \). A point \( q \) dominates another point \( p \) if \( p \)’s \( x \) and \( y \) values are (resp.) no less than those of \( p \) (i.e., \( p.x \geq q.x \land p.y \geq q.y \)), and at least one of them is strictly greater (i.e., \( p.x > p.q.x \land p.y > p.q.y \)). The so-called k-skyband for the point set \( D \) is the subset of points that are dominated by fewer than \( k \) others. Given \( o \in D \), we define \( q(o) \) to test its membership in the k-skyband using the following SQL condition:

\[
\text{(SELECT COUNT(*) FROM } D \text{ WHERE } \sum_0^q \text{ AND } y \text{ OR } 0 < k \text{) }
\]

Note that this predicate involves an aggregate subquery parameterized by \( o \). The number of points in the k-skyband is then the number of points satisfying \( q \). Here, object enumeration is efficient (just scan \( D \)), while predicate evaluation is costly in comparison (without specialized indexes).

Alternatively, we can write the whole k-skyband size query using a self-join and nested aggregation, without explicitly referring to \( q \):

\[
\text{(SELECT COUNT(*) FROM (SELECT o1.id FROM D o1, D o2 WHERE o2.x > o1.x AND o2.y > o1.y \text{ AND (o2.x > o1.x OR o2.y > o1.y)) < k}) }
\]

**Example 3 (relevant document count).** Consider a set of documents in table \( D(id, text) \). Each document, based on the content of its \( text \), can be associated with zero or more labels from a predefined set of labels of interest. For example, during electronic discovery for a legal proceeding, \( D \) can be a set of emails and documents, and one such label may indicate whether a document is in support of or against a particular action. Let \( labels(text) \) denote a function that examines a document and returns the subset of labels that it is associated with. We mark a document as highly relevant if it is associated with at least \( k \) labels. The following query returns the number of highly relevant documents:

\[
\text{(SELECT COUNT(*) FROM D WHERE \text{len(labels(o.text))} > k)}
\]

Here, \( q \) is the \( WHERE \) predicate, but it involves a complex black-box function \( labels \) whose evaluation can be very expensive. For example, if labels are highly specialized for a given proceeding, there may not exist good automated labeling procedures and we would have to evaluate \( labels \) manually. In general, the predicate
that determines whether a document is relevant can be even more complicated than counting how many labels it is associated with, but our problem formulation and solutions are designed to work with arbitrarily complicated \( q \).

### Handling More General SQL Queries

An observant reader will notice the similarity between the last query in Example 2 and the one counting points with few neighbors in Example 1. Despite the latter query’s lack of an explicit per-object predicate, it is not hard to see that we can define \( q(o) \) for \( o \in D \) as the following complex SQL condition involving an aggregate subquery (analogous to Example 2 above):

\[
\text{(SELECT COUNT(*) FROM D WHERE SQRT(POWER(o.x-x,2)+POWER(o.y-y,2)) <= d) <= k)}
\]

More generally, suppose we are interested in counting the number of results for the following SQL aggregate query:

\[
\text{SELECT } \theta \text{ FROM L, R -- (Q1) WHERE } \theta_L, \theta_{LR} \text{ GROUP BY } G_L \text{ HAVING } \phi;
\]

In the above, \( G_L \) is the list of group by columns, \( L \) denotes the list of tables with columns in \( G_L \), and \( R \) denotes the list of other tables in the join with no group-by-columns; \( \theta_L \) refers to the part of the \( WHERE \) condition that be evaluated over \( L \) alone, \( \theta_{LR} \) refers to the remaining part of the \( WHERE \) condition, and \( \phi \) refers to the \( HAVING \) condition; finally, \( E \) is the list of output expressions for each group. The problem of counting the number of results can be formulated by defining the set \( O \) of objects as:

\[
\text{SELECT DISTINCT } G_L \text{ FROM } L, R -- (Q2) \text{ and the predicate } q(o) \text{ as:}}
\]

\[
\text{exists (SELECT } G_L \text{ FROM } L, R -- (Q3) \text{ WHERE } \theta_{LR} \text{ AND } G_L \neq \theta_L \text{ GROUP BY } G_L \text{ HAVING } \phi).
\]

Again, the key takeaway is that our problem formulation is general enough to support complex queries involving joins and aggregates (besides the final counting). Our approach works well as long as the set of objects is cheap to enumerate (i.e., the local selection \( \theta_L \) in (Q2) is easy to evaluate), while the per-object predicate (Q3) is relatively expensive (which is usually the case because of join and aggregation).

### 3. BASELINE METHODS

We present a number of baseline methods for estimating \( C(O, q) \). While these methods are not new, we note that some connections to our problem (e.g., quantification learning and sampling-based data cleaning) have never been made explicit or evaluated previously.

#### 3.1 Sampling-Based Methods

##### Simple Random Sampling (SRS)

The problem of estimating \( C(O, q) \) using sampling has been studied extensively in the context of estimating proportions \([24]\). A straightforward method is simple random sampling (SRS). Let \( S \subseteq O \) denote the set of \( n \) objects drawn randomly without replacement from the set \( O \) of all \( N \) objects. For each \( o \in S \), we evaluate \( q(o) \). Then, an unbiased estimator of \( C(O, q) \) is \( \hat{p}N \), where the estimated proportion

\[
\hat{p} = \frac{1}{n} \sum_{o \in S} q(o)
\]

There are a number of ways to derive a confidence interval for this estimation. The most popular one is the Wald interval, which approximates the error distribution using a normal distribution: the \( (1 - \alpha) \) confidence interval for \( \hat{p} \) in this case is

\[
\hat{p} \pm z_{\alpha/2} \sqrt{\frac{\hat{p}(1-\hat{p})}{n}} \cdot \frac{N-n}{N-1}.
\]

The usual caveats apply: if \( q \) is highly selective or highly non-selective, the Wald interval is unreliable because normal distribution approximation fails; one can use the more reliable Wilson interval instead. See standard sampling literature \([24]\) for details.

##### Stratified Sampling (SSP and SSN)

Stratified sampling is a method that works especially well when the overall population can be divided into subpopulations (straata) where objects are homogeneous within each stratum. For example, if there is a way to divide \( O \) into two strata where one contains mostly positive objects and the other contains mostly negative objects, we can sample the two strata independently and use much fewer samples overall than SRS to achieve the same confidence interval. The problem, of course, is that we do not know the outcome of each \( q(o) \) unless we first evaluate it. A practical solution is to choose some attributes of \( o \) whose values are readily available and likely correlated with the outcome of \( q(o) \); we can then stratify \( O \) according to these surrogates.

In our case, a natural choice for surrogates would be the attributes of \( o \) used in computing \( q(o) \); e.g., for Example 1 we would choose \( x \) and \( y \) and grid the 2d space into the desired number of strata.

Suppose we are given a partitioning of \( O \) into \( H \) strata \( O_1, O_2, \ldots, O_H \), where \( N_h = |O_h| \) denotes the size of each stratum \( h \), and an allocation of samples \( n_1, n_2, \ldots, n_H \), where \( n_h \) is the number of samples allotted to stratum \( h \). Stratified sampling randomly draws the allotted number of samples from each stratum; denote these samples by \( S_h = \cup_{h=1}^{H} S_h \), where \( n_h = |S_h| \). For each stratum \( h \), using \( S_h \), we can derive an unbiased estimator for the proportion \( \hat{p}_h \) of positive objects therein (as described for SRS above). Then, an unbiased estimator of \( C(O, q) \) is \( \hat{p}N \), where

\[
\hat{p} = \sum_{h=1}^{H} W_h \hat{p}_h
\]

is the estimated overall proportion and \( W_h = n_h/N_h \) is the weight of stratum \( h \). The variance in \( \hat{p} \) is

\[
\text{Var}(\hat{p}) = \sum_{h=1}^{H} \frac{W_h^2 S_h^2}{n_h} - \frac{n}{\sum_{h=1}^{H} W_h S_h^2},
\]

where \( S_h \) is the standard deviation of \( n_h \) (i.e., of the multiset \( \{q(o) \mid o \in O_h\} \)). The \( (1 - \alpha) \) confidence interval for \( \hat{p} \) is

\[
\hat{p} \pm z_{\alpha/2} \sqrt{\text{Var}(\hat{p})} \cdot \frac{N-n}{N-1}.
\]

A simple strategy is proportional allocation, where the number of samples allotted to each stratum is proportional to its size, i.e., \( n_h \propto N_h \). We refer to stratified sampling with proportional allocation as SSP. A more sophisticated alternative, Neyman allocation, optimally allocates samples according to \( n_h \propto N_h S_h \), which minimizes \( \text{Var}(\hat{p}) \). We refer to this alternative as SSN. In practice, as we do not know \( S_h \) in advance, SSN proceeds in two stages:

1. Randomly draw a set \( S' \) of samples to evaluate \( q \) with, and use them to derive an estimate of \( S_h \) for each stratum \( h \). Then calculate the Neyman allocation using these estimates.
2. Randomly draw the allotted number of samples from each stratum.

#### 3.2 Learning-Based Methods

Since \( q \) is expensive to evaluate, it is natural to consider learning a binary classifier \( f: O \rightarrow \{0, 1\} \) to approximate the behavior of

1. Standard caveats apply: given the desired total number of samples, we ensure that no stratum is allotted more samples than it contains, and that no stratum is allotted fewer than a prescribed minimum number of samples (even if its estimated standard deviation is close to 0); we do so by rebalancing the allocation after meeting these constraints.

3
We can draw a random sample $S$ from $O$, evaluate $q$ on them to obtain the ground truth, and then use the results to train the classifier. The classic classification problem strives to classify each input object correctly, but for our problem, we are concerned only with the number of objects whose ground-truth labels are 1. The resulting problem is an instance of quantification learning \[6\], whose goal is to estimate the class distribution as opposed to individual labels. While specialized algorithms are possible, it is appealing to adapt classic classification algorithms for quantification learning, thereby leveraging a rich palette of mature techniques. In this section, we first explore how, given a classifier $f$ that approximates $q$, we can use quantification learning to estimate $C(O, q)$.

We will not delve into specific classification algorithms here, because they are not this paper’s focus; our methods can work with any of them. For feature selection, we use a simple heuristic that selects the attributes of $o$ referenced in $q$, e.g., columns of $L$ referenced by $\theta_{LR}$ in (Q1) (Section 2). We also note that training can be improved by active learning \[4\] as we discuss later.

**Classify-and-Count (QLCC)** A straightforward and natural approach is Classify-and-Count \[5\], which we refer to as QLCC. Suppose we randomly select $S \subseteq O$ as training data and let $C_S = C(S, q)$ denote the count of positive objects therein. After learning $f$ from $S$, we evaluate $f(o)$ for each “test object” $o \in O \setminus S$. Let $C_{obs} = \sum_{o \in O \setminus S} f(o)$ denote the “observed count” of $f$ over the test data. We simply return $C_{obs} + C_S$ as the estimate for $C(O, q)$. Should the classifier be accurate over the test data, this estimate will be accurate as well. However, it should be clear that QLCC is susceptible to classification errors and can produce wildly skewed estimates when false positive/negative counts are imbalanced.

**Adjusted Count (QLAC)** To mitigate this problem, a recommended approach is Adjusted Count \[5\], which we refer to as QLAC. The basic idea is to further adjust $C_{obs}$ using the rates of true and false positives estimated empirically from the training data. In more detail, we use $k$-fold cross validation on the samples $S$ to compute $\hat{tpr}$ and $\hat{fpr}$, the estimated true and false positive rates, respectively. Then, we obtain an “adjusted count” $C_{adj}$ of $f$ over the test data by adjusting the observed count $C_{obs}$ as follows:

$$C_{adj} = \frac{C_{obs} - \hat{fpr} \cdot |O \setminus S|}{\hat{tpr} - \hat{fpr}}. \quad (2)$$

Finally, we return $C_{adj} + C_S$ as the estimate for $C(O, q)$.

**Active Learning** To improve the training of the classifier, we apply uncertainty sampling from active learning. Given the high cost of labeling objects (evaluating $q$), note that not all labeled objects are equally important to training; the idea is to prioritize labeling objects that the classifier is most “uncertain” about. Many classifiers, besides predicting the class label, also compute a numeric score that indicates how “confident” they are in their predictions. For our setting of a binary classifier, suppose the classifier provides a scoring function $g: O \rightarrow [0, 1]$: if $g(o) = 1$ (or 0), the classifier is totally confident in predicting $g(o)$ to be 1 (or 0, resp.); a value strictly between 0 and 1, on the other hand, indicates uncertainty. For some classifiers (e.g., random forest), one can intuitively interpret $g(o)$ as the probability that $q(o) = 1$, but in general, $g(o)$ may not have a probabilistic interpretation. Regardless, the scoring function $g$ gives us a way to select the “most uncertain” objects to label. We assume that, compared with $q$, $g$ is cheap to evaluate (in practice it is often a byproduct of classification).

In more detail, suppose we have a labeling budget (in terms of the total number of objects on which to evaluate $q$). We first spend a portion of this budget to draw a set of objects $S_0$ and train an initial classifier with scoring function $g_0$. Next, we select another set of objects $S_1 \subseteq O \setminus S_0$ according to $g_0$, focusing on objects that the initial classifier is most uncertain about. The most straightforward method for selecting $S_1$ is to evaluate $g_0$ for all objects in $O \setminus S_0$, and select the desired number of objects with the smallest value for $|g_0(o) - 0.5|$ (i.e., deviation from the “toss-up”). In practice, instead of considering all of $O \setminus S_0$, we randomly draw a large enough number of objects from $O \setminus S_0$ to evaluate $g_0$, and select among them objects with the smallest value for $|g_0(o) - 0.5|$. We then evaluate $q$ for the set $S_0 \cup S_1$ as training data. In general, we can augment the training data in this fashion multiple times until we exhaust the total labeling budget.

As a concrete example, Figure 1 shows two steps of augmenting the training data for Example 1. The classifier here is a simple nearest-neighbor classifier with $x$ and $y$ values as features. The training data initially consists of 2500 randomly drawn objects; each step adds 100 more objects using the uncertainty sampling idea above. The classifier scores over the feature space are shown as heat maps. As can be seen intuitively from these maps, augmenting training data by drawing objects near the decision boundary is very effective in “sharpening” the decision boundary and improving classification accuracy.

Depending on the classification algorithm used, retraining with more data may add overhead, which impacts the overall efficiency (recall our ultimate goal of estimating $C(O, q)$ quickly). As we have observed in our experiments, however, just one augmentation/retraining step gives sufficient improvement (especially for our new learning-to-sample methods in Section 4 which rely less on classifier accuracy). Hence, we recommend a single augmentation/retraining step in practice, with $S = S_0 \cup S_1$.

**3.3 Learning with Sample-based Correction**

One idea for combining learning and sampling is to follow QLCC (Classify-and-Count) with another phase, where we randomly sample additional objects, evaluate $q$ on them, assess the errors in the learned classifier $f$, and correct the result of Classify-and-Count accordingly. We call this method QLSC, for “quantification learning with SampleClean,” as it is inspired by the work of \[25\] on using sampling for data cleaning\(^2\). More precisely, recall that QLCC samples $S \subseteq O$, learns $f$, and estimates the positive count over

\(^2\)While SampleClean \[25\] deals with the different problem of evaluating aggregates over dirty data, its techniques can be adapted to our quantification learning setting by conceptually regarding the labels produced by the learned classifier as dirty data; “cleaning” a dirty label involves sampling the object and paying the cost of evaluating $q$. Specifically, QLSC
remaining objects as \( C_{\text{obs}} = \sum_{o \in \mathcal{O} \setminus S} f(o) \). QLSC then proceeds with drawing (uniformly at random) another set \( S' \) of objects from \( \mathcal{O} \setminus S \), and for each \( o \in S' \) computes the error \( f(o) - q(o) \). The average error \( \bar{e} \) over \( S' \) gives an unbiased estimator for the average error over \( \mathcal{O} \setminus S \), so we can correct the count over \( \mathcal{O} \setminus S \) as \( C_{\text{obs}} - \bar{e}|\mathcal{O} \setminus S| \). Adding \( C_S \) (positive count in \( S \)) yields the overall estimate. Confidence intervals can be derived as in Section 5.1 because the second phase of QLSC is basically SRS.

QLSC is similar to QLAC (Section 3.2) in that both seek to correct the result of QLCC by assessing its errors on labeled samples. However, QLAC produces only a point estimate while QLSC can provide confidence intervals.

4. LEARNING-TO-SAMPLE METHODS

In the previous section, we have seen how sampling and learning can be applied to problem of estimating \( C(O, q) \). Learning is attractive for its ability to "generalize" knowledge of \( q \) to unsampled objects, but it does not offer the guarantees provided by sampling (e.g., confidence intervals), and its accuracy depends heavily on the quality of the classifier it learns. A natural question is whether we can combine learning and sampling to get the "best of both worlds." QLSC (Section 3.3) represents a baseline approach towards this goal: it uses sampling to correct the count predicted by the classifier, but its sampling scheme does not take advantage of the learned model in any way, and a poor classifier would result in a poor starting point.

This section proposes two methods that combine learning and sampling more effectively. Both methods proceed in two phases. The first phase is learning, and is identical for the two methods: we randomly sample objects, evaluate \( q \) on them, and train a binary classifier, as we did in Section 3.2. However, we are not going to use this classifier to get a count (as a starting point or otherwise). Instead, we assume that the classifier provides a scoring function \( g : \mathcal{O} \rightarrow [0, 1] \); if \( g(o) = 1 \) (or 0), the classifier is totally confident in predicting \( q(o) = 1 \) (or 0, resp.); a value strictly between 0 and 1, on the other hand, indicates uncertainty (e.g., 0.5 means a toss-up). For some classifiers (e.g., random forest), one can intuitively interpret \( g(o) \) as the probability that \( q(o) = 1 \), but in general, \( g(o) \) may not have a probabilistic interpretation. Regardless, the scoring function \( g \) gives us a way to gauge the certainty in the predicted labels. We assume that, compared with \( q \), \( g \) is cheap to evaluate (in practice it is often a byproduct of classification).

The second phase is sampling, but differs between the two methods. The first method, Learned Weighted Sampling (LWS), is the more straightforward one of the two. Treating \( g(o) \) as a guess of how much each object \( o \) contributes to \( C(O, q) \), LWS samples objects with higher \( g(o) \) with higher probability. The second method, Learned Stratified Sampling (LSS), uses \( g \) to guide the partitioning of objects into strata, with the goal of reducing the variance of estimates using stratified sampling.

The novelty of these two methods lies in their use of learning to inform sampling. Thanks to sampling, we still get accurate guarantees in the form of confidence intervals. At the same time, we get the benefit of learning without relying on it for correctness. A good classifier leads to more efficient sampling designs; on the other hand, a poor classifier leads to a less efficient sampling design, but we still have unbiased estimates with confidence intervals. As we will see, between the two methods, LSS is even more robust and less dependent on the quality of the learned classifier than LWS.

The remainder of this section describes the second phase for these two methods in detail. Let \( \mathcal{S} \) denote the samples used in the first phase for learning a classifier with scoring function \( g \). We now focus on estimating \( C(\mathcal{O} \setminus \mathcal{S}, q) \) in the second phase. In the following, we will abuse notation for simplicity: we shall refer to \( \mathcal{O} \setminus \mathcal{S} \) simply as \( O \) instead, and let \( N = |\mathcal{O}| \).

4.1 Learned Weighted Sampling

The second phase of LWS can be seen as a form of probability-proportional-to-size (PPS). In general, PPS relies on a "size measure" that is believed to be correlated to the variable of interest. Objects with large size measures are deemed more important in estimation; hence, objects are drawn with probabilities proportional to their size measures. In our case, the variable of interest is the result of \( q(o) \), so the learned \( g(o) \) can serve as the size measure. However, to guard against an overconfident (and potentially inaccurate) classifier, we adjust the sampling probabilities so every \( o \) has some chance of being sampled (even if \( g(o) = 0 \)). Specifically, we assign each \( o \) an initial sampling probability \( \pi(o) = \max(g(o) \epsilon) \), where \( \epsilon > 0 \) is a (small) prescribed threshold. We then sample objects from \( O \) according to \( \pi \) without replacement, evaluate \( q \) on the sampled objects, and estimate \( C(O, q) \).

There are a number of estimators available from the literature [14], including the popular Horvitz-Thompson estimator. We use the Des Raj estimator, whose calculation is simpler and can provide "ordered" estimates, i.e., running estimates of mean and variance as samples are being drawn. Let \( o_1, o_2, o_3 \ldots \) denote the sequence of objects drawn according to \( \pi \) without replacement. We compute the following quantity after drawing each \( o_i \) (with the summations below yielding 0 in case of \( i = 1 \):

\[
p_i = \frac{1}{\pi} \left( \sum_{j=1}^{i-1} q(o_j) + \frac{q(o_j)}{\pi(o_j)} \left( 1 - \sum_{j=1}^{i-1} \pi(o_j) \right) \right). \tag{3}
\]

The estimate for \( C(O, q) \) after drawing the \( n \)-th sampled object would be \( \hat{p}^{(n)} N \), where the estimated proportion \( \hat{p}^{(n)} \) of positive objects is simply the average of all \( p_i \)'s so far:

\[
\hat{p}^{(n)} = \frac{1}{n} \sum_{i=1}^{n} p_i.
\]

And the variance in \( \hat{p}^{(n)} \) can be estimated as follows:

\[
\hat{\text{Var}}(\hat{p}^{(n)}) = \frac{1}{n(n-1)} \sum_{i=1}^{n} (p_i - \hat{p}^{(n)})^2.
\]

LWS is very efficient when the learned classifier is accurate and confident. To see why, suppose the true proportion of positive objects in \( O \) is \( p \). For an accurate and confident classifier, assuming an arbitrarily small \( \epsilon \), \( \pi(o) \) would be arbitrarily close to 0 if \( q(o) = 0 \), or \( \frac{1}{\hat{p}_i} \) otherwise. Therefore, each sampled object \( o_i \) will have \( q(o_i) \approx 1 \) and \( \pi(o_i) = \frac{1}{\hat{p}_i} \). Plugging these into (3) and simplifying the equation yields \( p_i = p \) for all \( i \), so the estimate \( \hat{p}^{(i)} \) at every step will be perfectly accurate.

On the other hand, LWS’s efficiency can suffer with a poor classifier. Even though it still produces unbiased estimates (regardless of the choices of \( \pi(o)^{s} \)’s), it may require many more samples to achieve a tight confidence interval if it gets the priorities wrong.

Another indication that LWS may not be best for our setting is its preference for objects with high \( g(o) \). Intuitively, focusing instead on objects with \( g(o) \) in the toss-up range reveals more information. Note that traditionally, PPS applies to the more general setting where the variable of interest can be of any value; hence, it is natural to focus on objects with potentially higher contribution to the result. In our setting, however, the value of interest, \( q(o) \), is either 0 or 1. This limited range makes our problem easier, as we...
do not need to worry about cases where inclusion or exclusion of objects with extremely high values can seriously impact the estimates. At the same time, this more constrained setting also enables the possibility for better sampling designs, which we explore next.

4.2 Learned Stratified Sampling

As discussed in Section 4.1, the quality of the learned classifier can adversely impact the efficiency of LWS, because the values of scoring function \( g \) directly control the sampling probabilities. We now present LSS, which uses \( g \) more conservatively, and in a way that naturally encourages exploration of uncertain outcomes (as opposed to certain positives).

Following the learning phase, LSS conceptually sorts the objects in \( O \) by \( g \) (say, in increasing score order). At a high level, LSS applies stratified sampling to \( O \), where stratification is done according to this ordering; i.e., each stratum covers objects whose \( g \) scores fall into a consecutive range. More specifically, the second phase of LSS proceeds in two stages:

1. Randomly draw \( S^1 \subseteq O \) to evaluate \( q \), and use the results to design a sampling scheme for the second stage—namely, the partitioning of \( O \) into strata as well as an allocation of second-stage samples among these strata.
2. Randomly draw \( S^{II} \subseteq O \setminus S^1 \) to evaluate \( q \), according to the sampling scheme designed by the first stage, and use the results to estimate \( C(O, q) \).

Several points are worth noting:

(Versus LWS) While LWS uses the actual \( g \) values in its sampling design, LSS uses only the ordering of \( g \) values among objects. Hence, LSS relies less on the learned classifier. We will validate this observation with experiments in Section 5.

On the other hand, the ordering induced by \( g \) is useful to LSS because it intuitively brings together objects with similar levels of uncertainty, and in particular encourages putting confidently positive objects and confidently negative objects into separate strata with low within-stratum variances.

(Versus Basic Stratified Sampling) While the second phase of LSS uses stratified sampling, this phase differs from the baseline methods in Section 3.1 in important ways: (i) stratification in LSS is based on the learned \( g \) instead of surrogate object attributes; (ii) LSS uses \( S^1 \) to jointly design stratification and allocation; in contrast, SSN only uses \( S^1 \) to design allocation (given stratification), while SSP does not have a first stage.

(Samples in Learning and Sampling Phases) The samples we draw in the sampling phase of LSS (\( S^1 \cup S^{II} \) above) are separate from those drawn in the learning phase. Since the samples from the learning phase already affect (through the learned \( g \)) the ordering of \( O \) for stratification, we choose to use new, independent samples (\( S^1 \)) for sampling design in order to minimize reliance on the classifier quality.

The remainder of this section discusses how we design the sampling scheme for the second stage in detail. Formally, we define the design problem as follows. Consider an ordered set \( O \) of objects \( o_1, o_2, \ldots, o_N \) ordered by \( g \) with ties broken arbitrarily, which can be efficiently computed as we assume that the classifier is easy to execute. A stratification of \( O \) into \( H \) strata, specified by \((N_1, N_2, \ldots, N_H)\) where \( \sum_{h=1}^{H} N_h = N \), defines the partitioning of \( O \) into subsets \( O_1, O_2, \ldots, O_H \). Here \( O_1 \) objects with indices \( \leq N_1 \), and \( O_h, h \geq 2 \) denotes the subset of objects whose indices fall within the interval \([\sum_{j=1}^{h-1} N_j, \sum_{j=1}^{h} N_j]\).

Recall from Section 3.1 that \( \vartheta \) gives the variance in the estimator of \( C(O, q)/N \) for stratified sampling, given the stratification \((N_1, N_2, \ldots, N_H)\) and a sample allocation \((n_1, n_2, \ldots, n_H)\) where we draw \( n_h \) objects from \( O_h \). However, we do not know the \( S_h \) terms in \( \vartheta \) in advance, since they denote the standard deviation of the actual \( q(o) \) values of the objects \( o \in O_h \) that are expensive to compute, so LSS instead seeks to minimize the variance of \( C(O, q) \) given by \( \vartheta \) estimated using the first-stage samples \( S^1 \).

More precisely, suppose the first-stage sample \( S^1 \) consists of \( m \) objects \( o_1, o_2, \ldots, o_m \) where \( 1 \leq t_1 < t_2 \cdots < t_m \leq N \). We aim to find a stratification \((N_1, N_2, \ldots, N_H)\) to minimize the objective given in (5) below that estimates the variance in the estimator of \( C(O, q) \) using \( n \) samples in total in the second stage.

Here we assume \( S_h^1 = O_h \cap S^1, m_h = |S_h^1| \), \( n_h \) is number of second-stage samples in \( O_h \), \( \sum_{h=1}^{H} n_h = n \), and the variances \( s_h^2 \) using the first-stage samples \( S^1 \) are estimated as

\[
s_h^2 = \frac{1}{m_h-1} \sum_{o \in S_h^1} (q(o) - C(S_h^1, q)/m_h)^2. \tag{4}
\]

Then the variance of the estimated \( C(O, q) \) obtained by simplifying \( \vartheta \) is given by:

\[
V(N_1, N_2, \ldots, N_H) = \sum_{h=1}^{H} \frac{N_h s_h^2}{n_h} - \sum_{h=1}^{H} N_h s_h^2. \tag{5}
\]

The remainder of this section describes our algorithms for computing the optimal stratification given \( S^1 \). Note that the optimality of stratification depends on the allocation strategy used. We first present the case of using Neyman allocation, which minimizes the variance for a given stratification. In this case, LSS gives the overall optimal sampling design that jointly considers stratification and allocation. Then, we briefly discuss the case of proportional allocation, which is simpler but not optimal for a given stratification. In this case, we would find the stratification that makes proportional allocation most effective; the optimization problem is much easier than the case of Neyman allocation.

Optimizing the Stratification

Recall from Section 3.1 that under Neyman allocation using \( S^1 \), \( n_h = n(N_h s_h)/\left(\sum_{h=1}^{H} N_h s_h\right) \). Hence, we can further simplify (5), the minimization objective, as follows:

\[
V(N_1, N_2, \ldots, N_H) = \frac{1}{n} \left(\sum_{h=1}^{H} N_h s_h^2\right)^2 - \sum_{h=1}^{H} N_h s_h^2. \tag{6}
\]

A naive algorithm would compute \( V \) for all possible stratifications \((N_1, N_2, \ldots, N_H)\) and pick the best, but the number of possibilities is \( \Omega(N^H) \), and computing \( V \) involves going over \( S^1 \), which is expensive even for small number of partitions (e.g., when \( H = 3 \)). Before presenting our algorithms, we describe some ideas useful to combat these challenges.

First, note that in the expression for \( V \) in (6), the \( s_h \) terms depend only on the subset of objects \( S_h^1 \) sampled in \( S^1 \) in each stratum \( h \), and the precise locations of stratum boundaries between these sampled points only affect the \( N_h \) terms. This observation suggests that we may be able to first consider the partitioning of \( S^1 \) among strata, and then decide where precisely the stratum boundaries lie among \( O \). Later in this section, we will start with an algorithm that uses this strategy, where given the partitioning of \( S^1 \), the optimal \( N_h \)'s can be solved directly and (almost) exactly in the case of \( H = 3 \). Building on the insights revealed in this simple case, we then present two general algorithms for any \( H \) providing different trade-offs between speed and accuracy. Both of these algorithms tame complexity by restricting the potential locations of the stratum boundaries.

Second, we can speed up the computation of \( V \) significantly using precomputation. By sorting the \( m \) objects in \( S^1 \) by \( g \), we can compute a prefix-sum index \( \Gamma \), such that \( \Gamma(k) = \sum_{j=1}^{k} q(o_j) \) (for...
Given $o_h$ as the last sampled object in $O_1$ and $o_j$ as the first sampled object in $O_3$, we can readily compute $s_1, s_2, s_3$ in (6) using the precomputed index $\Gamma$: 

\[ s_1^2 = \frac{V(0)}{r} \left( 1 - \frac{V(0)}{r} \right), \quad s_2^2 = \frac{V(1) - V(0)}{r} \left( 1 - \frac{V(1) - V(0)}{r} \right), \quad \text{and} \quad s_3^2 = \frac{V(n) - V(1)}{r} \left( 1 - \frac{V(n) - V(1)}{r} \right). \]

Then, noting that $N_2 = N - N_1 - N_3$, we can write $V(N_1, N_2, N_3)$ as a bivariate quadratic function $f(N_1, N_3)$ of the form 

\[ a_3 N_3^2 + a_2 N_3 + a_1 N_3 + a_0, \]

where coefficients $a_1, \ldots, a_6$ are computed from $s_1, s_2, s_3, n$, and $N$ (see Appendix A for detailed derivation). Our goal is to minimize $f(N_1, N_3)$ subject to the following constraints:

- $\max\{N_i, t_1\} \leq N_i \leq t_{i+1} - 1$; i.e., the last sampled object in $O_i$ is indeed the $i$-th one in $S^i$, and $|O_i| \geq N$.
- $\max\{N_i, N - t_j + 1\} \leq N_i \leq N - t_{j-1}$; i.e., the first sampled object in $O_i$ is the $j$-th in $S^i$, and $|O_i| \geq N$.

These constraints define a 2-dimensional polygon $R$ with at most 5 sides. We optimize the function $f$ over $R$ using a standard algebraic method by considering (i) the critical points of $f$, and (ii) the boundary of $R$.

To find the critical points we set the partial derivatives of $f$ to zero and solve the resulting linear system of equations. If the solution is inside $R$, we consider it a candidate. We then optimize $f$ for each side (1-facet) of $R$, which only involves optimizing a univariate quadratic function. We consider these solutions for the sides of $R$ as candidates too. Finally, for each candidate, we find its closest integer coordinate point in $R$ and evaluate $f$; we then pick the best integer-coordinate solution.

We repeat the above procedure for each pair of sampled objects, and in the end return the stratification with the overall minimum variance (see Appendix A for additional details and the pseudocode). We call this algorithm DirSol (for direct solve). The following theorem summarizes its time complexity and accuracy.

**Theorem 1.** Given an ordered set $O$ of $N$ objects and a sampled subset $S^i$ of $m$ objects, let $v^*$ denote the minimum value of estimated variance defined in (9) achievable using $n$ samples under stratified sampling with $H = 3$ strata where each stratum contains at least $N_i$ objects. Assuming $N_i > n$, DirSol runs in $O(N \log m + n^2)$ time and finds a stratification resulting in estimated variance $v \leq (1 + \frac{2}{N} + \frac{2}{N} \sqrt{\log 2}) v^*$.

Note the assumption of $N_i > n$ above; without it, the approximation factor would be arbitrarily bad. In practice, however, this assumption is weak and often holds in practice: e.g., if we take a 5% sample of $O$ in the second stage, this assumption means that each stratum in $O$ contains at least 5% of $O$.

The algorithm is almost exact, except that the boundaries of the strata we want to find are integers, so rounding an optimum fraction solution to its closest integer solution may lose some accuracy. As for running time, we can sort all objects in $S^i$ and precompute $\Gamma$ in $O(m \log m)$ time. The indices of sampled objects within the ordered $O$ can be computed in $O(N \log m)$ time, with one pass over $O$ that checks each object against a balanced search tree constructed over the $g$ values of the $m$ sampled objects. The algorithm considers $O(m^2)$ pairs of sampled objects, and for each pair, it is able to minimize $f$ in $O(1)$ time, by computing derivatives and considering only a constant number of candidate solutions. Therefore, overall, our algorithm takes $O(N \log m + m^2)$ time to compute the optimal stratification.

Finally, we note that this algorithm can be extended to more than 3 strata by trying all possible size-$(H-1)$ subsets of $S^i$ and optimizing an $(H-1)$-variate quadratic function subject to linear constraints. However, the resulting algorithm will be expensive when
H and m = |S| are large. In the following, we present two less expensive approximation algorithms that work for any H. The first one is slower than the other but it has a better approximation ratio.

**LogBdr:** Given a partitioning of the sampled objects, consider two consecutive sampled objects \( o_i \) and \( o_{i+1} \) that are put into different strata (there are \( H - 1 \) such pairs of objects). When deciding where exactly to draw the boundary between \( o_i \) and \( o_{i+1} \), the algorithm only considers the set \( B_h \) of candidate boundary indices \( t_h, t_{h+1}, t_h^2, t_{h+1}^2, t_h^2 + t_{h+1}^2, \ldots \) up to \( t_k \); we add \( t_{k+1} = 1 \) if it is not already in \( B_h \). Choosing a particular index \( i \) from \( B_h \) means the stratum containing \( o_i \) ends with \( o_i \). Then the algorithm is simple. We just check all candidate stratifications formed by choosing one index from each of the \( H - 1 \) sets of candidate boundary indices.

We call this algorithm LogBdr (for logarithmic number of candidate boundary indices). The following theorem summarizes its time complexity and accuracy (proof is in Appendix B).

**Theorem 2.** Given an ordered set \( O \) of \( N \) objects and a sampled subset \( S \) of \( m \) objects, let \( v^* \) denote the minimum value of estimated variance defined in (6) achievable using \( n \) samples under stratified sampling with \( H \) strata where each stratum contains at least \( N \) objects. Let \( N^* \) denote the size of stratum \( s \) in this optimum solution. Assuming \( N > n \), LogBdr runs in \( O(N \log m + \frac{Hm^{H-1} \log H - 1}{N^*} \cdot N) \) time and finds a stratification resulting in estimated variance \( v \leq \max \{4, 2 + 2 \max_{1 \leq t \leq H} \log \frac{N}{N^*} \} v^* \).

We can further improve the approximation ratio if we increase the running time. More specifically, instead of considering candidate boundary indices in \( B_h \) that are powers of 2 away from the sampled object index \( t_h \), we can consider those are powers of \( (1 + \epsilon) \) for a small parameter \( 0 < \epsilon < 1 \). The approximation ratio becomes \( \max \{ (1+\epsilon)^2, (1+\epsilon)^2 - \epsilon \max_{1 \leq t \leq H} \frac{N}{N^*} \} \) and the running time becomes \( O(N \log m + \frac{Hm^{H-1} \log H - 1}{N^*} \cdot N) \).

**DynPgm:** While the previous algorithm, LogBdr, works for any \( H \), it is expensive due to the \( m^{H-1} \) term in its running time. While \( H \) is usually not large in practice, for a large enough \( m \) (say, hundreds) the term \( m^{H-1} \) can be prohibitive even if \( H = 5 \). Here, we present a faster algorithm with a larger approximation ratio that depends on \( H \).

The algorithm is based on dynamic programming. A straightforward application of dynamic programming would be to create an array \( A \) with \( N \) rows and \( H \) columns, where \( A[i, h] \) represents the best we can do with \( h \) strata among the first \( i \) objects. Indeed, dynamic programming has been used previously for finding suitable stratifications over the data, where the problems were separable, i.e., the solution of \( A[i, h] \) could be derived by examining the optimum solutions for \( A[j, h-1], j < i \). In our case, however, a straightforward application would not work because our objective function renders the problem non-separable. To see why, note from (6) that

\[
V(N_1, \ldots, N_H) = \frac{1}{n} \sum_{i=0}^{H-1} N_i N_{i+1}^2 + \sum_{h=1}^{H} N_h \sigma_h^2 + \frac{1}{n} \sum_{i=0}^{H-1} N_i \left( \sum_{h=i+1}^{H} N_h \sigma_h^2 \right).
\]

While the first two summations are separable, the third (with nesting) is not: intuitively, the additional contribution to \( V \) from the next stratum \( h \) depends on the sum \( \sum_{h=1}^{H} N_i \sigma_i^2 \) computed over the previous strata, but this sum is not what the optimum solution would have minimized—we call this sum the auxiliary sum.

To work around the difficulty of handling the effect of this auxiliary sum, we select a set \( T \) of possible bounds on it, namely, \( T = \{2^t \mid 0 \leq t \leq \lceil \log(mH N) \rceil \} \) if the auxiliary sum is greater than 1 and \( T = \{t \in \mathbb{Z} \mid 0 \leq t \leq 1 \} \) for a parameter \( \varepsilon \), if the sum is less than 1. Since we do not know the value of the auxiliary sum upfront, we try all these possible values. Then, for each \( t \in T \), we run a dynamic programming procedure operating under the constraint that \( N_h \sigma_h^2 \leq t \) for each \( h \). Intuitively, these auxiliary sum constraints help us bound the quality of our solutions even though we are not optimizing for the auxiliary sum directly. To further reduce complexity, we also apply the same idea as in LogBdr to limit the set of candidate boundary indices to consider. Here, we will consider more indices but without increasing the asymptotic complexity. Specifically, for each sampled object \( o_i \in S \), we consider indices \( t_h, t_h^2, t_h^3, t_h^2 + t_{h+1}^2, t_h^2 + t_{h+1}^2, \ldots \) up to \( t_k \); as well as indices \( t_h - 1, t_h^2 - t_{h+1}^2, t_h^2 - t_{h+1}^2, \ldots \) down to \( (t_h - 1) \) (but not including \( t_h - 1 \)). We denote the ordered set of all candidate boundary indices (induced by all sampled points) by \( B = \{b_1, b_2, \ldots \} \). Clearly \( |B| = O(m \log N) \). Furthermore, for each \( b_i \), we denote by \( \ell_i \) the value \( k \) such that the \( k \)-th sampled object is the last sampled one among \( o_1, o_2, \ldots, o_{b_i} \); we can easily record all \( \ell_i \)'s when constructing \( B \).

Now we can describe the dynamic programming procedure that runs for each \( t \in T \). Let \( A[i, h] \) be an array with \( B \) rows and \( H \) columns, where \( A[i, h] \) stores the variance of the best stratification we found for \( h \) strata over the first \( i \) objects in \( O \). Let \( X_i \) be an array of the same dimension as \( A \), where \( X[i, h] \) stores the overall auxiliary sum corresponding to the solution represented by \( A[i, h] \). Then we have

\[
A[i, h] = \min_{1 \leq j < i, \sum_{j \leq h} s^2 \leq t} \left\{ A[j, h-1] + \frac{1}{n} N_j s_j^2 + \frac{1}{n} N_j s_j X[j, h-1] \right\},
\]

where \( N_j = b_i - b_j \) is the size of stratum \( h \) (containing objects \( o_{b_j+1}, \ldots, o_{b_i} \)) being considered, and \( s_j^2 \) is the estimated variance for stratum \( j \), which can be computed using the prefix-sum index \( s_j = \sum_{0 \leq k < j} s_k \). The array entry \( X[i, h] \) can be updated accordingly.

After running the dynamic programming procedure for all \( t \in T \), we return the best solution found (minimizing \( A[i, |B|] \)). Overall, we try \( O(\log(mH N) + \frac{1}{t}) = O(\log(N + \frac{1}{t}) \log H) \) values of \( t \), and for each \( t \), the dynamic programming procedure takes \( O(Hm^2 \log^2 N) \) time. The total running time, including precomputation, is \( O(N \log m + \log(N + \frac{1}{t}) Hm^2 \log^2 N) \).

The proof of the next theorem can be found in Appendix C.

**Theorem 3.** Given an ordered set \( O \) of \( N \) objects and a sampled subset \( S \) of \( m \) objects, let \( v^* \) denote the minimum value of estimated variance defined in (6) achievable using \( n \) samples under stratified sampling with \( H \) strata where each stratum contains at least \( N \) objects, and let \( \varepsilon \) be any parameter with \( 0 < \varepsilon < 1 \). Assuming \( N \geq 4n \), DynPgm runs in \( O(N \log m + (\log(N + \frac{1}{t}) Hm^2 \log^2 N)) \) time and finds a stratification resulting in estimated variance \( v \leq \frac{12}{8} v^* + \frac{12}{8} \varepsilon ) \) or \( v \leq \frac{12}{8} v^* + \varepsilon \).

**DynPgm:**

Recall from Section 3.7 that under proportional allocation, \( n_i = \frac{N_i}{N} \). Hence, we can further simplify [5], the minimization objective, as follows:

\[
V(N_1, \ldots, N_H) = \frac{N-n}{n} \sum_{h=1}^{H} N_h \sigma_h^2.
\]

This objective is much simpler than [6] for Neyman allocation. The resulting optimization problem is indeed separable, and can be solved readily by dynamic programming.
We still carry out the same precomputation (e.g., the prefix-sum index \( \Gamma \)), and also use the same idea behind DynPgmp, LogBdr to select the ordered set of candidate boundary indices \( B = \{ b_1, b_2, \ldots \} \), where \( |B| = O(m \log N) \). The dynamic programming algorithm then proceeds as follows. Let \( A \) be an array with \( |B| \) rows and \( H \) columns, where \( A[i,h] \) represents the best we can do with \( h \) strata over the first \( b_i \) objects in \( \mathcal{O} \). We have \( A[i,h] = \min_{t_s < t < t_s + 1} \{ A[j,h-1] + \frac{\log N_j,s_j}{j} \} \), where \( N_j,s_j = b_i - b_{i-1} \) is the size of stratum \( h \) being considered, and \( s_{j,i} = t_s + \frac{\log (t_s + 1 - t_s)}{t_s - t_s + 1} \) is the estimated variance for this stratum.

We call this algorithm DynPgmp (for dynamic programming for stratification with proportional allocation). With analysis similar to DynPgmp (except here we only run the dynamic programming procedure once), we see that the running time of DynPgmp is \( O(N \log m + H m^2 \log^2 N) \), where the two terms can be attributed to precomputation and dynamic programming, respectively. The dynamic programming procedure finds the optimum stratification whose boundaries are restricted to \( B \), which still yields a good approximation ratio of 2.

The proof of the next theorem can be found in Appendix [1]

**Theorem 4.** Given an ordered set \( \mathcal{O} \) of \( N \) objects and a sampled subset \( S^\alpha \) of \( m \) objects, let \( v^\alpha \) denote the minimum value of estimated variance defined in \( [7] \) achievable using \( n \) samples under stratified sampling with proportional allocation over \( H \) strata. DynPgmp runs in \( O(N \log m + H m^2 \log^2 N) \) time and finds a stratification resulting in estimated variance \( v \leq 2 v^\alpha \).

As with LogBdr and DynPgmp, we can improve DynPgmp’s approximation ratio at the expense of its running time, by considering candidate boundary indices that are powers of \( 1 + \epsilon \) (instead of 2) away from the indices of sampled objects. The resulting approximation ratio would become \( (1 + \epsilon) \) and running time \( O(N \log m + H \frac{\log \epsilon}{\epsilon} \log^2 N) \).

5. **Experiments**

Most of our experiments are based on three scenarios, each with its own real-world dataset and counting query template:

**(Sports)** The data contains yearly performance statistics for players in the Major League Baseball. We focus on pitching statistics, which exclude a portion of the players. We consider the \( k \)-skyband size query in Example 2, where each point is a player-year combination (there are about 47,000 of them), and \( x \) and \( y \) refer to runs and home runs.

**(Neighbors)** The data comes from KDD Cup 1999, where the goal was to learn a predictive model that could distinguish legitimate and illegitimate (intrusion attacks) connections to a machine. The original dataset contains 4.9 million records with 41 features and a binary label. We removed many sparse rows, resulting in 73,000 points. We consider the query in Example 2 that counts points with few neighbors.

**(Text)** We consider the relevant document count query in Example 2. Since we do not want to manually evaluate the predicate ourselves in experiments, we use the LSHJC dataset [20], which provides ground-truth labels (Wikipedia categorization) for 2.4M documents from Wikipedia. The same dataset was used in [18]. In our experiments, each algorithm is charged a cost for revealing the true label, which in practice would be expensive.

To experiment with different selectivities of the predicate \( q \), we adjust query parameter settings (\( k \) for Sports; \( k \) and \( d \) for Neighbors; \( k \) for Text). We also create synthetic datasets based on Sports to study how data distributions affect learned models and the performance of various algorithms; for details see Section 5.2.

We compare the following algorithms:

- **Sampling-based (Section 3.1):** simple random sampling (SRS) and stratified sampling (SSP, with proportional allocation, and SSN, with Neyman allocation in two stages). For stratified sampling (which applies to Neighbors and Sports but not to Text), we use attributes \( x \) and \( y \) as surrogates; each stratum is a rectangle in the 2d \( x-y \) space. Unless otherwise specified, we stratify using a uniform \( \sqrt{H} \times \sqrt{H} \) grid over the ranges of \( x \) and \( y \) values in the dataset. By default \( H = 4 \).
- **Learning-based (Section 3.2):** quantification learning (QLCC, without adjustment, and QLAC, with adjustment).
- **Learning with sampling-based correction (Section 3.3):** QLSC.
- **Learning-to-sample (Section 4):** learned weighted sampling (LWS) and learned stratified sampling (LSS). Unless otherwise specified, for LSS we implement a simplified version of LogBdr, which considers candidate boundaries that map to equally spaced ticks over \([0, 1]\) (the range of \( g \) scores). By default, \( H = 4 \) and the spacing between candidate boundaries is 0.05; for the distributions of \( g \) scores that arise in practice, these boundaries already provide fine enough resolution for \( H = 4 \), so more sophisticated choices of candidates in LogBdr are not needed.

For learning-based and learn-to-sample algorithms, we use standard implementations of classifiers from scikit-learn. For Neighbors and Sports, we experiment with \( k \)NN (\( k \)-nearest neighbors, where \( k \) is not to be confused with our query parameter), RF (random forests), and NN (a simple two-layer neural network); by default, we use RF with 100 estimators. For Text, we use a naive Bayes classifier with standard full-text features. For QLSC, LWS, and LSS, by default we devote 25% of their allotted samples to training (and including design, if applicable).

Since the estimates of result counts are uncertain, for each experimental setting, we run each algorithm 100 times, and record the distribution of estimates it produces. Recall that unlike sampling-based and learn-to-sample algorithms, those based on learning alone provide no accuracy guarantees by themselves. Nonetheless, the distributions of estimates they produce allow us to evaluate their accuracy empirically. When appropriate, we show distributions using violin plots [4]. We would like our estimates to be unbiased, so ideally the violin plots would be centered around the actual result count. Furthermore, we would like the estimates to have low variance, which means narrower interquartile ranges as well as shorter and wider plots. In some figures, we use MAE (mean absolute error) as a single numeric measure to quantify and summarize an error distribution, so we can report more results than violin plots.

For Neighbors and Sports, while our queries can be executed directly over a database system, they run slowly even if we construct all appropriate standard indices and enable the maximum level of optimization (on PostgreSQL and another commercial system). To enable faster experiments, we implemented the evaluation of \( q \) in Python in main memory. Since our experiments specify sampling budgets in terms of numbers (or percentages) of samples, our results are platform-neutral and easy to translate into time savings on different underlying platforms. The overhead of learning, as we will show later with experiments, is small compared to the cost of labeling samples (evaluating \( q \), even for the in-memory Python implementation; the overhead will be even smaller in the SQL setting.

5.1 **Overall Comparison with Real Datasets**

\(^5\)A violin plot shows the probability density at different values; additionally, a white dot marks the median of all data, a thick black line spans the lower and upper quartiles.
We begin with experiments that compare various algorithms using the three scenarios with real datasets, Neighbors, Sports, and Text. Both LSS and LWS used a random forest classifier with estimators and a 25%;75% training:sampling split. Figure 2 compares the MAE of various algorithms when we vary the result size (via query parameters) while keeping the sample size fixed. Figure 3 compares the MAE of various algorithms when we vary the sample size while keeping the result size fixed.

As it turns out, the learned classifier performs pretty well for Neighbors and Sports, but pretty poorly for Text, leading to very different results. We shall focus on Neighbors and Sports first. F1 scores for the learned classifiers average higher than 0.8 in these scenarios (with small result sizes being more difficult). We make several observations. First, learning-based methods are very competitive here thanks to high classifier quality. In fact, QLCC sometimes even delivers the smallest errors even without any adjustment or correction. But to keep things in perspective, QLCC and QLAC do not provide any guarantees; once QLCC uses sampling to provide correction and guarantees, MAE actually takes a small hit because of the extra overhead. Second, algorithms without any learning component, namely SRS and SSP are clearly not as competitive here, with much higher MAE than others. Third, LSS (highlighted) has consistently low MAE; it is nearly always the leader or not far from the leader, and bear in mind that it offers statistical guarantees, which QLCC does not. LSS also consistently leads QLSC by a good margin. Fourth, the comparison between LWS and LSS is difficult, as in some cases LWS leads LSS. The quality of the learned classifier for Neighbors and Sports is the main factor here. To better understand the situation, we take a closer look at some data points with violin plots showing distributions.

In Figure 1, we get a more detailed sense of the variability in estimates. LSS and LWS are consistently no worse and often better than SRS and SSP. Between LSS and LWS, we make two observations. First, when selectivity is low, we expect all sampling-based methods to have some trouble as the particular number of positives that come up by chance in each run will have a large impact on relative error. For Sports, LWS dodged this issue with a very good classifier that allows it to draw in a very targeted fashion. In contrast, LSS, as it places much less trust in the learned model compared with LWS, misses the opportunity. Second, LWS is not without its own problems. In Neighbors, where prediction becomes slightly more challenging, we see LWS underestimating with XS result size; as it turns out, the classifier at those points happens to generate more false negatives. In other words, LWS depends far more on model quality than LSS does—it can benefit more, but also can get hurt more. This effect will be magnified for the Text scenario, which we focus on next.

The Text tells a completely different story. In this case, classification is hard. Therefore, QLCC, QLAC, and QLSC fare very poorly here, because their performance is too dependent on starting point produced by QLCC. Correction is also difficult. From one representative run (with 857k resize size), true TPR and FPR are .53 and .85, while the estimated TPR and FPR are .35 and .95. Even with sampling-based correction, QLSC still underperforms other algorithms. In contrast, SRS, which does not use learning, actually shines here. Finally, LSS tracks SRS closely. It actually underperforms SRS a bit, which is understandable because learning phase is essentially not that useful, wasting 25% of the samples. However, the impact on the sampling design is limited. Closer examination reveals that it basically degenerates to SRS for the remaining 75% of the samples. This experiment highlights the sensitivity of QLCC, QLAC, and QLSC toward poor models.

5.2 Comparison with Synthetic Datasets

Results in Section 5.1 show just three data points along the spectrum of classifier quality. Neighbors and Sports have good classifiers but Text has a bad one. What happens in between? To understand how different algorithms are affected by varying degrees of difficulty in using a learned model to approximate a predicate, we design our next set of experiments by injecting additional “noise” into the Sports scenario to adjust the difficulty of classification. Recall from Example 2 that for each object o, we compute a count subquery with o.x and o.y, and compare the resulting count, say c, with k. Now, we create an additional “noise” table keyed on distinct (x, y) values, where each (x, y) is associated with a noise count drawn randomly from another distribution. Instead of comparing c with k, we use another subquery to look up the noise count c’ for (o.x, o.y), and have the predicate combine the original and noise counts into (1 − α)c + αc’ to compare with k. By adjusting α ∈ [0, 1], we control how much noise contributes to the outcome of the predicate: α = 0 corresponds to the original Sports scenario, where we know we can learn a good model; α = 1 means the predicate is simply comparing independent random noise, which is mostly challenging to predict.

We experiment with two noise distributions. One is a Gaussian with standard deviation of 1 truncated and discretized. The other is derived from a Zipf distribution with parameter s, where each draw is used to index into a randomly permuted array of possible noise counts derived from the real count values; large s means some (random) noise count will be far more popular than others.

We compare SRS, QLSC, and LSS, representing sampling-based, learning-based (but with sampling-based correction), and learn-to-sample algorithms, respectively. Figure 5 shows how they compare in terms of MAE when we vary α for synthetic datasets generated using Gaussian noise. Note that when α increases, the result size tends to decrease (but it is random depending on the particular dataset being generated), so MAE for SRS tends to decrease accordingly, although its relative error actually increases. The main observation from this figure is that when α is small, good model qualities make LSS and QLSC outperform SRS. However, as α increases, model quality starts to take a toll on LSS and QLSC. Nonetheless, LSS consistently outperforms QLSC, and it is not far behind SRS even when the predicate outcome is almost completely dictated by noise. Upon closer examination, we see that when α = 1, LSS basically degenerates to random sampling in the sampling phase, and it is not surprising that it is slightly worse than SRS because it has wasted 25% of its samples on learning.

Figure 6 shows how the three algorithms compare when we vary the Zipf parameter for synthetic datasets generated using Zipf noise. The results can be difficult to interpret because of the variability in each particular instance of the randomly generated dataset, and the fact that skewness does not necessarily make classification harder. However, once we overlay the quality (F1 score) of learned classifier for QLSC and LSS, a clear pattern emerges: model quality clearly influences the performance of methods that use learning, but LSS is far more resilient than QLSC (consider s = 7, for example). Again, LSS is the most consistent performer among all three—it is not far from SRS when the model is very poor, and it is not far from QLSC when the model is very good.

5.3 Running Time and Overhead

Before making a closer examination of LSS, we take a brief look at the running times of our approaches. Both LWS and QL methods (QLAC, QLCC, QLSC) are simpler than LSS, which has more overhead in stratification. Thus, we focus on LSS. In Figure 7, we plot the overhead added by using LSS when compared with SRS.
There are three distinct sources of overhead in LSS: *Learning* represents the time to train the classifier; *Design* includes the time to compute the optimal stratified sampling scheme; *Application* accounts for the overhead in applying the chosen scheme, which involves picking objects from their associated strata. (Note that we already charge the samples used by LSS for learning and sampling design towards the total number of samples, which is set to be the same when comparing with other approaches.) In Figure 7 we also list the fraction of overall running time consumed by overhead at the top of each bar. Note these are miniscule (below 0.2%) compared with the overall cost, dominated by the predicate evaluation over samples. Such a low overhead implies that if we give simpler approaches such as SRS additional samples to account for the overhead of LSS, the number of additional samples would be too low to make any difference.

5.4 Closer Looks at LSS

Next, we test a variety of facets involved in LSS: how strata are laid out, the number of strata, allocation of samples for learning/design vs. estimation, and how the underlying classifier affects final estimation quality.

**Strata Layout Strategy** First, we study the impact of stratification strategy on LSS. Instead of using more sophisticated algorithms to look for optimal bucket boundaries (optimal-width), what if we use simpler strategies? In particular, fixed-width simply make all strata equal in width; fixed-height simply ensures that all strata contain the same number of objects. Figure 8 shows the results, using 4 strata. It is no surprise that fixed-height produces poor results for stratified sampling, as each strata may be forced to contain a mixture of labels; in particular, for skewed datasets where one label occurs more often (XS and XXL), fixed-height has much higher variance in its estimates. Fixed-width fares better, but our optimal-width (which LSS uses by default) makes further gains—its interquartile range (IQR) is generally lower than the two simpler approaches.

**Number of Strata** In this experiment, we investigate the effect of the number of strata on estimation quality when using LSS and SSP, both of which use stratified sampling. We vary the number of strata with 4, 9, 25, 49, and 100 strata available. The results are summarized in Figure 9. Overall, as expected, increasing the number of strata tends to improve estimation quality, but not substantially so. Here, with XS result size and a large number of strata, SSP becomes competitive against LSS. The reason is that with superfine uniform gridding of the x-y space, the few positive objects eventually concentrate into a few strata, making SSP effective; in comparison, LSS may occasionally produce an outlier estimate, even though its overall variance is still competitive. Aside from these few extreme settings, however, LSS generally outperforms SSP, and often by significant margins as shown in Figure 9.

**Sample Split** Next, we test the effect of sample allocation on the quality of estimates produced by LSS. We vary the percentage of samples allocated to classifier training and sampling design from 10%, 25%, 50%, to 75%. A 10% split means 10% of the total samples are devoted to learning and design, while the rest (90%) of the samples are used to produce the result estimate. We fix the number of strata at 4. Figure 10 summarizes the results. We see that at 75%, too few samples are devoted to estimation, so the result quality tends to suffer. Conversely, at 10%, too few samples are devoted to learning and design, and the result quality may also suffer. Both middle proportions (25% and 50%) consistently produce the most reliable estimates with lowest IQR’s and fewer outliers.

**Choice of Classifier** As LSS is driven by the scores produced by a classifier, it is naturally dependent on the classifier itself. We tested LSS with four classifiers: k-Nearest Neighbors (KNN, with \( k = 3 \)), simple two-layer neural network (NN, with 5 nodes per layer), random forest (RF, with 100 estimators), and a dummy classifier (Random) that assigns arbitrary random scores to objects. Random can be viewed as a worst case scenario for LSS as the desired effect of stratification (producing homogeneous strata) is completely lost. Across classifiers, we use 25% of the samples for learning and sampling design, and there are 4 strata. As we can see from the results in Figure 11, consistent with intuition, a classifier that performs better than Random produces better estimates. On the other hand, even if a classifier performs poorly (such as Random), LSS still produces reasonable estimates.

6. RELATED WORK

**Sampling for Approximate Query Processing (AQP)** Sampling is a fundamental problem in databases and has been studied over more than three decades [21, 20, 4]. Random samples are one of the key types of *synopses* [5] frequently used for AQP. Sampling for complex queries has been a long-standing challenge. In particular,
sampling over joins is non-trivial, because simply joining independent samples of participating tables is ineffective [20, 4]. This problem has received much attention over the years, with representative works such as ripple join [7], wander-join [17], and more recently, sampling multi-way acyclic and cyclic joins [26]. The focus of our work is on counting queries with complex predicates. Even though our predicates can include joins as discussed in Section 2, our techniques differ because of different problem assumptions. First, some work on sampling over joins, e.g., [4], aims at producing a random sample of the result tuples (i.e., answering a reporting query), while we aim at estimating the result count (i.e., answering a counting query). Second, to make our approach general, we adopt a rather simple evaluation model, where sampling a candidate object \( o \) to be counted involves evaluating \( q(o) \) exactly, without additional sampling or approximation. In contrast, much of the work on sampling over joins assumes specific forms of join predicates or availability of indexes to avoid enumerating all join results for \( o \). On the other hand, all queries in our experiments are too complex for these approaches to handle, because these queries use constructs such as self-joins, complex non-equality join predicates, subqueries containing GROUP BY and HAVING, as well as UDFs.

\textit{BlinkDB} [1] and \textit{VerdictDB} [22] are examples of recent AQP systems aimed at supporting approximate processing of general, ad hoc queries. While these systems deliver very fast response time thanks to optimizations such as precomputation and parallelization, handling the full complexity of SQL remains challenging. For instance, \textit{VerdictDB} does not support self-joins out of the box; our best attempt at adapting the query in Example 2 to run on it resulted in poor estimates compared with other approaches we experimented with in Section 5.

A number of papers are related to ours in the use of sampling. [19] considers stratified sampling design for both streaming and stored data, and improves upon the Neyman allocation. [8] estimates the size of a query result by partitioning the query result and estimating the sum of the partition sizes. In our setting, each partition would be associated with one object, which contributes either 0 or 1 to the sum. [8] focuses on deriving a sequential sampling procedure, and considers both uniform random sampling and stratified sampling. However, unlike our work, it does not consider how to design stratification in a way to maximize sampling efficiency. Many other sampling papers are concerned with aggregates such as \textit{SUM}, which are more susceptible to sample biases than just counting queries. [12] studies robust stratified sampling for low-selectivity aggregate queries, and uses a pilot sampling phase to estimate variance as we do for \textit{SSN} and \textit{LSS}. A combination of outlier-indexing with weighted sampling has been used in [3] to approximate aggregate results, and in [2], where differently biased subsamples can be dynamically selected to answer a query. [13] estimates the results of aggregates over SQL queries with subqueries involving \((\text{NOT IN/EXISTS})\); notably, it proposes a low-variance estimator by learning a model from data using Bayesian statistical techniques. Compared with [13], our approach is simpler, uses off-the-shelf methods, and relies much less on the quality of the learned models. With the exception of [13], none of the work above applies any machine learning to help with estimation or to inform the sampling design.

Sampling has also been used for answering queries from dirty data with data cleaning [25]. In Section 3.3 we have discussed this connection and introduced the method \textit{QLSC} inspired by \textit{Sample-Clean} [25]. Experiments in Section 5 show that our learn-to-sample

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**Figure 4:** Distributions of estimates. Each row has a different sample size (1%, 2%), and each column has a different result size.

**Figure 5:** Varying \( \alpha \); synthetic datasets with Gaussian noise; \( k = 15000 \). Grey dashed line shows the result size (scale on right).

**Figure 6:** Varying Zipf parameter \( s \); synthetic datasets with Zipf noise; \( \alpha = 0.6 \); \( k = 15000 \). Grey dashed line/band show the F1 scores of the classifier (scale on right).

**Figure 7:** Execution time overhead (in seconds) vs. sample size (in thousands) for \textit{LSS}, broken down by sources of overhead.
approach is more effective and less dependent on classifier quality.

Use of Machine Learning There has been a flurry of recent research on the use of machine learning in database systems. One related line of work is the use of machine learning for selectivity estimation, e.g., \cite{15,9}, which can be seen as approximate counting queries. This line of work typically precomputes and maintains data summaries to support query optimization, or more ambitious optimizations across all components of a database system, e.g., SageDB \cite{16}. Since their goal is to use estimates for optimization instead of answering counting queries per se, their estimates typically do not come with any guarantees. In contrast, we strive to provide statistical guarantees on our approximate answers.

Finally, two recent papers are very similar to our approach in spirit. To reduce the cost of evaluating expensive UDFs that arise frequently in machine learning pipelines, Probabilistic Predicates (PP) \cite{18} use learned classifiers to pre-filter data before processing them further. Given a set of such classifiers and an accuracy requirement (minimum fraction of positives to retain), a query optimizer devises a plan that uses appropriate classifiers with optimal score cutoffs to pre-filter the data: any object scored lower than the cutoff by the classifier is dropped. A key difference between this work and ours is the problem definition: they target reporting queries while we target counting queries. This difference leads to our different use of the classifier scores; applying PP to our setting would result in poor estimates. Furthermore, PP gives no statistical guarantees on the actual recall, and its performance is far more susceptible to bad classifiers because of its heavy reliance on classifier scores. Earlier work by Joglekar et al. \cite{11} similarly tackles queries involving selections with expensive UDFs. By identifying attributes whose values are correlated with UDF results, and grouping objects by the values of such attributes, they judiciously choose the appropriate actions to take for each group of objects (e.g., accept all, return all, or sample some). Like our approach, the use of sampling enables probabilistic guarantees, but the key difference remains that they target reporting instead of counting queries.

7. CONCLUSION AND FUTURE WORK

In this paper, we have developed new techniques to estimate the results of counting queries with complex filters. Our techniques are based on a simple yet powerful idea: replace an expensive filter with a cheap classifier that approximates the filter. This cheap classifier can then be used in a number of different ways with different trade-offs. A key challenge is that too much reliance on the classifier makes result quality highly susceptible to bad classifiers. However, one novel technique we proposed, learned stratified sampling, delivers consistently good estimates compared with other alternatives. It is very resilient against bad classifiers, thanks to how it combines machine learning and sampling—the learned classifier.
is used in a limited but helpful way to design a stratified sampling scheme which in turn produces the estimate. This resiliency makes the technique easy to apply in practice, because we are much less concerned with training a perfect model: a good model will make sampling more efficient, but even if the model is poor and/or the filter is fundamentally hard to approximate, the technique still delivers unbiased estimates with statistical guarantees comparable to random sampling. There is an abundance of future work. In particular, learned stratified sampling is quite conservative by design—to ensure independence, it avoids using the samples it acquired in the learning phase when computing the final estimate. However, there may be ways in which such samples can be safely used. Second, some of the queries we considered in this paper (such as skyband sizes and neighbor counts) have highly specialized solutions. Although our goal is to develop general solutions that can work for far more complex queries, it will still be interesting to carry out a direct comparison with the specialized solutions for these specific queries. Finally, a promising direction is to extend and fully evaluate our approach in an online aggregation setting.

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APPENDIX

A. DETAILS ON DirSol

We have
\[ f(N_1, N_3) = \frac{1}{n} \left[ N_{1, s_1} + N_{3, s_3} + (N - N_1 - N_3)s_2 \right]^2 \]
\[ - \frac{1}{n} \left[ N_{1, t_1} + N_{3, t_3} + (N - N_1 - N_3)t_2 \right] \]
\[ = \frac{1}{n} \left[ (s_1 - s_2)^2 N_1^2 + (s_3 - s_2)^2 N_3^2 + \frac{2}{n} \left[ (s_1 - s_2)N_{1, s_2} - (s_2 - s_2)^2 \right] N_1 + \frac{2}{n} \left[ (s_3 - s_2)N_{3, s_2} - (s_2 - s_2)^2 \right] N_3 \right] \]
\[ + \frac{2}{n} \left[ (s_3 - s_2)N_{s_2} - (s_2 - s_2)^2 \right] N_3 + \frac{N^2}{n} s_2^2 - N s_2. \]

In addition, recall the constraints on \( N_1, N_3 \) that we have and define a polygon \( R \) on the plane with at most 5 edges.

Let \( f(N_1, N_3) = a_1 N_1^2 + a_2 N_3^2 + a_3 N_1 N_3 + a_4 N_1 + a_5 N_3 + a_6 \), where \( a_1 = \frac{(s_1 - s_2)^2}{N_1}, a_2 = \frac{(s_3 - s_2)^2}{N_3}, a_3 = \frac{2(s_1 - s_2)(s_3 - s_2)}{N_1 N_3}, a_4 = \frac{2(s_1 - s_2)N_{1, s_2}}{n} - (s_2 - s_2)^2, a_5 = \frac{2(s_3 - s_2)N_{3, s_2}}{n} - (s_2 - s_2)^2, \) and \( a_6 = \frac{N^2}{n} - N s_2. \)

Our goal is to minimize \( f \) inside the polygon \( R \) defined by the constraints on \( N_1, N_3 \).

Let \( T \) be the list of the possible points that minimize \( f \). We set \( T = \emptyset \).

In order to minimize the quadratic function we find the critical points by computing the partial derivatives and set them to 0. \( \frac{\partial f}{\partial N_1} = 0 \Leftrightarrow 2a_1 N_1 + a_3 N_3 + a_4 = 0, \) and \( \frac{\partial f}{\partial N_3} = 0 \Leftrightarrow 2a_2 N_3 + a_3 N_1 + a_5 = 0. \) We solve this linear system of two unknowns.

We consider three cases. If the linear system has a unique solution \( N_1, N_3 \) then we check if the point \((N_1, N_3)\) lies in \( R \). If this is the case, we store the point \((N_1, N_3)\) in \( T \), otherwise we do not add any pair in \( T \). If the linear system has infinite solutions then it holds that in any solution \( N'_1, N'_3 \) of the system, \( 2a_1 N'_1 + a_3 N'_3 + a_4 = 0. \) This function defines a line on the 2-dimensional space of \( N_1, N_3 \).

We check if the line \( 2a_1 N_1 + a_3 N_3 + a_4 = 0 \) intersects the \( R \). If this is the case then let \( q = (q_1, q_2) \) be one intersection point. We add the point \((q_1, q_2)\) in \( T \). Notice that \( f \) takes the same value for all points on the line \( 2a_1 N_1 + a_3 N_3 + a_4 = 0 \), hence it is sufficient to store only one point. If the line does not intersect \( R \) then we do not add any pair in the list. Finally, if the linear system has no solution then we do not add any pair in the list.

So far we only searched for the critical points of the function \( f \). In case that those critical points do not lie in \( R \) or if those points are saddle points or global maxima, the function \( f \) is minimized over the boundary of \( R \). We continue our algorithm assuming the minimization of \( f \) on the boundary of \( R \). Then, for each side of \( R \) we do the following. We only describe it for the side where \( N_1 = \max \{N, t_1\} \) and without loss of generality assume that \( N_1 = t_1 \). The rest of the sides of \( R \) can be processed in the same way. Since, \( N_1 = t_1 \), we have to minimize the function \( f(t_1, N_3) = a_2 N_3^2 + (a_3 t_1 + a_5) N_3 + a_4 t_1 + a_5 t_1^2 + a_6 \), which is a quadratic function with one variable. We can easily check the minimum value of the function \( f(t_1, N_3) \), by computing the derivative. Let \((t_1, N_3)\) be the pair that minimizes \( f(t_1, N_3) \). We add \((t_1, N_3)\) to \( T \).

After computing \( T \), we check all points in \( T \) to find the optimum: Let \((x_1, x_3)\) be a point in \( T \). We evaluate the function \( f \) on a point \((x'_1, x'_3) \in R \) which is the closest point to \((x_1, x_3)\) with integer coordinates. In the end, we keep the integer values \((N_1, N_3)\) with the minimum \( f(\tilde{N}_1, \tilde{N}_3) \) over all pairs in \( T \). We also have \( \tilde{N}_2 = N - \tilde{N}_1 - \tilde{N}_3 \).

We repeat the above procedure for each pair of sampled points and in the end we return the boundaries that give the overall minimum variance. You can see the pseudocode of our algorithm in Algorithm 1.

Algorithm 1 Pseudocode

1: procedure PSEUDOCODE
2: Sort \( M \)
3: Compute the array \( \Gamma \)
4: \( (y_1, y_2) = \emptyset, r^* = +\infty \)
5: for each pair \((i, j)\) with \( m_i \leq i < m_j \leq m_i + 1 \) do
6: \( s_1 = \frac{\Gamma(i)}{\Gamma(i+1)} \left( 1 - \frac{\Gamma(i)}{\Gamma(i+1)} \right) \)
7: \( s_2 = \frac{\Gamma(j)}{\Gamma(j+1)} \left( 1 - \frac{\Gamma(j)}{\Gamma(j+1)} \right) \)
8: \( s_3 = \frac{\Gamma(m-j)}{\Gamma(m-j+1)} \left( 1 - \frac{\Gamma(m-j)}{\Gamma(m-j+1)} \right) \)
9: Define polygon \( R \) based on the constraints:
10: \( \max \{N, t_i\} \leq N_i \leq t_i + 1 \)
11: \( \max \{N, N_i-t_i+1\} \leq N_3 \leq N - t_i - 1 \)
12: \( N_1 + N_3 \leq N - N_i \)
13: \( a_1 = \frac{1}{(s_1 - s_2)^2} \)
14: \( a_2 = \frac{1}{(s_3 - s_2)^2} \)
15: \( a_3 = \frac{2(s_1 - s_2)(s_3 - s_2)}{n} \)
16: \( a_4 = \frac{2(s_1 - s_2)N_{1, s_2}}{n} - (s_2 - s_2)^2 \)
17: \( a_5 = \frac{2(s_3 - s_2)N_{3, s_2}}{n} - (s_2 - s_2)^2 \)
18: \( a_6 = \frac{N^2}{n} - N s_2 \)
19: Define \( f(N_1, N_3) = a_1 N_1^2 + a_2 N_3^2 + a_3 N_1 N_3 + a_4 N_1 + a_5 N_3 + a_6 \)
20: Let \( T \) be the set of critical points of \( f \) in \( R \) along with the candidate solutions over each side of \( R \):
21: \( (y_1, y_2) = \emptyset, r = +\infty \)
22: for \((x_1, x_3)\) in \( T \) do
23: Let \((x'_1, x'_3)\) be the closest point from \((x_1, x_3)\) with \( x_1, x'_3 \in Z, \) and \((x'_1, x'_3)\) in \( R \)
24: if \((x_1, x'_3) < r \) then
25: \( y_1 = x_1, y_3 = x'_3 \)
26: \( r = f(x'_1, x'_3) \)
27: end if
28: end for
29: if \((y_1, y_3) < r^* \) then
30: \( y'_1 = y_1, y'_3 = y_3 \)
31: \( r^* = f(y'_1, y'_3) \)
32: end if
33: end for
34: \( N_1 = y'_1, N_3 = y'_3, N_2 = N - N_1 - N_3 \)
35: return \((N_1, N_2, N_3)\)
36: end procedure

Assume that \((x_1, x_3)\) is the pair that minimizes the function \( f \) and \((N_1, N_3)\) is the closest integer coordinates point. Furthermore, let \( N'_1, N'_3 \) be the optimum integer values that minimize the function \( f \). Let \( v^* \) denote the minimum value of estimated variance defined in (9) achievable using \( n \) samples under stratified sampling with \( H = 3 \) strata where each stratum contains at least \( N \) objects.

Lemma 1. Assuming that \( N_i > n \), DirSol algorithm returns the boundaries of three strata with variance \( v \), such that \( v \leq (1 + \frac{2}{N_i} + \frac{2}{N_i-n} + \frac{4}{N_i(n-N)})v^* \).
Proof. First, we observe that \( |x_1 - N_1|, |x_3 - N_3| \leq 1 \) (notice that the intersection of the line \( N_1 + N_3 \leq N - N_2 \) with the rectangle defined by \( \max\{N, t_i\} \leq N_1 \leq t_i + 1, \max\{N, N - t_i + 1\} \leq N_3 \leq N - t_1 + 1, \) we can find integer coordinates so we can always find integer coordinates \( N_1 \in R \) within distance 1). Let also \( x_2 = N - x_1 - x_3, N_2 = N - N_1 - N_3 \) and \( N_2' = N - N_1' - N_2' \). In the worst case if \( N_1 = x_1 - 1 \) and \( N_3 = x_3 - 1 \) then \( N_2 = x_2 + 2 \). For simplicity we analyze the function 

\[
g(z_1, z_2, z_3) = \frac{1}{n}(z_1s_1 + z_2s_2 + z_3s_3) - \frac{1}{n}(z_1s_1' + z_2s_2' + z_3s_3')
\]

which is equivalent with the function \( f \). In particular, notice that 

\[
f(x_1, x_2) = g(x_1, x_2, x_3) \text{ and } f(N_1, N_2) = g(N_1, N_2, N_3)
\]

We have \( g(x_1, x_2, x_3) \) with \( g(N_1, N_2, N_3) \) term by term. We have,

\[
N_2s_2^2\left(\frac{N_2^2}{n} - 1\right) \leq (x_2 + s_2^2)\left(\frac{x_2}{n} - 1\right)(1 + \frac{2}{x_2} + \frac{2}{x_2 - n} + \frac{4}{x_2(x_2 - n)})
\]

\[
\leq x_2s_2^2\left(\frac{x_2}{n} - 1\right)(1 + \frac{2}{N_2 - n} + \frac{2}{N_2 - n} + \frac{4}{N_2(N_2 - n)})
\]

With the same way, it is easy to observe that \( N_1s_1^2\left(\frac{N_1^2}{n} - 1\right) \leq x_1s_1^2\left(\frac{x_1}{n} - 1\right)(1 + \frac{2}{N_1 - n} + \frac{2}{N_1 - n} + \frac{4}{N_1(N_1 - n)}) \) and \( N_3s_3^2\left(\frac{N_3^2}{n} - 1\right) \leq x_3s_3^2\left(\frac{x_3}{n} - 1\right)(1 + \frac{2}{N_3 - n} + \frac{2}{N_3 - n} + \frac{4}{N_3(N_3 - n)}) \).

It remains to bound the terms \( \frac{1}{n}N_1s_1N_2s_2, \frac{1}{n}N_1s_1N_3s_3, \) and \( \frac{1}{n}N_2s_2N_3s_3 \). We start by expanding the term \( \frac{1}{n}N_1s_1N_2s_2 \). We have,

\[
\frac{1}{n}N_1s_1N_2s_2 \leq \frac{1}{n}(x_1 + 1)s_1(x_2 + 2)s_2
\]

\[
= \frac{1}{n}x_1s_1x_2s_2(1 + \frac{2}{x_2} + \frac{2}{x_1} + \frac{2}{x_1x_2})
\]

\[
\leq \frac{1}{n}x_1s_1x_2s_2(1 + \frac{2}{N_1 - n} + \frac{2}{N_2 - n} + \frac{4}{N_1(N_1 - n)})
\]

Similarly, it is easy to see that \( \frac{1}{n}N_1s_1N_3s_3 \leq \frac{1}{n}x_1s_1x_3s_3(1 + \frac{2}{N_1 - n} + \frac{2}{N_3 - n} + \frac{4}{N_1(N_1 - n)}) \) and \( \frac{1}{n}N_1s_1N_3s_3 \leq \frac{1}{n}x_1s_1x_3s_3(1 + \frac{2}{N_1 - n} + \frac{2}{N_3 - n} + \frac{4}{N_1(N_1 - n)}) \).

We have that \( g(x_1, x_2, x_3) \leq g(N_1^*, N_2^*, N_3^*) = v^* \), so we conclude that

\[
g(N_1, N_2, N_3) \leq \left(1 + \frac{2}{N_1'} + \frac{2}{N_2'} + \frac{2}{N_3'} + \frac{4}{N_1(N_1' - n)}\right)g(N_1^*, N_2^*, N_3^*)
\]

That concludes the proof of Theorem 7.

\[\square\]

That concludes the proof of Theorem 7.

B. DETAILS ON LogBdr

Lemma 2. Assuming that \( N_i > n \), LogBdr algorithm returns the boundaries of \( k \) strata with variance \( v \), such that \( v \leq \max\{4, 2 + 2 \max_{1 \leq i \leq H} \frac{N_i'}{N_i^*} v^*\} \), where \( N_i^* \) is the size of the \( i \)-th stratum in the optimum solution.

Proof. We assume that the optimum allocation contains \( N_1',...,N_H' \) points in stratum \( 1,...,H \), respectively. Let \( S' \) be the set that contains the last sampled object in each stratum defined by \( N_1',...,N_H' \). Since the LogBdr algorithm considers all possible ways to partition the sampled points it will definitely consider the partitioning where the sampled objects in \( S' \) are the last sampled points in each stratum. Let \( t_1,...,t_{H-1} \) be the boundaries of the optimum strata. Let \( t_i' \) be the leftmost point in \( B_i \) which is at the right side of \( t_i \). Let \( N_1,...,N_H \) be the sizes of the strata we get using the points \( t_i' \) as the boundary points. We observe that \( N_i \leq 2N_i^* \) for all \( i \). Indeed, consider the size \( N_i^* \). Notice that in order to get \( N_i \)’s we always move the left boundaries of the strata to the right, so that makes the strata smaller. Now consider the right boundaries of the strata. From the way that we constructed \( B_i \), there always be a point \( t_i' \in B_i \) such that the number of points between \( o_i \) and \( t_i' \) is at most twice the number of points between \( o_i \) and \( t_i \). In addition by using the boundary points \( t_i' \) instead of the optimum \( t_i \), notice that we do not change the estimator \( s_i \) for stratum \( i \) for each \( i \leq H \).

The rest of the proof is similar to the proof of Lemma 1. Let \( g(x_1,...,x_H) \) be the function as we defined in the proof of Lemma 1. Let \( N_i',...,N_H' \) be the sizes that are found by our algorithm. Since we return the boundaries with the smallest variance, it holds that \( g(N_1',...,N_H') \leq g(N_1,...,N_H) \). Finally, we compare \( g(N_1,...,N_H) \) with \( g(N_1^*,...,N_H^*) \), term by term as we did in the proof of Lemma 1.

For any pair \( i,j \) we have \( \frac{1}{n}N_is_is_js_j \leq 4\frac{N_i^*}{n}N_i^*s_is_j \). For any \( i \), we also have,

\[
N_is_i^2\left(\frac{N_i^2}{n} - 1\right) \leq 2N_i^*s_i^2\left(\frac{2N_i^*}{n} - 1\right) = N_i^*s_i\left(\frac{N_i^2}{n} - 1\right)(2 + \frac{N_i'}{N_i^*} - \frac{N_i'}{N_i^*}).
\]

In any case we conclude that,

\[
g(N_1',...,N_H') \leq \max\{4, 2 + 2 \max_{1 \leq i \leq H} \frac{N_i'}{N_i^*} v^*\} g(N_1^*,...,N_H^*).
\]

That concludes the proof of Theorem 8.

C. DETAILS ON DynPgm

We show the approximation factor we get from algorithm DynPgm. Let \( N_1^*,...,N_H^* \) be the cardinalities of the strata in the optimum solution with variance \( v^* \).

Lemma 3. There exist strata with boundaries assuming the points in \( B \) and sizes \( \bar{N}_1,...,\bar{N}_H \) such that \( V(\bar{N}_1,...,\bar{N}_H) \leq \max\{4, 2 + 2 \max_{1 \leq i \leq H} \frac{N_i'}{N_i^*} v^*\} \) and \( 2N_i^* \geq \bar{N}_i \geq \bar{N}_i^*/2 \) for each \( i \leq H \).

Proof. Let \( t_i \) be the right boundary of stratum \( i \) in the optimum solution. Let \( t_i' \in B \) be the leftmost object at the right of \( t_i \). We construct the strata with cardinalities \( \bar{N}_1,...,\bar{N}_H \) by considering the objects \( t_i' \) for each \( i \) as boundaries. As we discussed in the slower algorithm for any \( H \) we have \( V(\bar{N}_1,...,\bar{N}_H) \leq \max\{4, 2 + 2 \max_{1 \leq i \leq H} \frac{N_i'}{N_i^*} v^*\} \).
max\(4.2 + 2 \max_{1 \leq h \leq H} \frac{N_j - N_i}{N_j} v^*\) and \(2N_j^* \geq \bar{N}_i\) for each \(i \leq H\). Assume that \(p_i, p_{i+1}\) be the two consecutive points in \(M\) such that \(w(p_i) < w(t_i) < w(p_{i+1})\) (if \(t_i \in M\) then the result follows). If there are \(y\) points in \(P_i\) and \(p_i\) we have the guarantee that between \(p_i\) and \(t_i\) there are at most \(2\) points. Since \(B\) contains all points in the order of powers of two from \(o_{i+1}\) to \(o_i\) it also follows that \(\bar{N}_i \geq N_i^*/2\) for each \(i \leq H\). \(\square\)

For simplicity we consider that for each \(i\), \(N_i^* \geq 4n\). We can generalize the results even if \(N_i^*\) is less than \(4n\), however the analysis of the first layer will be more tedious. Hence, from the above lemma we have that \(V(N_1, \ldots, N_H) \leq \frac{14}{3} v^*\).

Let \(v'\) be the minimum variance of an allocation assuming the objects in \(B\) when the size of the \(l\)-th stratum is \(N_l \geq 2n\) for each \(l \leq H\). Notice that the solution \(\bar{N}_1, \ldots, \bar{N}_H\) satisfies the inequalities \(\bar{N}_l \geq 2n\) because \(\bar{N}_l \geq N_l^*/2 \geq 2n\), hence the optimum allocation \(N_1, \ldots, N_H\) (and variance estimators \(s_1^2, \ldots, s_H^2\)) using objects from \(B\) with the additional constraint that \(N_l^* \geq 2n\) satisfies that \(V(N_1, \ldots, N_H) \leq \frac{14}{3} v^*\).

Let \(L = \sum_{i=1}^H N_i s_i^2\) be the auxiliary sum of the optimum allocation in \(B\) with the constraint \(N_l \geq 2n\). We also assume that the \(j\)-th stratum with size \(N_j^*\) has its right boundary on \(b_j \in B\). We define \(I = \{i_1, \ldots, i_H\}\). Next, we prove that the dynamic programming algorithm returns a good approximation.

First, assume that \(\sum_{i=1}^H N_i s_i^2 \geq 1\). Notice that \(\sum_{i=1}^H N_i s_i^2 \leq \sum_{i=1}^H N_i m \leq H N m\), so \(HN m\) is an upper bound on any auxiliary sum. Hence, in \(T\) there should always be a value \(t\) such that \(L \leq t \leq 2L\). Furthermore, let

\[
O(i, j) = \frac{1}{n} (\sum_{k=1}^i N_k s_k^2) - \frac{1}{n} \sum_{k=1}^i N_k^* s_k^2.
\]

**Lemma 4.** If \(L \geq 1\), for each \(i, j \in I\) we have that \(A[i, j, k] \leq (8j - 7)O[i, j, k] + 4\frac{1}{n} \sum_{y=1}^H (y - 1) (N_y s_y^2) \sum_{y=1}^H N_y s_y^2\).

**Proof.** We prove it by induction on the number of buckets. For \(j = 1\) we have from the definition that \(A[i_1, 1]\) has the optimum variance so \(A[i_1, 1] = \frac{1}{n} (N_i s_i^2) - N_i s_i^2\), and the inequality holds. Assume that this is true for \(A[i_{j-1}, j - 1]\). We will prove it for \(A[i_j, j']\). We have

\[
A[i, j, j'] \leq \frac{1}{n} N_j^2 s_j^2 - N_j s_j^2 + A[i, j - 1, j - 1] - \frac{2}{n} N_j s_j \sum_{l=1}^j N_l s_l.
\]

Since at each step we consider a stratum with \(N_i = s_i \leq t\), we have that \(X_i[i_{j-1}, j - 1] \leq (j - 1) t \leq 2(j - 1) \sum_{l=1}^j N_l s_l\) so

\[
A[i, j, j'] \leq \frac{1}{n} N_j^2 s_j^2 - N_j s_j^2 + A[i_{j-1}, j - 1] + \frac{4(j - 1)}{n} \sum_{l=1}^j N_l s_l^2.
\]

In addition we have,

\[
N_j s_j \sum_{l=1}^H N_l s_l = N_j s_j \sum_{l=1}^{j-1} N_l s_l + (N_j) s_j + \sum_{l=j+1}^H N_l s_l,
\]

so

\[
A[i, j, j'] \leq \frac{1}{n} N_j^2 s_j^2 - N_j s_j^2 + A[i_{j-1}, j - 1] + \frac{4(j - 1)}{n} \sum_{l=1}^j N_l s_l^2 + (N_j) s_j^2 + \sum_{l=j+1}^H N_l s_l^2.
\]

We focus on the expression \(\frac{1}{n} N_j^2 s_j^2 - N_j s_j^2 + \frac{4(j - 1)}{n} (N_j) s_j^2\). This can be written as \(N_j (s_j^2) + A[j-1, j] \leq (8j - 7)(\frac{1}{n} N_j^2 s_j^2 - N_j s_j^2)\). Finally,

\[
(2j - 1) - \frac{1}{2} N_j s_j \sum_{l=1}^{j-1} N_l s_l \leq (8j - 7) - \frac{1}{2} N_j s_j \sum_{l=1}^{j-1} N_l s_l,
\]

and

\[
A[i, j, j] \leq (8j - 7)O[i, j, j] + 4\frac{1}{n} \sum_{y=1}^H (y - 1) (N_y s_y^2) \sum_{y=1}^H N_y s_y^2,
\]

so we conclude that

\[
A[i, j, j] \leq (8j - 7)O[i, j, j] + 4\frac{1}{n} \sum_{y=1}^H (y - 1) (N_y s_y^2) \sum_{y=1}^H N_y s_y^2\sum_{y=1}^H N_y s_y^2.
\]

**From the lemma above, we have,**

\[
A[i_{H}, H] \leq (8H - 7)O[i_{H}, H] + \frac{1}{n} \sum_{y=1}^H 2(y - 1) (N_y s_y^2) \sum_{y=1}^H N_y s_y^2\sum_{y=1}^H N_y s_y^2.
\]

Notice that

\[
O[i_{H}, H] = \frac{1}{n} \sum_{a=1}^H N_a s_a^2 - \sum_{a=1}^H N_a (s_a)^2 \sum_{a=1}^H N_a (s_a)^2 = \sum_{a=1}^H N_a (s_a)^2 \left( \frac{N_a}{N} - 1 \right) + \frac{2}{n} \sum_{y=1}^H (N_y s_y^2) \sum_{y=1}^H N_y s_y^2 \sum_{y=1}^H N_y s_y^2,
\]

where

\[
\sum_{a=1}^H N_a (s_a)^2 \left( \frac{N_a}{N} - 1 \right) \geq 0 \text{ and } \frac{2}{n} \sum_{y=1}^H (N_y s_y^2) \sum_{y=1}^H N_y s_y^2 \sum_{y=1}^H N_y s_y^2 \geq 0.
\]

Each term \(\frac{2}{n} \sum_{y=1}^H (N_y s_y^2) \sum_{y=1}^H N_y s_y^2 \sum_{y=1}^H N_y s_y^2\) for \(l\) such that \(y + 1 \leq l \) exists in \(O[i_{H}, H]\), so we have

\[
A[i_{H}, H] \leq (10H - 9)O[i_{H}, H] = (10H - 9)V(N_1, \ldots, N_H).
\]

Since \(V(N_1, \ldots, N_H) \leq \frac{14}{3} v^*\), we conclude that the solution we get in the dynamic programming algorithm has variance at most \(\frac{14}{3} (10H - 9) v^*\).

Finally, we assume that \(\sum_{l=1}^H N_l s_l^2 < 1\). The proof is similar to the previous case. Notice that in \(T\) there should always be a value \(t\) such that \(L \leq t \leq L + \varepsilon\). Similar to Lemma we can show:

**Lemma 5.** If \(L \leq 1\), for each \(i, j \in I\) we have that \(A[i, j, j] \leq (4j - 3)O[i, j, j] + 2\frac{1}{n} \sum_{y=1}^H (y - 1) (N_y s_y^2) \sum_{y=1}^H N_y s_y^2 + \frac{16}{n} \sum_{y=1}^H (y - 1) N_y s_y^2\).
Proof. We prove it by induction on the number of buckets. For \( j = 1 \) we have from the definition that \( A_r[i, 1] \) has the optimum variance so \( A_r[i, 1] = \frac{1}{n} (N_i'(s_i')^2 - N_i'(s_i')^2) \), and the inequality holds. Assume that this is true for \( A_r[i_{j-1}, j-1] \). We will prove it for \( A_r[i_{j}, j] \).

\[
A_r[i_{j}, j] \leq \frac{1}{n} N_j'^2 s_j'^2 - N_j'^2 s_j'^2 + A_r[i_{j-1}, j-1] + \frac{2}{n} N_j'^2 s_j' X_r[i_{j-1}, j-1].
\]

Since at each step we consider a stratum with \( N_i \cdot s_i \leq t \), we have that \( X_r[i_{j-1}, j-1] \leq (j-1)t \leq (j-1) \left( \sum_{i=1}^{H} N_i'(s_i' + \varepsilon) \right) \) so

\[
A_r[i_{j}, j] \leq \frac{1}{n} N_j'^2 s_j'^2 - N_j'^2 s_j'^2 + A_r[i_{j-1}, j-1] + \frac{2(j-1)}{n} N_j'^2 s_j'.
\]

In addition we have,

\[
N_j'^2 s_j' \sum_{i=1}^{H} N_i s_i' = N_j'^2 s_j' \sum_{i=1}^{H} N_i s_i' + (N_j')(s_j')^2 + N_j'^2 s_j' \sum_{i=1}^{H} N_i s_i',
\]

so

\[
A_r[i_{j}, j] \leq \frac{1}{n} N_j'^2 s_j'^2 - N_j'^2 s_j'^2 + A_r[i_{j-1}, j-1] + \frac{2(j-1)}{n} (N_j' s_j' + (N_j')(s_j')^2)
\]

\[
+ \frac{2(j-1)}{n} N_j'^2 s_j' \sum_{i=1}^{H} N_i s_i'.
\]

We focus on the expression \( \frac{1}{n} N_j'^2 s_j'^2 - N_j'^2 s_j'^2 + \frac{2(j-1)}{n} (N_j')(s_j')^2 \).

This can be written as \( N_j'(s_j')^2 \left( \frac{2(j-1)}{n} N_j' - 1 \right) \). Since \( N_j' \geq 2n \) we have that \( (2(j-1)N_j') \geq 1 \) and \( \frac{1}{n} N_j'^2 s_j'^2 - N_j'^2 s_j'^2 + \frac{2(j-1)}{n} (N_j')(s_j')^2 \geq (j-3) \frac{1}{n} N_j'^2 s_j'^2 - N_j'^2 s_j'^2 \).

Finally,

\[
(j-1)\frac{1}{n} 2N_j'^2 s_j' \sum_{i=1}^{H} N_i s_i' \leq (j-3)\frac{1}{n} 2N_j'^2 s_j' \sum_{i=1}^{H} N_i s_i',
\]

and

\[
A_r[i_{j-1}, j-1] \leq (j-4)O[i_{j-1}, j] + 2\frac{1}{n} \sum_{i=1}^{H} (y-1) N_i' s_i' \sum_{i=1}^{H} N_i' s_i' + \frac{2}{n} \sum_{i=1}^{H} (y-1) N_i' s_i'.
\]

so we conclude that

\[
A_r[i_{j}, j] \leq (j-4)O[i_{j}, j] + 2\frac{1}{n} \sum_{i=1}^{H} (y-1) N_i' s_i' \sum_{i=1}^{H} N_i' s_i' + \frac{2}{n} \sum_{i=1}^{H} (y-1) N_i' s_i'.
\]

From the lemma above, we have,

\[
A_r[i_{H}, H] \leq (4H-3)O[i_{H}, H] + \frac{1}{n} \sum_{y=1}^{H} 2(y-1) N_i' s_i' \sum_{i=1}^{H} N_i' s_i' + \frac{2}{n} \sum_{y=1}^{H} (y-1) N_i' s_i'.
\]

D. DETAILS ON DynPgmP

Lemma 6. DynPgmPalgorithm returns the boundaries of \( k \) strata with variance \( v \), such that \( v \leq 2v^* \).

Proof. DynPgmPalgorithm returns the optimum answer with respect to points in \( B \), since the objective function is decomposable. Let \( N_1', \ldots, N_H \) be the sizes of the optimum strata. Because of the selection of \( B \) and Lemma 2, the dynamic programming algorithm always consider a solution where the size of each stratum is \( N_h' \leq 2N_h' \) for each \( h \leq H \), and the estimated variance in each stratum is the same as in the optimum solution. Hence, we can easily observe that \( N_h' s_h'^2 \leq 2N_h' s_h'^2 \). Let \( v^* \) be the variance of such a solution (with sizes \( N_1', \ldots, N_H' \)). Since \( B \) returns the best solution we have that \( v \leq v^* \leq 2v^* \).

That concludes the proof of Theorem 4.