An asymptotically optimal, online algorithm for weighted random sampling with replacement

MICHAŁ PIOTR STARTEK
University of Warsaw, Faculty of Mathematics, Informatics, and Mechanics
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Abstract

This paper presents a novel algorithm solving the classic problem of generating a random sample of size $s$ from population of size $n$ with non-uniform probabilities. The sampling is done with replacement. The algorithm requires constant additional memory, and works in $O(n)$ time (even when $s >> n$, in which case the algorithm produces a list containing, for every population member, the number of times it has been selected for sample). The algorithm works online, and as such is well-suited to processing streams. In addition, a novel method of mass-sampling from any discrete distribution using the algorithm is presented.

1 Introduction

Assume that we are given a population of elements $P = \{e_i\}_{i=0}^{n-1}, n \in \mathbb{N}$ (at least at first, the problem of infinite populations will be elaborated on later), along with a sequence of probabilities of each element of $P$, denoted $\{p_i\}_{i=0}^{n-1}$, such that $\sum_{i=0}^{n-1} p_i = 1$, and a single number $s$, the sample size, which might be greater or lower than $n$. The task is to compute a random sample of size $s$ from the population $P$, such that each element $X_i$ from the sample is one of the elements of $P$, each with its corresponding probability. Note that without loss of generality we can (and will) assume that $P = \{0, ..., n-1\}$

The algorithm assumes a non-naive (constant-time) implementation of procedures for sampling single random numbers from the beta (in the easy case, where $\alpha$ and $\beta$ parameters are integer and $\geq 1$), and binomial distributions, as
ALGORITHM 1: The naive sampling algorithm

Input: The sequence of probabilities $p_{i_{n=0}^{n-1}}$, desired sample size $s$
Output: A multiset $R$ containing the random sample

1. Compute array $\{S_i\}_{i=0}^{n-1} = \sum_{j=0}^{i-1} p_j$;
2. $R =$ new empty multiset;
3. repeat $s$ times
   4. Randomize $X \sim \mathcal{U}(0,1)$;
   5. Find greatest $k$ s.t. $S[k] < X$ using binary search ;
   6. Add $k$ to $R$
4. until;
8. $R$ contains the result ;

well as lack of numerical errors. Some consideration to mitigating the effects of numerical inaccuracies will be given in later sections.

The algorithm is best presented (as the author feels) by starting from the naive algorithm, and iteratively refining it, until the desired time and memory complexity are reached.

2 The naive algorithm

The naive algorithm (which, despite its non-optimal costs, in practice is reasonably efficient, and is used, in its second variant, for example by the numpy numeric library for Python) is based on a crucial idea, which will be used also in the novel version presented here. The idea is based on a geometrical intuition: if an interval $[0, 1]$ is divided into parts with lengths $p_i$, then sampling a random number $X$ from the uniform distribution $\mathcal{U}(0,1)$ and picking the subinterval of $[0,1]$ into which it falls (and the corresponding element of $P$) results in a choice of a single element of $P$ with the desired probability distribution. Efficient finding of the selected subinterval is facilitated by precomputing an array of cumulative sums of probabilities, then performing a binary search on it.

The algorithm consumes $O(n)$ time for initialization (lines 1 and 2), then $O(s \log(n))$ time for the actual sampling, and $O(n)$ memory space for additional data structures (not counting the $O(s)$ for the result).

3 Omitting the computation of cumulative sums table

The first modification of the algorithm makes it possible to skip the necessity to precompute the array of cumulative sums in line one. Instead it samples all the necessary random numbers $X_i \sim \mathcal{U}(0,1)$, sorts the $X$ array, and then processes the $p_i$ sequence at the same time as $X$, in fashion similar to the merge step of the mergesort algorithm.
ALGORITHM 2: The sampling algorithm without cumulative sums table

**Input:** The sequence of probabilities $p_{i=0}^{n-1}$, desired sample size $s$

**Output:** A multiset $R$ containing the random sample

1. $R =$ new empty multiset;
2. $idx = 0$;
3. $cumulativeProbSum = 0.0$;
4. Randomize $X \sim U(0, 1)^s$;
5. Sort $X$ in ascending order;
6. **foreach** $x \in X$ **do**
7.  **while** $cumulativeProbSum < x$ **do**
8.    $cumulativeProbSum += p[idx]$;
9.    $idx += 1$
10. **end**
11. Add $idx - 1$ to $R$;
12. **end**
13. $R$ contains the result;

The algorithm runs in $O(s \log(s) + n)$ time, (which is not an improvement over the previous version): lines 4 and 5 take a total of $O(s \log(s))$, the outer loop runs $s$ times, while the inner loop runs a total of $n$ times (as the variable $idx$ is bound by $n$). The algorithm uses $O(s)$ memory.

4 Omitting the sorting

The algorithm might be further improved if the table $X$ could be generated in an already sorted order. This is, in fact, possible: it is a well-known fact that if $X_0, ..., X_{n-1} \sim iid U(0, 1)$, then $min(X_0, ..., X_{n-1}) \sim Beta(1, n)$, and is the first element of the sought table [1]. Since the variables are independent, then, after sampling the minimum using this method, it is easy to see that the remaining variables (under condition that they have to be not less than the minimum) are distributed according to $U(M, 1)$, where $M$ is the minimum. The second-lowest variable might be sampled with the same method after rescaling $U(M, 1)$ to $U(0, 1)$, and so on.

In fact, this allows us to drop the step of precomputing the table $X$ altogether, and to just compute the consecutive variables "on the go", making the algorithm capable of online operation, as well as improving the runtime.

The algorithm runs in $O(n + s)$ time, and requires constant additional memory if working online: in that case, every intermediate result is immediately provided to the calling procedure for consumption (and possibly, immediately discarded), instead of being explicitly stored in $R$. 
ALGORITHM 3: The online algorithm

Input: The sequence of probabilities \( p_{i=0}^{n-1} \), desired sample size \( s \)
Output: A multiset \( R \) containing the random sample

1. \( R = \) new empty multiset;
2. \( idx = 0 \);
3. \( \text{cumulativeProbSum} = 0.0 \);
4. \( \text{currentX} = 0.0 \);
5. for \( i \) in \( s, \ldots, 1 \) do
6.     \( \text{currentX} = \text{Beta}(1, i) \times (1.0 - \text{currentX}) \);
7.     while \( \text{cumulativeProbSum} < \text{currentX} \) do
8.         \( \text{cumulativeProbSum} = p[idx] \);
9.         \( idx++ \);
10. end
11. Add \( idx - 1 \) to \( R \);
12. end
13. \( R \) contains the result;

The case of \( s \gg n \)

The practical speed of the above algorithm is constrained by the speed of the sampling from the beta distribution, the remaining operations being trivial in comparison. This provides an opportunity for optimization: if the population is small with respect to the number of samples required, then the algorithm will have to sample from the beta distribution many times for any population member. This can be avoided by changing the reasoning: instead of asking "where will the next \( X_i \) be?" we can ask "how many \( X \)es will we encounter while going through the current \( p_i \)?". The answer to that, for \( p_i \) is the binomial distribution: \( \text{Binom}(s, p_i) \). For further \( p_i \)s the answer is the same distribution, only conditioned on the number of \( X \)es and the population probability already consumed: \( \text{Binom}(s - |X_{used}|, p_i/(1.0 - \sum_{j=0}^{i-1} p_j)) \). This is in fact a standard algorithm for sampling from multinomial distribution (which is exactly the same problem as random sample with replacement: only the former terminology is most often used in contexts where \( s \gg n \), and the latter otherwise).

The provided algorithm runs in \( O(n) \) time (assuming that \( R \) behaves like a counter, and increasing the count of a given item is done in constant time), and in constant memory. It is capable of working online. It should be noted, that although it achieves the optimal theoretical asymptotic runtime, its practical implementation will be very inefficient when \( s \ll n \): even if a sample consisting only of one element is desired, it will perform \( n \) expensive operations of sampling from binomial distribution.

A practical algorithm

The previous two algorithms are opposites in terms of their practical pessimistic case: the one using beta distribution has to randomize once per each requested
**ALGORITHM 4:** The online algorithm for \( s > n \)

**Input:** The sequence of probabilities \( p_{i=0}^{n-1} \), desired sample size \( s \)

**Output:** A multiset \( R \) containing the random sample

1. \( R = \) new empty multiset;
2. \( \text{idx} = 0 \);
3. \( \text{cumulativeProbSum} = 0.0 \);
4. for \( i \) in \( 0, ..., n - 1 \) do
5.   Randomize \( N \sim \text{Binom}(s, p[i]/(1.0 - \text{cumulativeProbSum})) \);
6.   Add \( i \) to \( R \) with multiplicity \( N \);
7.   \( s = s - N \);
8.   \( \text{cumulativeProbSum} = \text{cumulativeProbSum} + p[i] \);
9. end
10. \( R \) contains the result ;

The algorithm is still online (although presented in non-online form for readability), works in constant memory if online (results are immediately consumed by caller, instead of being stored in \( R \)). A careful reader might notice that the algorithm as presented runs in pessimistic \( O(n + s) \) time. The pessimistic
**ALGORITHM 5**: The final algorithm

**Input**: The sequence of probabilities \( p_{n=0} \), desired sample size \( s \)

**Output**: A multiset \( R \) containing the random sample

1. \( R = \text{new empty multiset; } \)
2. \( idx = 0; \)
3. \( \text{cumulativeProbSum} = 0.0; \)
4. \( \text{currentPosition} = 0.0; \)
5. While \( s > 0 \) do
6.   \( \text{cumulativeProbSum} = p[idx]; \)
7.   While \( (\text{cumulativeProbSum} - \text{currentPosition}) \ast s/(1.0 - \text{currentPosition}) < 1.0 \) do
8.     \( \text{currentPosition} = \text{Beta}(1.0, s) \ast (1.0 - \text{currentPosition}); \)
9.     While \( \text{cumulativeProbSum} < \text{currentPosition} \) do
10.       \( idx++; \)
11.       \( \text{cumulativeProbSum} = p[idx]; \)
12.   end
13.   Increase multiplicity of \( idx \) in \( R \) by 1;
14.   \( s-- = 1; \)
15.   If \( s == 0 \) then
16.     Terminate algorithm, \( R \) contains the result
17. end
18. end
19. Randomize \( N \sim \text{Binom}(s, (\text{cumulativeProbSum} - \text{currentPosition})/(1.0 - \text{currentPosition})); \)
20. Increase multiplicity of \( idx \) in \( R \) by \( N; \)
21. \( s-- = N; \)
22. \( idx++ = 1; \)
23. \( \text{currentPosition} = \text{cumulativeProbSum}; \)
24 end
25 \( R \) contains the result;

If the algorithm encounters an element of the population with probability small enough that it decides to use the beta mode, but, due to bad luck, proceeds to draw \( O(s) \) infinitesimal samples from the beta distribution before leaving the element and proceeding forward. This may be easily avoided by adding a hard condition that would force a binomial mode after a constant number of consecutive beta samples. This was omitted from the main code presented here for readability, and also because it is not a concern for any practical application. However, with the hard limit, the algorithm can perform at most \( n \) binomial samples (as each binomial sample increases the \( idx \) variable - which is bounded by \( n \) - and with the hard limit it is possible to perform at most \( O(n) \) beta samples) - therefore its runtime is bounded by \( O(n) \).
7 Practical notes

The algorithms presented here depend heavily on good implementations of functions for sampling from binomial and from beta distribution.

In particular, anyone undertaking the implementation of the algorithm is advised to write a custom version of function for sampling from $\beta(\alpha, \beta)$ distribution: the algorithm always samples with $\alpha = 1$, and in this case, the distribution has an explicit, invertible CDF - and so, a custom sampler using the inverse CDF method will always be faster than a sampler from any scientific library which has to handle the general case.

Regarding the binomial distribution, the C++11 function for sampling as implemented by the GNU project’s libstdc++ (standard C++ library on most Unix systems) is inadequate for the task as it seems to have non-constant complexity with regard to its parameters. In any tests performed I have used the function as implemented by the Boost library which seems to work not only faster than libstdc++’s, but also runs in constant time.

Regarding the numerical stability of the algorithm, the algorithm computes a cumulative sum of all encountered probabilities, which is of course tricky. If precise numerical correctness is required, then the summation should be done using Kahan’s \cite{Kahan} or even Shewchuk’s \cite{Shewchuk} summation algorithms. However, for most if not all practical purposes imaginable, this is not necessary. Special care must be taken, however, as sometimes, due to numerical errors, the last sampling from binomial distribution might be performed with probability of success slightly greater than 1 - the programmer must ensure that the sampling function just assumes 1 instead of crashing.

As a side note: the algorithm does benefit slightly from having its input data sorted (in either ascending or descending order, doesn’t matter): it casues the algorithm to perform less switches between beta and binomial mode, and so, it minimises the number of elements which are partially dealt with in binomial mode, and partially in beta mode. The very slight speed benefit does not justify spending the computational time (and especially the loss of asymptotic optimality and the ability to work online) needed to sort the data. However, this means that in order to avoid any bias in runtime tests described further, the input data for all tests was randomly shuffled.

8 Comparison with other sampling methods and runtime tests

The algorithms presented in this paper have been implemented in C++11 programming language for purposes of testing and speed comparison. These are compared with the implementation of standard Walker’s alias method \cite{Walker} as implemented by the R programming language (later referred to under name "Walker-R"), the full implementation of R’s sampling function (which examines the data, heuristically chooses between Walker’s algorithm or a naive algorithm, and the runs it), referred to as "full-R", an alternative, standalone implemen-
Figure 1: Comparison of runtimes of various random choice algorithms. The various versions of the novel algorithm proposed in this work are marked with large dots, some example algorithms are marked with small dots, competing algorithms used by various scientific libraries are marked with crosses.
| Algorithm          | Pessimistic runtime | Additional memory used | Calls to RNG | Can work online |
|-------------------|---------------------|------------------------|--------------|-----------------|
| Algorithm 1 (numpy) | $O(n + s \log n)$   | $O(n)$                 | $O(s)$       | No              |
| Algorithm 2       | $O(n + s \log s)$   | $O(s)$                 | $O(s)$       | Yes             |
| Algorithm 3       | $O(n + s)$          | $O(1)$                 | $O(s)$       | Yes             |
| Algorithm 4       | $O(n)$              | $O(1)$                 | $O(n)$       | Yes             |
| Algorithm 5       | $O(n + s)$          | $O(s)$                 | $O(s)$       | Yes             |
| Walker’s algorithm | $O(n + s)$          | $O(n)$                 | $O(s)$       | No              |

Table 1: A comparison of properties of sampling algorithms

The implementation of Walker’s algorithm in C by ransampl library, and with numpy’s implementation which follows Algorithm 1. The novel algorithm proposed in this work (Algorithm 5) has been tested in two versions, one which produces an array of size $s$ (the sample with repetitions), referred to as the "Alg5-array" algorithm, and one which produces the multiset (with integer counts instead of the repetitions). The multiset was implemented either as a hashtable (using standard C++ unordered_map data structure) or trivially as an array of size $n$. The implementation using the former is referred to as "Alg5-HT" in plots, the one using the latter as "Alg5-Pop". Similarly, Algorithm 4 has been implemented and tested both outputting an array with repetitions and multiset (based on an array, hashtable implementation was produced but skipped in effort to avoid complicating the plots further). A summary of theoretical properties of each of the algorithms is presented in Table 5.

The R functions are written in C code, and the code for these functions is reused, slightly modified to remove dependencies on R’s internals. Numpy, although written in Python, is compiled to native code using Cython, and as such, should run at near-native speeds, like the rest of the tested algorithms, without suffering overhead due to Python being an interpreted, high-level language.

The algorithms have been tested on three different random populations, one drawn from uniform distribution $\mathcal{U}([0, 1])^n$, representing population with mostly equal probabilities, one drawn from a geometric sequence starting with 1.0 and ending at $10^{-100}$, representing a population with skewed probabilities. The third type of population is generated by applying a Gaussian PDF function to $n$ points evenly spaced between 0.0 and 10 times the stdev of the Gaussian function. This is meant to simulate the usual application of sampling function in modelling in population genetics (which in fact was the inspiration for this research): in population genetics models, selection and reproduction of modelled organisms is often done precisely by randomly sampling with replacement of $n$ organisms (that reproduce and pass their offspring to a next generation) from a population of $n$. The probability of a given organism being chosen to reproduce is proportional to its fitness function - which is often Gaussian.

Each population type (uniform, geometric and Gaussian) is rescaled so that it sums to 1.0, and randomly shuffled. The results of the tests are presented on
It is evident from the results of the tests that not only is the proposed algorithm asymptotically optimal, but, unlike Algorithm 4 it is also efficient in practice, outperforming the competing methods in most scenarios, by as much as several orders of magnitude in some cases. In the single pessimistic case, where the distribution of probabilities in the population is close to uniform and $s \approx n$, although it runs slightly slower, it still remains competitive, moreover, the difference in runtime grows smaller as $s = n \to \infty$, and it overtakes the Walker’s method at $s = n \approx 10^8$ (data not shown).

The algorithm is able to adapt to the input data and use any skew from uniform distribution to its advantage, to increase its runtime, as evidenced by the tests on Gaussian and especially geometric populations. Unlike the popular algorithms it works in constant additional memory, and is capable of online operation.

An implementation of this algorithm in a few programming languages may be downloaded from [http://bioputer.mimuw.edu.pl/~mist/stats](http://bioputer.mimuw.edu.pl/~mist/stats)

9 Application: mass sampling from any discrete distribution

As the proposed algorithm is online, it may accept an infinite sequence of states as its population, and can still be expected to produce a sample in finite time, without exhausting the whole sequence. As such, one application is immediately obvious: mass sampling of iid variates from any discrete distribution. All one needs to do is to exhaustively walk through the configuration space of the distribution, preferably (though not necessarily) in order of decreasing probability mass function (PMF), and feed the resulting sequence into the proposed algorithm. The result is a sample from the input distribution of any desired size.

The advantage of the proposed solution is that the input distribution does not need to have an easily invertible CDF, only a computable PMF. The runtime is usually sublinear, wrt. to the sample size, but that depends on the exact properties of the distribution being sampled, distributions with light tails being faster to sample from than heavy-tailed ones. As an example: generating a sample of size $10^9$ from Poisson distribution with $\lambda = 10000.0$ using R programming language’s `rpois` function takes about 90 seconds, while using the scheme proposed above elapses 0.7 seconds. Such an algorithm itself consumes constant memory plus any memory needed for datastructures needed to walk through the configuration space (trivially constant in case of distributions with integer support, at worst a linear "visited" hashtable plus a linear priority queue when the configuration space is complicated, and needs to be traversed in a Dijkstra-like fashion [2]). The algorithm works online, in the meaning that the generated part of the sample is immediately available for consumption, before computations proceed to generate the rest of it.
This could be used to provide an alternative implementation of sampling functions in many programming languages, most of which accept an argument denoting sample size, but then proceed to generate even a large sample in a naive, iterative fashion. One point worth noting, however, is that the algorithm, as presented, returns the sample sorted in the order in which the configuration space was traversed. If this is undesirable, a Fisher-Yates shuffle \[3\] may be performed on the resulting stream, at the cost of loss of online property.

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