Adaptive threshold sampling and unbiased estimation

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Abstract

Sampling is a fundamental problem in both computer science and statistics. A number of issues arise when designing a method based on sampling. These include statistical considerations such as constructing a good sampling design and ensuring there are good, tractable estimators for the quantities of interest as well as computational considerations such as designing fast algorithms for streaming data and ensuring the sample fits within memory constraints. Unfortunately, existing sampling methods are only able to address all of these issues in limited scenarios.

We develop a framework that can be used to address these issues in a broad range of scenarios. In particular, it addresses the problem of drawing and using samples under some memory budget constraint. This problem can be challenging since the memory budget forces samples to be drawn non-independently and consequently, makes computation of resulting estimators difficult.

At the core of the framework is the notion of a data adaptive thresholding scheme where the threshold effectively allows one to treat the non-independent sample as if it were drawn independently. We provide sufficient conditions for a thresholding scheme to allow this and provide ways to build and compose such schemes. Furthermore, we provide fast algorithms to efficiently sample under these thresholding schemes.

1 Introduction

For sampling problems, there are three primary issues to deal with:

- How to select "good" data
- How to do so quickly with limited space
- How to turn the data into useful quantities or summaries

In computer science and statistics, various methods have been proposed to address one or two issues at a time. However, few are able to simultaneously

address all three as a solution to one issue can introduce difficulties in another. In computer science applications, the problems are often algorithmic in nature. Sampling is often used to reduce extremely large datasets into a summary that has fixed size [27], [1], [22], [15], [2]. In statistics, sampling is used to choose which measurements to take, with the goal of obtaining the most accurate estimate with the least amount of data. The resulting problems typically center around sampling design and estimation [13], [21], [6]. However, solutions to the problems can quickly become computationally intractable.

One particularly important problem when building systems that employ sampling is ensuring that the space required by the sample does not exceed the system's capacity. This space constrained sampling does not allow data points to be drawn independently. As a consequence, estimation of quantities of interest can be difficult, since exact inclusion probabilities may be intractable to compute in non-uniform sampling designs or the naive estimator is derived under the assumption of independence.

To see this, note that when weighted sampling is performed under the presence of space constraints, independence of the samples is broken, and the resulting probability distributions are typically intractable to work with. For example, in simple weighted sampling without replacement, each item is sampled in proportion to its weight, removed from the set of candidates, and the process is repeated k times. After each step, the sampling probabilities change dependent on the previous items selected. As a result, computing the probability of a given sample requires summing over $k!$ possible permutations. Computing the marginal probability that an item is included in the sample requires summing over the $\binom{n-1}{k-1}$ different samples that include that item. In the language of graphical models, after conditioning on the threshold, moralization of the graph yields a fully connected clique and an extremely high treewidth of n.

Thus, solving the second problem of sampling quickly with limited space results in complications with the first problem of selecting "good" data non-uniformly as well as the third problem of estimation of quantities of interest. A common solution in existing work is to assume that one has prior knowledge of the data set. This allows one to set inclusion probabilities for an independent Poisson sample that approximately yield a desired sample size. While reasonable given repeated workloads, this is a highly unrealistic for a general purpose system which may be ingesting new datasets or datasets that can vary greatly in size over time. Furthermore, this problem is more difficult when balancing the memory usage of samples for many sets of data [2].

We propose a class of sampling methods that we call *adaptive thresholding sampling schemes*. We show how such schemes can be used to generate sampling designs which have efficient algorithms for sampling. Furthermore, estimation is simple as the resulting samples can be treated almost like conditionally independent samples given the threshold with an easily computable pseudo-inclusion probability. This allows such schemes to address all three areas of concern: sampling design, algorithms, and estimation.

While the use of adaptive thresholds is not new, previous schemes only generate a subset of sampling designs and provide the theoretical justification for the

small, but important, class of Horvitz-Thompson estimators. Our work extends the sampling designs that can be efficiently generated and demonstrates how to construct theoretically justified estimators. Furthermore, our work includes a substantial number of existing sampling schemes and makes the proofs of their associated unbiasedness estimators trivial. These include work in database join size estimation [7], approximate distinct counting [18], multi-objective sampling [8], frequency-capped sampling [9], and others.

Our paper is structured as follows. First, we provide some background and intuition behind our contributions. We describe priority sampling and its connections to order sampling with fixed shape and the Horvitz-Thompson estimator to show how it works. We then introduce our contributions, what we call the distribution substitution trick and adaptive sampling schemes. Whereas priority sampling gives a set of adjusted weights and shows that they are uncorrelated, our application of the distribution substitution trick in theorem 4 states that the sample can often be treated as an independent sample conditional on the threshold. This has significant consequences as it shows that unbiased estimators for independent samples can often immediately yield an unbiased estimator for an adaptive threshold sample. The condition under which this holds depends on the amount interaction between sampled points allowed by the thresholding scheme and the amount of interaction required by the estimator.

In addition to unbiasedness, we examine the consistency properties of a adaptive thresholding schemes. This includes cases where an estimator of interest includes too many interactions or the thresholding scheme uses information not allowed by the distribution substitution trick.

We then examine sampling designs and give methods to verify the conditions required for the distribution substitution trick to hold. This provides another set of contributions as it gives procedures to generate and compose designs that satisfy the conditions by manipulating the threshold. This covers existing designs including weighted reservoir sampling described by [22] and [15], Wegman's sampling method of [18], and multi-objective sampling [8]. It also simplifies and improves other sampling algorithms such as adaptive reservoir sampling [2]. We further demonstrate its use by constructing several novel designs as well. For instance, we construct a stratified sample using a fixed memory budget but unknown item sizes and an unknown number of strata. More examples are given in section 8.

We also derive new algorithms for the sampling designs covered by basic priority sampling. In particular, we show that priority sampling can be converted into a simple reservoir sampling algorithm with a small modification to keep track of high weight items. When no weight is too large, the algorithm reduces to a simple reservoir sampling algorithm. We use this along with the earlier estimation theory on a streaming logistic regression example and show that we can choose points that are more informative than one chosen from a simple exponential decay model. In simulations, the resulting samples reduce the squared error by over half which is equivalent to having a sample size that is over twice as large.

For reference, a table of commonly used symbols is given in table 1.

2 Basic sampling design

The notion of weighted or unequal probability sampling is at the core of many sampling problems that improve upon simple random sampling. An ideal sampling scheme or design is able to sample the most informative items with the highest probabilities. For example, to estimate the join size of two tables it is sensible to sample keys in proportion to their multiplicity. A simple random sample can be inefficient when sampled elements contribute unequally to the final population estimate. For example, to estimate total corn production in a state, it is beneficial to favor sampling large, influential farms based on acreage or some other easily obtained measure of size. Such a scheme reduces the variance of the final estimate and is an example of an unequal probability sampling design. Some other sampling design choices that reduce variance include sampling without replacement and stratified sampling.

In unequal probability sampling designs, an unbiased estimate of the population total S is given by the Horvitz-Thompson estimator,

$$\hat{S} = \sum_i x_i \frac{Z_i}{\pi_i} \tag{1}$$

where Z_i indicates if the item x_i is included in the sample and $\pi_i = p(Z_i = 1)$ is the inclusion probability. If the inclusion probabilities $\pi_i \propto x_i$ and the sample size is fixed at k, it is clear that the variance of the estimator is minimized as $\hat{S}$ is constant. In surveys, the quantities of interest x_i are not available to the sampler, and a correlated surrogate is used to devise the inclusion probabilities. Likewise, in some database applications such as join size estimation where x_i may be the number of output records for the i^{th} join key, there may only be partial information about the size available, namely the multiplicity of the i^{th} key in one table. However, when generating a sample from a database simply to reduce computational costs, the exact value x_i is often available. In such cases, the main difficulties in sampling arise from the difficulty in computing the sampling probabilities π_i under sample size constraints and when sampling without replacement.

The statistics literature on sampling without replacement from a target distribution $\{\pi_i\}_i$ is considerable. Over 50 methods are described in [5] in 1982. Of particular interest is [24] which formalized the notion of order sampling schemes and derived asymptotic properties of these schemes. This provided a sampling scheme which was algorithmically efficient, allowed specifying target sampling probabilities for fixed size samples, and had good asymptotic estimation properties. In this scheme, the elements x_i are ordered by random independent priority variables $R_i \sim F_i$ for some distributions F_i, and the k items with the smallest priorities are included in the sample. Of particular interest is the case where items are weighted (x_i, w_i), and the priorities can be rescaled so that $\alpha(w_i)R_i \sim F$ are drawn from a common distribution F under some function of the weights α. If the weights w_i represent target inclusion probabilities, then $\alpha(w_i) = F^{-1}(w_i)$ results in an order sample with inclusion probabilities that

approximate the targets [25]. This class of sampling schemes is called *order sampling with fixed distribution shape* (OSFS). Although the method provides asymptotic approximation to the inclusion probabilities, their exact computation is difficult, and hence, deriving an unbiased estimator is similarly difficult.

2.1 Adaptive threshold sampling

Our work focus on a class of sampling methods that control inclusion in the sample by a data dependent threshold. This can control both the total size of the sample as well as individual inclusion probabilities.

An adaptive thresholding scheme is comprised of two parts. One associates each item x_i with some random quantity $R_i \in \mathcal{R}$ where $\mathcal{R}$ is a partially ordered set (poset). The second part defines a threshold τ_i taking values in $\mathcal{R}$ and is a random function of the data and random quantities $\{(x_j, R_j)\}_j$. The item x_i is included in the sample if $R_i < \tau_i$. This event is denoted by Z_i which is 1 if $R_i < \tau_i$ and 0 otherwise. To simplify exposition, we will take $\mathcal{R} = \mathbb{R}$ to be the reals unless otherwise noted.

2.2 Priority Sampling

Priority sampling [14] introduces a modification to order sampling where the smallest $k+1$ priorities are retained but only the smallest k are used for estimation. Surprisingly, this modification addresses the deficiency of OSFS as it greatly simplifies calculations and allows a unbiased estimators for the sum and variance to be derived. Priority sampling can be described as follows.

For simplicity, assume $x_i > 0$ for all i. In priority sampling, max-priorities are generated by taking $T_i = x_i/U_i$ where the U_i are i.i.d. $Uniform(0,1)$ random variates and the largest $k+1$ priorities are retained. This is equivalent to taking the $k+1$ smallest priorities defined by $R_i = 1/T_i = U_i/x_i$. The $(k+1)^{th}$ smallest R_i is the threshold τ. Define new variables $\tilde{X}_i = \max\{1/\tau, x_i\}$. Let $\mathcal{J}$ be the set of indices for the k smallest priorities. The estimate for the population sum $S = \sum_i x_i$ is given by $\hat{S} = \sum_{i\in\mathcal{J}} \tilde{X}_i$. It turns out that this estimator is unbiased. Furthermore, the $\tilde{X}_i$ can be shown to be uncorrelated. For the remainder of this paper, any priority will always be a min-priority.

How priority sampling works is unclear from its original description. It was described as magical by its creators [3]. The workings become evident once formulated in terms of order sampling with fixed shape. Since the priorities are invariant to scaling, one may rescale the weights $w_i \leq 1$. In that case $F^{-1}(w_i) = w_i$ where F is the cumulative distribution function (cdf) of a $Uniform(0,1)$ variable. Thus, $w_i R_i \sim F$ and priority sampling is an instance of order sampling with fixed shape. Since $F(x_i\tau) = \min\{1, x_i\tau\}$, the estimator for the population sum can be given in a form similar to the Horvitz-Thompson estimator.

$$\hat{S} = \sum_{i\in\mathcal{J}} \frac{x_i}{F(w_i\tau)}. \tag{2}$$

This leads to the following generalization which was noted by [10]. Given any order sampling scheme with cdfs F_i, let $\tau = R_{(k+1)}$ be the $(k+1)^{th}$ smallest priority and $\mathcal{J}$ be the indices of the k smallest priorities. An estimate of the population sum is given by equation 2.

3 Distribution Substitution Trick and Unbiasedness

Priority sampling provides a stronger unbiasedness guarantee than OSFS which only provides asymptotic results. The validity of these can be established by a simple technique we introduce and call the "distribution substitution trick." It further shows that the sample using only the k smallest ranked elements can be treated in almost the same manner as using an easy to analyze conditionally independent sample.

The distribution substitution trick is described as follows. Consider a set of functions $\mathcal{F}$ and probability measures P, Q where P is easy to sample from and Q easy to evaluate. If for all $f \in \mathcal{F}$, we have

$$\int g(x)dP(x) = \int g(x)dQ(x) \tag{3}$$

then any estimator in $\mathcal{F}$ which is unbiased under the assumption that Q is the sampling distribution is also unbiased when the true distribution is P. In other words, one can assume Q when the distribution is P in reality. The crucial restriction is that this only applies to a restricted class of functions $\mathcal{F}$.

For the cases we consider, the set of estimators of interest are functions of the sample plus a threshold and possibly some auxiliary information. Items which are not in the sample are discarded, and hence, not available for use in the estimator. To make computations easy, we typically choose Q so that the sampled items are modeled by independent draws.

3.1 General estimation for Priority Sampling

To see how the distribution substitution trick works, consider the case of priority sampling. We show how one can derive an estimator under the easy to work with assumption of independent Bernoulli sampling and then directly apply it to the sampling without replacement priority sampling scheme. For simplicity, assume the priorities are drawn $R_i \sim F_i$ with densities f_i. Let Z_i indicate if x_i is in the sample and $\mathcal{J}$ be the corresponding set of indices for the sampled items. Denote the threshold by τ, and let S be the index of the item selected as the threshold $x_S = \tau$. Denote by Λ_k the set of all possible combinations of up to k indices. Any estimator of an unknown parameter θ is a function g of the samples and threshold. It can be written as $g(\mathbf{Z}, \tau) = \sum_{\lambda \in \Lambda_k} \beta_\lambda(\mathbf{x}_\lambda, \tau) \prod_{j \in \lambda} Z_j$ for some functions β_λ. In other words, given a the threshold value, g is a k degree polynomial in the indicators $\mathbf{Z}$. The function g is an unbiased estimator if the

expectation $\mathbb{E}_P g(\mathbf{Z}, \tau) = \theta$. This expectation is difficult to compute due to the dependence of the indicators Z_i as well as the threshold τ. However, the distribution substitution trick may be easily applied to each term $\beta_\lambda(\mathbf{x}_\lambda, T) \prod_{j \in \lambda} Z_j$.

The probability density function for observing $\mathcal{J}$ with threshold τ is

$$p(\mathbf{z}, s, \tau) = f_s(\tau) \prod_{i \neq s} F_i(\tau)^{z_i} (1 - F_i(\tau))^{1 - z_i} \tag{4}$$

whenever $\sum_i z_i = k$ and 0 otherwise. Whenever $z_i = 1$ for all $i \in \lambda$, this constraint is equivalent to $\sum_{i \notin \lambda} z_i = k - |\lambda|$. Now consider the distribution $\tilde{P}_\lambda$ which first draws a threshold τ equal to the $k - |\lambda| + 1$ order statistic for the random priorities excluding those in λ, and then draws conditionally independent $Bernoulli(F_i(\tau))$ inclusion variables for those in λ. The probability of observing $\mathcal{J}$ with threshold τ is exactly the same under $\tilde{P}_\lambda$ as P. Thus, the expectation $\mathbb{E}_P g_\lambda = E_{\tilde{P}_\lambda} g_\lambda$ as the densities on the support of g_λ are identical.

To derive an unbiased estimator using the distribution substitution trick, consider a Horvitz-Thompson style estimator

$$\hat{S} = \sum_i x_i \beta(\tau) Z_i. \tag{5}$$

While $\mathbb{E}_P Z_i$ is difficult to compute, the distribution substitution trick allows one to easily compute the expectation under $\tilde{P}_{\{i\}}$. This gives that $\hat{S}$ is unbiased if $\mathbb{E}_{\tilde{P}_{\{i\}}} \beta_i(\tau) Z_i = 1$ which trivially holds if $\beta_i(\tau) = 1/F_i(\tau)$. The variance of this estimator is

$$\mathrm{Var}(\hat{S}) = \sum_{i,j} x_i x_j Cov\left(\frac{Z_i}{F_i(\tau)}, \frac{Z_j}{F_j(\tau)}\right) \tag{6}$$

Since the covariance depends only on pairwise inclusions $Z_i Z_j$, it follows that the variance can be estimated as

$$\begin{aligned} Cov\left(\frac{Z_i}{F_i(\tau)}, \frac{Z_j}{F_j(\tau)}\right) &= \mathbb{E}\frac{Z_i Z_j}{F_i(\tau) F_j(\tau)} - 1 \\ &= \begin{cases} \mathbb{E}_{\tilde{P}_{\{i,j\}}} \frac{1}{F_i(\tau)} - 1 & \text{if } i = j \\ 0 & \text{otherwise,} \end{cases} \\ \hat{\mathrm{Var}}(\hat{S}) &= \sum_i x_i^2 Z_i \left(\frac{1 - F_i(\tau)}{F_i(\tau)^2}\right). \end{aligned} \tag{7}$$

Note that this straightforward application of the distribution substitution trick already generates a novel result as this generalizes the variance estimator for priority sampling given in [14] by allowing for arbitrary weighting schemes rather than only probability proportional to size weights.

3.2 Substitution compatibility

The previous example demonstrated the value of the distribution substitution trick in deriving principled estimators. We now establish the conditions under

which it can be applied. This allows us both to identify the set of estimators that are available for use as well as the sampling designs one can generalize the methods to. We give a sufficient set of conditions called *substitution compatibility*.

For adaptive threshold sampling, we will consider a slightly richer class of estimators than the ones given for basic priority sampling in section 3.1. First, the threshold τ is vector valued to give per-item thresholds: $Z_i = 1$ if and only if $R_i < \tau_i$. Second, the coefficients β may also depend on some summarization M of the rejected items. For example, M may contain information on the total number or rejected items or equivalently, the number of items in the sample. The estimator may then be a function of the sample size. We will say a function is a *degree V estimator* if it has form

$$g(\mathbf{Z}, \tau, M) = \sum_{\lambda \in \Lambda_V} \beta_\lambda(\mathbf{x}_\lambda, \tau, M) \prod_{j \in \lambda} Z_j \tag{8}$$

for some constant V or random V that is a function of M and τ. This allows us to define substitution compatibility.

Definition 1 (Strong Substitution compatibility)**.** *Let $\mathcal{J}$ be a random sample from a thresholded sampling scheme P with continuous cdfs F_i and corresponding densities f_i and with thresholds τ_i. Let $\mathcal{F}$ be a class of degree n estimators using auxiliary information M. Let Q_τ be the distribution which draws a sample using independent Bernoulli$(F_i(\tau_i))$ draws. The threshold τ is* strongly substitution compatible with $\mathcal{F}$ *if for any function $g \in \mathcal{F}$ with coefficients $\beta_\lambda(\mathbf{x}_\lambda, \tau, M)$ some h_λ, the density*

$$p\left(\mathbf{R}_\lambda, \tau, M\right) = \prod_{i \in \lambda} f_i(R_i) h_\lambda(\tau, M) 1(R_i < \tau_i) \tag{9}$$

whenever $\beta_\lambda(\mathbf{x}_\lambda, \tau, M) > 0$. When this holds for the class $\mathcal{F}$ consisting of all degree V estimators where V is some function of τ, M, we say the thresholding scheme is strongly V substitution compatible*. When this holds for the class of estimators that are computable from the sample, so that the coefficient $\beta_\lambda(\mathbf{x}_\lambda, \tau, M) = 0$ whenever $|\lambda| > |\mathcal{J}|$, then we simply say the thresholding scheme is* strongly substitution compatible*.*

The important property of substitution compatibility is that it also yields a factorization for the inclusion probabilities. When this weaker factorization holds, we say the threshold is just (V) substitution compatible.

Lemma 2. *If τ yields the factorization in equation 9, then there is a corresponding factorization for the inclusion probabilities given by*

$$p\left(\prod_{i \in \lambda} Z_i = 1, \tau, M\right) = \prod_{i \in \lambda} F_i(\tau_i) h_\lambda(\tau, M) \tag{10}$$

Proof. Integrate over R_i for $i \in \lambda$. □

x_i, w_i	Value and weight of the i^{th} item
$R_i \sim F_i$	Min-priorities and their distribution
$R_{(i)}$	The i^{th} smallest priority
τ	Threshold
Z_i	Sample inclusion indicator
$\mathcal{J}$	Indices of sampled items
π_i	Inclusion probability $p(Z_i = 1)$
λ	Set of indices
Λ_k	Set of all combinations of indices with size k
$\mathbb{E}_P$	Expectation under distribution P
$\mathbf{x}_\lambda$	$(x_i : i \in \lambda)$
P	True sampling distribution
Q_τ	Independent $Bernoulli(F_i(\tau_i))$ distribution

Table 1: Table of symbols

We note neither V substitution compatibility and substitution compatibility imply the other. Clearly, 1 substitution compatibility is weaker than substitution compatibility as long as the sample is always non-empty. On the other hand, if the threshold is always R_1 so that $Z_i = 0$ always, the resulting threshold is not 1 substitution compatible as there is no compatible factorization for $p(Z_1 = 1, \tau, M)$. V substitution compatibility is more easily applied when designing estimators since it does not require knowing which combinations have 0 probability of occurring. Checking V substitution compatibility for a substitution compatible threshold can be easily performed.

Corollary 3. *For priorities $\{F_i\}$, let τ be a substitution compatible threshold with auxiliary information M. If for some function V of τ and M and for all subsets of indices λ with $|\lambda| \leq V$ one has that the support $p(Z_\lambda = \mathbf{1}, \tau, M) > 0$ whenever $F_i(\tau_i) > 0$ for all $i \in lambda$, then τ is V substitution compatible.*

In some cases, we will consider τ to be a thresholding rule rather than a random variable itself. In this case τ is a function taking the set of priorities as an argument, and $\tau(\mathbf{R})$ is the random threshold. In this case, the thresholding rule τ is said to be substitution compatible if and only if $\tau(\mathbf{R})$ is a substitution compatible threshold for any set of independent priorities.

3.3 Adaptive Threshold Sampling

We now formalize the example given in section 3.1 for deriving unbiased estimators under the sampling distribution.

Theorem 4 (Generalized Priority Sampling)**.** *Let P be a thresholded sampling scheme that is weakly substitution compatible for $\mathcal{F}$, and let θ be a population quantity to be estimated. If an estimator $\hat{\theta}(\mathcal{J}, \tau, M) \in \mathcal{F}$ is an unbiased estimator of θ under Q_τ so that $\overline{\theta}(\tau, M) := \mathbb{E}_{Q_\tau}\hat{\theta}(\mathcal{J}, \tau, M) = \theta$, then $\hat{\theta}(\mathcal{J}, \tau, M)$ is an unbiased estimator under P. More generally, for any estimator $\hat{\theta} \in \mathcal{F}$, one has $\mathbb{E}_P\mathbb{E}_{Q_\tau}\hat{\theta}(\mathcal{J}, \tau, M) = \mathbb{E}_P\hat{\theta}(\mathcal{J}, \tau, M)$.*

Proof. This immediately follows from the distribution substitution trick. □

In practical terms, this theorem states that for a large class of expectations of interest one can treat an adaptive threshold sample as if it were an independent Bernoulli weighted sample. The cost of doing so is the need to store an additional threshold value and the primary restriction is that the estimator can only utilize interactions of up to v items or whatever interactions are allowed by the function class.

This provides a simple recipe to deriving estimators under adaptive threshold sampling. Compute an unbiased or consistent estimator assuming the sample is an independent $Bernoulli(F_i(\tau))$ random sample with fixed threshold τ. That estimator is also unbiased or consistent under the true distribution P when it does not include too many interactions between items in the sample.

We apply this recipe to provide a simpler way to compute the unbiased subset sum variance estimator given in equation 7. An unbiased estimate of the variance of $Z \sim Bernoulli(p)$ is given by $Z(1-p)$. Under independent $Bernoulli(F_i(\tau))$ sampling, the Horvitz-Thompson estimator in equation 2 is a weighted sum of independent Bernoulli random variables and has an unbiased variance estimate $\sum_i Z_i(x_i/F_i(\tau))^2(1-F_i(\tau))$.

Although the recipe provides a simple way to derive a suitable estimator for an adaptive threshold sample, we note that not every estimator derived under independent Bernoulli Q_τ sampling can make use of the distribution substitution trick. For example, consider the simple linear regression estimator, $\hat{\beta} = (X^T ZX)^{-1} X^T ZY$ where the regression is on d variables and Z is a weighted diagonal selection matrix with $Z_{ii} > 0$ if item i is in the sample. When Z is the identity matrix, the population coefficients β are obtained. Due to the inverse term $(X^T ZX)^{-1}$, the resulting estimator is an n degree polynomial in Z. However, a priority sample has only k items in the sample. It is only k substitution compatible and not n substitution compatible.

However, a slightly different estimand does have an unbiased estimator which can also be used to give a nearly unbiased estimator for the regression coefficients. By Cramer's rule, it is easy to see that the entries of $|X^T ZX|(X^T ZX)^{-1}$ are degree $d-1$ polynomials in Z. Furthermore, the entries of $X^T ZY$ are degree 1 polynomials in Z. Thus, the population value $|X^T X|\beta$ has an unbiased estimate whenever $k \geq d$ as $|X^T ZX|\hat{\beta}$ is a degree d polynomial in Z. This estimator is also provably consistent when the data points (X_i, Y_i) are i.i.d. and $k \to \infty$. This is since $k \geq 2d$, so the variance is computable under Q_τ and goes to 0 . Since $|X^T ZX|$ is a degree d polynomial in Z, the distribution substitution trick can again be applied to show $\text{Var}|X^T ZX| = O(k)$, so that $|X^T ZX|$ is consistent. Hence, $\hat{\beta}$ is consistent as well.

In this case, the unbiased estimator is complex as it cannot be expressed by simply weighting in the Z matrix. However, as described in section 5.1, the distribution substitution trick can be applied to the loss function that generates the usual regression estimator $J(b) = \sum_i Z_i(Y_i - X_i b)^2$. Although the distribution substitution trick no longer directly provides unbiasedness properties for the estimator, it shows that the is still a principled estimator since it minimizes

a noisy version of the same loss function. One can obtain provably good properties as well since the same method used above in expressing the estimator as a ratio of d degree polynomials also proves that the weighted linear regression estimator is consistent. Section 5.2 gives further methods for obtaining an estimator for which the distribution substitution trick applies.

3.4 Threshold inclusion

In order to further improve the efficiency of an estimator, it is beneficial to also make use of information in the threshold. This can be accomplished by "forgetting" which item is the threshold and resampling it. This averaging can further reduce the variance of the estimator.

Theorem 5 (Threshold inclusion)**.** *Consider the conditions in theorem 4 and further assume that for all $i \in \mathcal{J}$ and some s, $\tau_i = R_s$. Let $\tilde{\mathcal{J}} = \mathcal{J} \cup \{s\}$ and $\tilde{\mathcal{J}}_{-j} = \tilde{\mathcal{J}}/\{j\}$ be the sample excluding j. The estimator*

$$\hat{\theta}'(\tilde{\mathcal{J}}, \tau) = \sum_{j \in \tilde{\mathcal{J}}} \hat{\theta}(\tilde{\mathcal{J}}_{-j}, \tau) p(R_j = \tau | \tilde{\mathcal{J}}) \tag{11}$$

is an unbiased estimator of θ under P.

Proof. Given in the appendix. □

In the case of a fixed size sample of size k, [10] provided this result which gives a sample of size $k + 1$. The weights used to combine the estimators is simple to compute and are given by $p(R_j = \tau | \tilde{\mathcal{J}}) \propto f_j(\tau)/F_j(\tau)$.

3.5 Streaming and Permutation invariance

Theorem 4 is somewhat abstract as the conditions under which it can be applied are not always obvious. Most of the remaining theory developed for the method revolves around establishing conditions and sampling schemes where the theorem can be applied.

A better intuition can be obtained by examining a simple situation with a streaming order sample and a corresponding a sequence of thresholds τ_i. In this case, the conditional inclusion probability $P(Z_i = 1 | \tau_{i-1}) = F_i(\tau_{i-1})$, and Z_i is genuinely a $Bernoulli(\tau_i)$ draw. However, the entire sequence of thresholds must be stored, and the theorem only holds for estimators of degree 1, such as Horvitz-Thompson estimators.

When the threshold is invariant to the order in which elements arrive, the estimated inclusion probability $F_i(\tau_i)$ has an intuitive meaning. Regardless of the actual order of arrival, one can treat the data as a stream where item i arrives last. Equation 9 states that the threshold τ_i can be viewed as a draw from some distribution that depends only on elements arriving before i, and hence the probability item i is added to the sample is $F_i(\tau_i)$. This same perspective holds when evaluating the joint inclusion probability of a set of items $\mathcal{J}$. In this

permutation invariant case, since all items in $\mathcal{J}$ can be moved to the end of the stream, it is easy to determine if the factorization in equation 9 exists for degree v estimators. There must exist some rule where the threshold can be set without peeking at the last v priorities.

4 Consistency

It is often the case that an estimator of interest is not unbiased in the first place. For example maximum likelihood estimators are often biased. However, they typically have a guarantee of consistency and asymptotic normality.

We show that another set of conditions give probabilistic and distributional guarantees rather than guarantees on the moments.

This has significant implications as it allows for parameter estimates even when the sampling scheme is not amenable for unbiased estimation as well as the computation of error estimates.

Here the tools we use are empirical process results. In particular, we use the convergence of the rescaled empirical distribution function to a Poisson process limit.

4.1 Poisson process limit

For a sequence of i.i.d. random variables from distribution F, the rescaled empirical process

$$N_c(t) = n(\mathbb{F}_n(c + t/n) - \mathbb{F}(c)) \tag{12}$$

converges to a Poisson counting process [16].

Our goal is to instead identify a limit random measure.

4.2 Gaussian process limit

Similarly, the process

$$\mathbb{G}n(t) = \sqrt{n}(\mathbb{F}_n(t) - F(t)) \tag{13}$$

converges to a Gaussian process G with $Cov(G(t_1), G(t_2)) = F(t_1)(1 - F(t_1))$ whenever $t_1 \leq t_2$.

4.3 Stopping times and In-sample thresholding rules

One advantage of using the

5 Estimation applications

5.1 Quantiles, functionals, and M-estimation

Although the original priority sampling paper focused on the subset sum problem, weighted sampling may be used to solve a much broader set of problems.

It may be used to solve any problem defined by an empirical distribution. Many quantities can be defined as a function of a c.d.f. G. For example, the median is defined as $median(G) = G^{-1}(1/2)$. The mean is defined as $mean(G) = \int x dG(x)$. In general, the plug-in estimator for a function of the cdf $\phi(G)$ is defined to be $\phi(\hat{G})$ where $\hat{G}$ is an empirical estimate of the c.d.f..

Suppose the weights $\{w_i\}$ are fixed and each item X_i is drawn independently from some c.d.f. G_i so that $X_i \sim G_i$. We consider the weighted c.d.f.

$$G(x) = \frac{1}{z} \sum_i w_i G_i(x). \tag{14}$$

In the case where X_i is fixed at x_i, then $G_i(x) = 1(X_i \leq x)$.

Theorem 6. *Given an adaptive threshold sample $\mathcal{J}$, the following are unbiased estimate empirical estimators of the weighted cdf*

$$\hat{G}(x) = \frac{1}{\alpha} \sum_{i \in \mathcal{J}} \frac{w_i}{F_i(\tau_i)} G_i(x) \tag{15}$$

$$\hat{\mathbb{G}}(x) = \frac{1}{\alpha} \sum_{i \in \mathcal{J}} \frac{w_i}{F_i(\tau_i)} 1(X_i \leq x) \tag{16}$$

where $\alpha = \sum_i w_i$. If α is replaced by $\hat{\alpha} = \sum_{i \in \mathcal{J}} w_i / F_i(\tau_i)$ then the estimators are consistent whenever $\hat{\alpha}$ is consistent.

Proof. These follow immediately from adaptive threshold sampling. Consistency follows from Slutzky's lemma. □

We note that provable convergence of the plug-in estimators from convergence of the empirical cdfs often depends on a stronger convergence result, namely a Glivenko-Cantelli result that provides uniform convergence of the cdf. Asymptotic normality can be established using a Donsker result. These results are outside the scope of this paper.

Another class of problems that can be solved with weighted samples are M-estimation problems. An M-estimator is the minimizer or maximizer of an objective function which can be expressed as the sum of functions on single data points so that it has the form given in equation 17. For example, the least squares estimator has objective $L(\theta) = \sum_i \|x_i - \theta\|^2$. When ℓ is the log-likelihood function, the estimator is the maximum likelihood estimator. Since the objective function is simply a sum over data points, the objective can be estimated using an adaptive threshold sample. This results in the trivial result.

Theorem 7 (M-estimation)**.** *Given a priority sample $\mathcal{J}$ with a 1-substitution compatible thresholding rule and an objective function of the form*

$$L(\theta) = \sum_i \ell(x_i, \theta), \tag{17}$$

the function

$$\hat{L}(\theta) = \sum_{i \in \mathcal{J}} \frac{w_i}{F_i(\tau)} \ell(x_i, \theta), \tag{18}$$

is an unbiased estimator of L for all θ.

M-estimators have the further property that the inverse Hessian of the objective function provides an estimate of the estimator's variance. Generalized priority sampling and 1 substitution compatibility also guarantees unbiasedness of the Hessian estimate. Thus, in addition to deriving an estimator using M-estimation, one also has an estimate of the variance of the resulting estimator.

5.2 U-statistics

The disadvantage of M-estimators is that although M-estimator objective functions are of degree 1 and hence, unbiased under the conditions of theorem 4, the M-estimator itself potentially includes interactions of all the items. Thus, we are unable to guarantee that expectations under the adaptive threshold sampling scheme match exactly those under a conditionally independent given τ Bernoulli scheme. However, almost any estimator can be modified to have at most v interactions by taking a v out of n bootstrap [4]. The v out of n bootstrap has the attractive property that it succeeds in cases where the bootstrap estimator fails when v grows sufficiently slowly relative to n.

To illustrate the v out of n bootstrap, again consider a linear regression model $Y = X\beta + \epsilon$ which has estimator $\hat{\beta} = (X^T Z X)^{-1} X^T Z Y$. Now consider the v out of n bootstrap estimator, $\hat{\beta}^{(v)} = \binom{n}{v}^{-1} \sum_S (X^T S Z X)^{-1} X^T S Z Y$ where the sum is over all diagonal selection matrices with exactly v entries with value 1. Since each term in the sum is a function of at most v sampled items, the estimator has degree at most v,

This v out of n bootstrap estimator is an example of an important class of statistics called U-statistics [20]. U-statistics are statistics of the form

$$U(\mathbf{x}) = \frac{1}{\binom{n}{v}} \sum_{\lambda} h(x_{\lambda(1)}, \ldots, x_{\lambda(v)}) \tag{19}$$

for some symmetric function h called the kernel and where the sum is over all combinations λ of size v out of n items. Other examples of U-statistics include the sample mean and variance, the Mann-Whitney U statistic used in nonparametric hypothesis testing, and Kendall's correlation coefficient τ. To illustrate their use, consider the U-statistic $\hat{\sigma}^2 = \frac{2}{n(n-1)} \sum_{i<j} (X_i - X_j)^2/2$ where $h(x_1, x_2) = (x_1 - x_2)^2$. This can be shown to be equal to the unbiased sample variance $\frac{1}{n-1} \sum_i (X_i - \overline{X})^2$. It is simple to prove its unbiasedness since it trivial to show that $\mathbb{E}(X_i - X_j)^2/2 = \sigma^2$ whenever $i \neq j$. For a degree 2 adaptive threshold sample, it follows that $\hat{\sigma}^2_{priority} = \frac{2}{n(n-1)} \sum_{i<j} Z_i Z_j \frac{(X_i - X_j)^2}{2F_i(\tau_i)F_j(\tau_j)}$ is also an unbiased estimator of the variance.

The importance of U-statistics is also captured by theorem 1 in [19] which states that there exists an unbiased estimator if and only if there exists an unbiased U-statistic. More precisely, for any family of distributions with parameter θ and i.i.d. draws $\{X_i\}_i$, there is an unbiased estimator for θ if and only if there is a kernel h with finite degree v such that $\mathbb{E}_P h(X_1, \ldots, X_v) = \theta(P)$ for all P in that family.

Another aspect in which U-statistics plays a pivotal role in the analysis of sampling methods is in determining when 1-substitution compatibility is sufficient to obtain the asymptotic limits for statistics that are not simple linear sums.

The Hajek's projection of a statistic T projects it into the set of linear statistics and is

$$\tilde{T} = \sum_i \mathbb{E}(T|X_i) - (n-1)\mathbb{E}T. \tag{20}$$

In this case, the expectation on the right $\mathbb{E}T$ typically contains the parameter being estimated. Although this makes it useless in estimating a parameter, it is useful when $\tilde{T}$ can be shown to have the same asymptotic distribution as T. In this case, T behaves *like* a simple linear statistic, and $1-$substitution compatibility is enough to ensure asymptotic correctness.

6 Concentration of the Threshold

The distribution substitution trick addresses the problem of unbiased estimation. In many cases, consistency of an estimator is sufficient. We examine the concentration of the threshold τ under an appropriate scaling.

7 Sampling design

Thus far, we have focused on the estimation properties of adaptive threshold sampling. This helps answer the question of how to make the best use of the sampled data. We now focus on the aspect of sampling design which helps answer the question of how to pick the best or most informative data. For adaptive threshold sampling, there are two mechanisms controlling the sampling design: the cdfs F_i and thresholds τ_i.

We focus on threshold rules and establishing conditions where the resulting threshold is substitution compatible. As an example, consider Wegman's adaptive sampling procedure [18]. In this scheme, a stream of items are given $Uniform(0, 1)$ priorities. Rather than always maintaining a fixed sample size with a threshold equal to the $(k+1)^{th}$ smallest priority, the threshold is cut in half whenever the number of retained elements exceeds k. This has computational benefits. A heap is not needed for fast update operations as threshold updates are less frequent but either require only a simple scan or removing a bucket containing all the elements to be dropped. The threshold in this scheme

can be expressed as the value $1/2^b$ where $1/2^b \leq R_{(k+1)} < 1/2^{b-1}$. This turns out to be a k substitution compatible thresholding rule as shown in corollary 10.

In general, the condition in which a threshold rule is substitution compatible is that it is not allowed to "peek" at priorities that are in the sample.

Theorem 8 (Leave-v-out thresholding)**.** *Let $\tau(\mathbf{R})$ be a threshold rule. Denote by $\mathbf{R}_{-\lambda}$ the set of priorities excluding those indexed by λ. If there exists a measurable threshold rule $\tau'[\lambda](\mathbf{R}_{-\lambda})$ such that for all $\lambda \in \Lambda_v$ and $i \in \lambda$, $\tau'[\lambda]_i(\mathbf{R}_{-\lambda}) = \tau_i(\mathbf{R})$ whenever $Z_j = 1$ for all $j \in \lambda$ then the threshold rule is strongly v substitution compatible.*

Proof. Since $\tau'[\lambda]$ is measurable, $\tau'[\lambda](\mathbf{R}_{-\lambda})$ has some distribution h_λ. Since $\tau'[\lambda](\mathbf{R}_{-\lambda})$ is independent of $\mathbf{R}_\lambda$, this has the distribution h_λ needed in equation 9 to establish substitution compatibility. □

Informally, the theorem states that a threshold rule is v substitution compatible when 1) there is a "shadow" threshold rule that makes no use of the items in the sample, and 2) the actual threshold rule agrees with the shadow whenever the items indexed by λ are in the sample.

When $|\lambda| = 1$, this condition is equivalent to the One-goodness condition described by [12] in distinct counting applications. The constant corresponding to inclusion is $F = \tau'_{-i}(\mathbf{R}_{-i})$. The value of the threshold is irrelevant when the i^{th} item is not in the sample.

The leave-v-out thresholding criterion can still be difficult to verify. For order samples which do not have per-item thresholds, a threshold rule that sorts the priorities and processes them from largest to smallest easily avoids peeking at the smallest priorities.

Theorem 9. *Consider $R_{(n)}, R_{(n-1)}, \ldots R_{(1)}$, the stochastic process on the order statistics of the priorities. If S is a stopping time with respect to this process, then for any threshold rule τ such that $\tau(\mathbf{R}) = f(R_{(n-S+1)}, \ldots, R_{(n)}) \leq R_{(n-S+1)}$ for some function f, defines a strongly $n - S$ substitution compatible threshold rule.*

Proof. Since $\tau(\mathbf{R}) \leq R_{(n-S+1)}$, it follows that $Z_i = 1$ if and only if $R_i < \tau(\mathbf{R})$. Let $\{\mathcal{F}_s\}$ be the sequence of filtrations defined by the stochastic process on the order statistics. By the definition of a stopping time, $1(S \leq n - v)$ and hence $\tau(\mathbf{R})1(S \leq n - v)$ are measurable with respect to the filtration $\mathcal{F}_{n-v}$. Together, these give a leave v out rule $\tau'[\lambda](\mathbf{R}_{-\lambda}) = \tau(\mathbf{R})$ if $S \leq n - v$ and $-\infty$ otherwise. □

Although a priority sample is typically processed by examining and retaining the smallest priorities rather than examining only the largest priorities as the theorem suggests, the theorem may still be applied dependent on the thresholding criterion. For example, in the case of priority sampling with fixed size k, the stopping time is the constant value $n - k$. Processing priorities from smallest to largest yields the same result as processing from largest to smallest

An example where one cannot simply use the smallest priorities would be to compute the a estimated mean by taking the smallest priorities and stopping when the estimated error in the mean estimate dips below a given tolerance. In this case, the estimated error can vary depend on order of the priorities under the threshold. The rule peeks into the "future" order of small priority items and hence is not a stopping time.

Corollary 10. *Suppose the threshold τ is permutation invariant, that it is invariant to the order in which items appear. If τ is a function of the order statistics $R_{(k+1)}, \ldots, R_{(n)}$ for some fixed v with $\tau(\mathbf{R}) \leq R_{(v+1)}$, then the threshold rule is strongly k substitution compliant.*

7.1 Composition of thresholding rules

One useful method of generating new thresholding rules is to combine thresholding rules. We consider two methods of composing thresholding rules. First, we consider the case where a set of candidate thresholds is generated, and the final threshold is generated as a function of these items. Second, we consider the sequential application of thresholding rules.

Theorem 11. *Given a set of priorities $\{R_i\}$ with strongly substitution compatible thresholds $\tau^{(1)}, \tau^{(2)}$, the threshold*

$$\tau_i^{(min)} = \min\{\tau_i^{(1)}, \tau_i^{(2)}\}$$
$$\tau_i^{(max)} = \max\{\tau_i^{(1)}, \tau_i^{(2)}\}$$

respectively define a strongly substitution compatible and strongly 1 substitution compatible threshold. If $\tau^{(1)}, \tau^{(2)}$ are strongly v substitution compatible, then so is $\tau^{(min)}$.

Proof. By the uniqueness of densities, $h_\lambda(\tau, M) = \int_D \prod_{i \notin \lambda} f_i(r_i) dr_i$ almost everywhere for some set D that depends on τ, M. When $R_i < \tau^{(min)}$ for all $i \in \lambda$, this factorization must exist for both thresholds, and taking the min of thresholds corresponds to taking the intersection of sets $D^{(1)}, D^{(2)}$. This induces a density $h_\lambda^{(min)}(\tau^{(min)}, M^{(min)})$ that yields the appropriate factorization. For $\tau^{(max)}$, if $\tau_i^{(max)} = \tau_i^{(1)}$, then the factorization for $\tau^{(1)}$ give strong 1 substitution compatibility. □

Theorem 12. *Let $\{R_i\}$ be a set of priorities, and let $\tau^{(1)}, \tau^{(2)}$ be strongly substitution compatible thresholding rules. Denote by $\mathcal{J} = \{i : R_i \leq \tau^{(1)}(\mathbf{R})\}$ the set of indices selected by the first thresholding rule. The threshold rule*

$$\tau^{(next)}(\mathbf{R}) = \tau^{(2)}(\mathbf{R}_\mathcal{J})$$

obtained by sequential application of the threshold rules defines a strongly substitution compatible threshold.

Proof. Since $\tau^{(1)}$ is strongly substitution compatible, the density for the priorities in the sample $\mathcal{J}$ have a factorization $p(\mathbf{R}_{\mathcal{J}}, \tau^{(1)}, M^{(1)}) = \prod_{i\in\mathcal{J}} f_i(R_i) h_{\mathcal{J}}(\tau^{(1)}, M^{(1)})$ when $R_i < \tau_i^{(1)}$ for all $i \in \mathcal{J}$. Otherwise, the density is 0. Since $p(\mathbf{R}_{\mathcal{J}}|\tau^{(1)}, M^{(1)})) \propto p(\mathbf{R}_{\mathcal{J}}, \tau^{(1)}, M^{(1)}))$, this implies that for all $i \in \mathcal{J}$, the R_i are conditionally independent given $\tau^{(1)}, M^{(1)}$. Let $\mathcal{J}'$ be the sample selected by the final threshold $\tau^{(next)}$. Since $\tau^{(2)}$ is substitution compatible, $p(\mathbf{R}_{\mathcal{J}'}, \tau^{(2)}, M^{(2)}|\tau^{(1)}, M^{(1)})$ $= \prod_{i\in\mathcal{J}'} f_i(R_i) h^{(2)}_{\mathcal{J}'}(\tau^{(2)}, M^{(2)}|\tau^{(1)}, M^{(1)})$. Multiplying times, $p(\tau^{(1)}, M^{(1)})$ and integrating over these nuisance variables yields the desired factorization. □

8 Sampling Applications

We demonstrate the usefulness of the theorems by constructing sampling schemes with desirable properties.

8.1 Distributed sampling

One application of an alternative thresholding rule arises when sampling is performed independently on nodes in a network, and a final sample is formed by merging the samples. Our theory improves upon existing distributed weighted sampling schemes by creating a thresholding rule that discards fewer samples and wastes less communication costs when merging the samples drawn at each node.

The weighted reservior sampling algorithms of [15] and [22] provide examples of priority based sampling schemes that can be merged. They are equivalent order sampling schemes as the priority of one is a log transformation of the other. [26] gives an optimal algorithm for order sampling with a fixed size k when nodes can coordinate their sampling rather than independently sampling. We consider the typical map-reduce setting where the worker nodes operate independently.

We start by presenting the more intuitive description in [22]. In a distributed system, each node samples k items using a order sample with fixed shape where the priorities $R_i \sim Exponential(w_i)$. Under such a scheme with m nodes, a total of mk elements are sampled but only k are retained when the final threshold is adjusted to the $(k+1)^{th}$ priority. An alternative threshold rule takes the minimum of the node thresholds. Theorem 11 gives that the resulting threshold is substitution compatible.

The savings of this scheme can be seen in the case of distributed simple random sampling. Suppose each of the m nodes sample k out of n points using uniformly distributed priorities. The thresholds for each node are distributed $Beta(k, n-k+1)$. If $m = 100, k = 1000, n = 10^6$, the mean $\mathbb{E}\tau^{(min)} \approx 0.97/100 \approx 1\%$. In contrast, taking the $(k+1)^{th}$ priority over the entire sample gives a threshold that is $Beta(k, mn-k+1)$ distributed with mean $k/mn = 10^{-5}$. In other words, the naive adaptation of priority sampling to the distributed case wastes 99.9% of the work. Other methods such as [23] try to reduce the waste at each node but fail if the resulting sample has fewer than k items. Out

thresholding strategy for merging removes the probability of a hard failure by allowing it to gracefully return a smaller sample with the desired weights.

8.2 Multi-objective sampling

Another application of alternative thresholds arises in multi-objective sampling [8]. In multi-objective sampling, the goal is to draw a single sample but provide control over the sample quality as measured by multiple objectives. This is represented by giving a single item multiple priorities, one per objective, indicating its importance for each objective. A simple method to draw a multi-objective sample is to take a priority sample for each objective and take the union of the samples. To reduce the size of the final sample, the scheme tries to maximize the overlap among the samples by maximizing the correlation of the priorities. This is achieved in order sampling by sharing a single $U_i \sim Uniform(0,1)$ variate for each item i, so that the jth priority for the i^{th} item is $R_i^{(j)} = F_{ij}^{-1}(U_i)$. Since U_i is shared, a small value for U_i encourages joint inclusion for all objectives.

To reduce this to a simple thresholding problem, note that all priorities for the i^{th} item are a function of the single uniform random variable U_i. Thus, inclusion is simple a thresholding operation on U_i where the threshold is $\max_j\{F_{ij}(R_i^{(j)})\}$. Theorem 11 gives that the resulting threshold is degree 1 substitution compliant so the Horvitz-Thompson style estimator is valid for the sample. However, it may happen that for some other item i' and objective j', that item would be rejected according to the j objective but is accepted by the j' objective, in other words, $R_{i'}^{(j)} \geq \tau^{(j)}$ and $R_{i'}^{(j')} < \tau^{(j')}$. Since $R_{i'}^{(j)}$ is among the rejected items for $\tau^{(j)}$ and is informative about $R_{i'}^{(j')}$ through U_i, it follows that $\tau^{(j)}$ peeked at the priority of item i'. The threshold is not 2 substitution compliant, and an unbiased variance estimator is not available.

One simple application of multi-objective sampling is in generating stratified samples. If the data is partitioned by strata, then one can apply a separate threshold rule to each strata. However, if data is stratified in two different ways, for example by age and by gender, the multi-objective sampling can a sample with appropriate minimum size for each stratification.

8.3 Stratified sampling

Another stratified sampling example can arise when there are an unknown number of strata or the size of each item is unknown. In this case, the size k for each stratum needed to fully utilize the available storage cannot be predetermined. Furthermore, to guarantee that stratified sampling improves upon simple random sampling, the size of the strata must be almost exactly proportional to their sizes.

One adaptive reservoir sampling algorithm [2] partially solves the problem. However, it has several shortcomings. It is unable to maintain a uniform sample whenever the reservoir size increased. It can only maintain an approximately uniform sample. Furthermore, whenever the reservoir size is increased from k

to $k+1$, the sampler is in an indeterminate state while processing $\Omega(n/k)$ items where n is the number of items seen thus far. We give a thresholding rule that solves these shortcomings.

Suppose there is a memory budget M. Given a stream of items (x_t, s_t) where s_t denotes the stratum for x_t, maintain a threshold $\tau_s(t)$ and count of items $n_s(t)$ for each stratum s. Denote by $k_s(t)$ the number of items in the sample for strata s at time t, and let $k_{tot} = \sum_s k_s(t)$. A sequential threshold process are defined by the following algorithm. If the stratum was not encountered before, initialize $\tau_{s_t} = 1$. If $R_t < \tau_{s_t}(t-1)$, then add (x_t, s_t, R_t) to the sample. If this violates the memory budget, choose the stratum that is most overallocated, in other words, the s' such that $k_{s'} - (k_{tot} - 1)n_{s'}(t)/t$ is maximized. Update the corresponding threshold to the maximum priority in that stratum to reduce its size by one. Repeat until the memory budget is satisfied.

8.4 Variance adapted sample sizes

The sampling schemes described so far have focused on controlling the size of the sample under hard memory constraints. Another feasible design is to control for the variance in the sample and choose an appropriate size. Suppose one must monitor a set of metrics in real time where some metrics are more noisy than others. The goal then is to allocate more space to noisy metrics. For simplicity, consider drawing a simple random sample for each metric where goal is to have the standard deviation in the mean estimate is approximately 1% of the true mean. This can be achieved by using the rejected items. Let $\mu_n(\tau_n), \sigma_n(\tau_n)$ be the sample mean and standard deviation of the rejected items if τ_n is the threshold after observing n items. For a simple random sample, approximately $\hat{k}_n = \frac{1}{\epsilon^2}\frac{\mu_n(\tau_n)^2}{\sigma_n(\tau_n)^2}$ items are needed to ensure the mean estimate's standard deviation is within $\epsilon\mu$ of the true mean μ. Update the threshold $\tau_{n+1} = \min\{\tau_n, \hat{k}_n/(n+1)\}$. Given $Uniform(0,1)$ priorities this will draw a sample approximately of size $\hat{k}_n$. This gives a substitution compatible threshold. When combined with multi-objective sampling, this can give a stratified sample which is appropriately sized for all strata.

9 Algorithms

The final problem we aim to address is how to select a sample efficiently.

9.1 Fast Sampling with a Priority Reservoir

We introduce a fast, memory efficient algorithm for basic priority sampling. The gist of the algorithm is that one can separate the samples into two parts: one which consists of items that are sampled with probability 1 given the threshold and one consisting of everything else. The items which are not sampled with probability 1 are a reservoir sample where the probability of inclusion for the n^{th} item is $F_n(\tau)$ instead of the usual $1/n$ where τ is the current threshold. The item

ejected from the reservoir is chosen uniformly at random. Under some regularity conditions on the weights, eventually no items are sampled with probability 1, and the algorithm degenerates to a simple modified reservoir sample.

An attractive property of basic priority sampling when expressed via min-priorities is that the priorities $R_i = U_i/w_i$ are easy to work with $Uniform(0, 1/w_i)$ random variables. In particular, the conditional distribution of the R_i given $R_i < \tau$ is $Uniform(0, \tau)$ whenever $\tau < 1/w_i$. This conditional distribution does not depend on the weight. Thus, the priorities may be thrown away as they can simply be regenerated as i.i.d. $Uniform(0, \tau)$ random variables. This leads to algorithm 1.

Algorithm 1 Fast priority reservoir sample with heavy items

```
function FastAddItemHeap(Reservoir, HeavyItems, τ, x, w)
    R ← Uniform(0, 1)/w
    if 1/w < τ then
        HeavyItems ← Add(HeavyItems, x, w, R)
    else if R < τ then
        Reservoir ← ReservoirAdd(Reservoir, x, w)
    end if
    if Size(Reservoir) + Size(HeavyItems) > k then
        τ_R ← τ × Beta(Size(Reservoir) − 1, 1)
        τ_H ← MaxPriority(HeavyItems)
        if τ_R > τ_H then
            τ ← τ_R
            Reservoir ← ReservoirDelete(Reservoir)
        else
            τ ← τ_H
            HeavyItems ← PopMax(HeavyItems)
        end if
    end if
end function
```

When the stream of weights is bounded above by M and there exists some constant δ such that $w_i > \delta$ infinitely often, then eventually the threshold τ is smaller than $1/M$, and no items fall into the heavy items category. At this point the algorithm reduces to simple reservoir sampling with a slightly modified inclusion rule and is given by algorithm 2.

The running time of an update is $O(1 + |H| \log |H|)$ where $|H|$ is the size of the heavy item set. Under the bounded weight conditions given above, the running time is $O(1)$ eventually.

The space requirement is $k|x| + (|H| + 1)|r|$ where $|x|$ denotes the storage size of an item and weight pair and $|r|$ is the storage size for a priority. There is a modest storage efficiency gain over heap based implementations since priorities are not stored for the reservoir.

Algorithm 2 Fast priority reservoir sample steady state

```
function FastAddItemSteadyState(Reservoir, τ, x, w)
    R ← Uniform(0, 1)/w
    if R < τ then
        if Bernoulli(k/(k + 1) = 1 then
            i ← RandomUniform(Size(Reservoir))
            Reservoir[i] ← (x, w)
        end if
        τ ← τ × Beta(k, 1)
    end if
end function
```

9.2 Lazy priority sampling

The fast priority sampling algorithm strongly exploits the properties of uniform random variables. It is not appropriate in all situations since it requires the priorities to be uniform random variates with a common minimum. Although a min-heap based solution is always available, the cost of adding or deleting a item from the sample is $O(\log k)$ where k is the size of the heap. At the cost of additional space, relaxed reservoir sampling [14] gives a constant $O(1)$ amortized update costs for fixed size samples.

For general threshold rules, a selection algorithm may still be used to lazily process the reservoir. However, the cost of the algorithm is dependent on several additional factors. In particular, it is dependent on the cost of computing and updating the threshold. Furthermore, items need not share the same threshold, so multiple thresholds may need to be updated. It is beneficial then to be able to update thresholds on the fly with constant cost for each rejected item. One way to do so it to make the threshold a function of an easily updated statistic S of the rejected items similar to the variance bounded threshold in section 8.4. Once a threshold is set, processing the reservoir takes $O(k)$ time where k is the size of the reservoir.

We give a simple "lazy" priority sampling algorithm. Given a current threshold τ, include a new item with probability given by τ. If the sample has reached some maximum capacity, then update τ and reject all items above the threshold. This can be seen as a modest generalization to the relaxed reservoir sampling algorithm in [14] and Wegman's adaptive sampling [18]. In the relaxed reservoir sampling algorithm $\tau_i = 1$ for new item i, and the threshold update sets the threshold to the $(k+1)^{th}$ smallest priority. In adaptive sampling, the threshold update simply reduces τ by half. The lazy sampling algorithm can be accelerated using buckets where each bucket stores priorities only in a limited range. In this case, the the threshold update cost is proportional to the size of the relevant buckets and not the entire reservoir.

Algorithm 3 Lazy priority sampling

```
function UPDATE(Reservoir, τ, S, x_n, R_n)
    if R_n < τ_n then
        Reservoir ← Add(Reservoir, x_n, R_n)
    end if
    if OverCapacity(Reservoir) then
        τ ← UpdateThreshold(τ, S, Reservoir)
        Reservoir ← {(x_i, R_i) : R_i < τ_i}
    end if
    return (Reservoir, τ, S)
end function
```

9.3 Amortized running times

Although the heap based implementation requires $O(\log k)$ time per addition or deletion of an item, only the items that are less than the threshold update the sample. In the case of a uniform sampling design, only $O(k \log n)$ items update the sample in expectation for an amortized cost of $O(n + k \log k \log n)$, since the size of the data n typically dominates, the amortized cost remains constant. For the fast priority sampling algorithm, the running time depends on the number of items in the heap. In the worst case, all items are in the heap. However, if n is large so that the threshold is small and the weights are bounded, then no items are in the heap with high probability. In this case, the update cost is $O(1)$ unamortized. The cost of the lazy priority sampling algorithm 3 depends on the properties of the threshold update, and the cost of updating the threshold.

If updating the threshold takes linear time and half of the items are evicted after the update then the algorithm has an amortized $O(1)$ update cost even if the inclusion probability of new items is 1. If the inclusion probability of new items is α^D where D is the number of threshold updates and the capacity of the reservoir has a finite bound, then there are approximately $\log_\alpha n$ updates and a threshold update cost of $O(k)$. The overall time complexity is $O(n + k \log n / \log \alpha)$ still yields an amortized cost of $O(\log \alpha)$ per item when $k / \log \alpha = O(n / \log n)$. In the case where buckets are used, k is replaced by the size of the bucket.

10 Streaming logistic regression

We give an example which brings together several components of the theory together. Consider the problem of streaming logistic regression with weights that decay exponentially over time. This combines the theory for estimation that goes beyond simple aggregation, the theory of sampling design using a time adapted thresholding, and a fast sampling algorithm with constant update costs and minimal storage overhead. In order to choose an efficient subsample, we draw a weighted subsample using local case-control sampling [17]. This

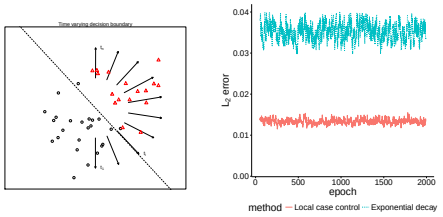

Figure 1: Left: The optimal decision boundary, given by the arrows, evolves counterclockwise over time with the positive (red) examples to the left of the arrow. The arrow at time t_1 is in the opposite direction of that at t_n, so the optimal prediction at t_n is the opposite of that at t_1. Right: The more advanced sampling design of local case-control sampling reduces the L_2 error in the logistic coefficients by a factor of 2.6 compared to simple exponential decay. The needed sample size to achieve a given error is also correspondingly reduced.

sampling method chooses items based on their degree of "surprise." An item with response y_i and covariates x_i is selected with probability $\tilde{p}(x_i)$ if $y_i = 0$ and $1-\tilde{p}(x_i)$ otherwise where $\tilde{p}$ is a pilot estimate of the classification probability. In other words, the scheme is likely to select items which the model misclassifies.

For the logistic regression data, we consider a model on two variables that evolves over time. The true decision boundary at time t is given by the line with angle πt that passes though the origin. This model evolves significantly over time since the class label probabilities at time 0 are the opposite of those at time 1. Formally, the model is given by

$$\beta_1 = c \cdot sin(\pi t), \qquad \beta_2 = c \cdot cos(\pi t)$$
$$p(y(t) = 1|x) = logistic(\beta_1(t)x_1 + \beta_2(t)x_2).$$

The $\mathbf{x}$ covariate values are independent standard normal. Time ranges from 0 to 1 with arrival times following a homogeneous Poisson process on the time interval $(0, 1)$ conditional on the total number of points being 1 million. Since well separated classes require few data points to obtain an accurate decision boundary, the scaling of the coefficients $c = 2.8$ was chosen to provide a moderately difficult problem with an optimal average prediction error of 17%. The evolving decision boundary is illustrated in figure 1.

Since we use exponential decay, we can apply the theory for forward decay [11] so that no priority needs to be recomputed. Furthermore, the shape is the cdf of a $Uniform(0, 1)$, so the fast reservoir sampling algorithm can be applied. Heavy items can be avoided by adjusting the weights to not be too large. A small regularization is also added to prevent near 0 weights. Furthermore, we know that under independent Bernoulli sampling with probabilities $F_i(\tau)$, the inverse probability weighted M-estimator is consistent [28]. The k-out-of-n unweighted bootstrap is also consistent as $m \to \infty, m/n \to 0$ [4]. Thus, if the model parameters were not changing over time, then the estimator would be consistent. This highlights three of this paper's contributions: weighted sampling of informative points and good (time varying) properties, a fast algorithm for priority sampling, and provably good estimation.

For the simulation, we initialized the coefficients of the logistic model by fitting a simple weighted estimator on the first 1000 items. The current model is used as a pilot estimate for the classification probabilities for small batches of 50 items. This allows us to apply local case control sampling. The coefficients are refit after each batch. The results are then compared to the estimates that would be obtained from strictly using weighting without any data reduction from sampling.

The simulation results in figure 1 show that applying the more efficient local-case control sampling method reduces the L_2 error by a factor of 2.6 when compared to exponential decay sampling. Since the variance of an estimator scales as c/k for some constant c, reducing error by a factor of 2.6 is equivalent to requiring only $1/2.6 \approx 38\%$ as many samples.

11 Conclusion

Our paper tackles the three issues that are needed for a good sampling procedure: selecting informative data points, doing so efficiently, and being able to correctly make use of the data. We do so by developing a common framework we call adaptive threshold sampling. Within this framework, the key insight to develop the needed theory is the distribution substitution trick.

The contributions of most practical significance are two-fold. First, they allows the easy generation of complex sampling designs with attractive properties. We give several examples of these in section 8. Since these designs can depend on the response variable of interest and induce selection bias, the second contribution is that this selection bias can be removed when estimating a quantity of interest even when using a more complex estimator than a simple aggregation. These are, of course, subject to some technical conditions. The bulk of the paper provides the tools to meet these conditions while performing the analysis of interest.

The most important technical contribution to be the identification of the distribution substitution trick and the resulting theorem 4. It shows that for any function of the samples that does not have too many interactions, one can effectively treat the thresholded sample as an independent sample when computing expectations. This has significant implications as it provides a general and computationally tractable method for deriving principled estimators for the resulting weighted samples without replacement. We demonstrate in section 5 that a wide range of useful estimators are covered. In contrast, prior work required computation of intractable unconditional inclusion probabilities or only solved a specific problem such as the subset sum problem.

Our other major contributions are in the theorems and recipes that simplify the design of adaptive threshold sampling schemes. We derive rules for generating thresholds and proving that they are V substitution compatible to satisfy sufficient conditions for unbiased estimation. These are shown to both encompass existing sampling schemes as well as enable derivation of new ones with attractive properties. These include the ability to merge distributed samples,

adaptively resize stratified samples, satisfy multiple objectives when sampling, appropriately size using the variance, as well as others. We also provide a new algorithm with $O(1)$ update time for efficiently sampling from one large class of priority sampling schemes.

These contributions are illustrated empirically in a logistic regression problem that evolves over time. The sampling design accomplishes 3 goals. It obeys a fixed memory budget, it selects the most informative points, and it weights recent items more heavily as they are more relevant. The sample itself is chosen using the fast reservoir sampling algorithm. Finally, the validity of the v out of n bootstrap and weighted M-estimation to ensure good estimates. This is shown to substantially outperform simple exponential time decay.

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A Proofs

Theorem 5 (Threshold inclusion)**.** *Consider the conditions in theorem 4 and further assume that for all $i \in \mathcal{J}$ and some s, $\tau_i = R_s$. Let $\tilde{\mathcal{J}} = \mathcal{J} \cup \{s\}$ and $\tilde{\mathcal{J}}_{-j} = \tilde{\mathcal{J}}/\{j\}$ be the sample excluding j. The estimator*

$$\hat{\theta}'(\tilde{\mathcal{J}}, \tau) = \sum_{j \in \tilde{\mathcal{J}}} \hat{\theta}(\tilde{\mathcal{J}}_{-j}, \tau) p(R_j = \tau | \tilde{\mathcal{J}}) \tag{21}$$

is an unbiased estimator of θ under P.

Proof. By theorem 4 and the tower rule

$$\begin{aligned}
&\mathbb{E}_P \hat{\theta}(\tilde{\mathcal{J}}_{-j}, \tau) p(R_j = \tau | \tilde{\mathcal{J}}) \\
&\quad = \mathbb{E}_P \mathbb{E}_P (\hat{\theta}(\tilde{\mathcal{J}}_{-j}, \tau) p(R_j = \tau | \tilde{\mathcal{J}}) | R_j = \tau, \tilde{\mathcal{J}}) \\
&\quad = p(R_j = \tau | \tilde{\mathcal{J}}) \mathbb{E}_P (\hat{\theta}(\tilde{\mathcal{J}}_{-j}, \tau) | R_j = \tau, \tilde{\mathcal{J}}) \\
&\quad = \theta \cdot p(R_j = \tau | \tilde{\mathcal{J}})
\end{aligned}$$

Summing over $j \in \mathcal{J}$ yields that the estimator is unbiased. □