3

Random Sampling

"So much of life, it seems to me, is determined by pure randomness."
Sidney Poitier

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This lecture attacks a simple-to-state problem which is the backbone of many randomized algorithms, and admits solutions which are algorithmically challenging to design and analyze.

Problem. *Given a sequence of items $S = (i_1, i_2, \ldots, i_n)$ and a positive integer $m \leq n$, the goal is to select a subset of m items from S uniformly at random.*

Uniformity here means that any item in S has to be sampled with probability $1/n$. Items can be numbers, strings or general objects either stored in a file located on disk or streaming through a channel. In the former scenario, the input size n is known and items occupy n/B pages, in the latter scenario, the input size may be even unknown yet the *uniformity* of the sampling process must be guaranteed. In this lecture we will address both scenarios aiming at efficiency in terms of I/Os, extra-space required for the computation (in addition to the input), and amount of randomness deployed (expressed as number of randomly generated integers). Hereafter, we will make use of a built-in procedure `Rand(a,b)` that randomly selects a number within the range $[a, b]$. The type of the number, it is either real or integer, will be clear from the context. The design of a good `Rand`-function is a challenging task, however we will not go into its details because we wish to concentrate in this lecture on the sampling process rather than on the generation of random numbers; though, the interested reader can refer to the wide literature about (pseudo-)random number generators.

Finally we notice that it is desirable to have the positions of the sampled items in *sorted* order because this speeds up their extraction from S both in the disk setting (less seek time) and in the stream-based setting (less passes over the data). We do not want to detail further the sorting issue here, which gets complicated whenever $m > M$ and thus these positions cannot fit into internal memory. In this case we need an external-memory sorting algorithm, which is indeed an advanced topic of a subsequent lecture. If instead $m \leq M$ we could deploy the fact that positions are integers in a fixed range and thus use radix sort or any other faster routine available in the literature. Chapter **??** will deeply deal with such sorting problems, so we refer the interested reader there.

3.1 Disk model and known sequence length

We start by assuming that the input size n is known and that $S[1, n]$ is stored in a file on disk which cannot be modified because it may be the input of a more complicated problem that includes the

Algorithm 5: Drawing from all un-sampled positions

1: Initialize the auxiliary array $S'[1,n] = S[1,n]$;
2: **for** $s = 0, 1, \ldots, m-1$ **do**
3: $p = \texttt{Rand}(1, n-s)$;
4: select the item (pointed by) $S'[p]$;
5: swap $S'[p]$ with $S'[n-s]$.
6: **end for**

current one as a sub-task. The first algorithm we propose is very simple, and allows us to arise some issues that will be attacked in the subsequent algorithmic solutions.

At each step the algorithm selects one item from S', and replaces it with the last item of that sequence. This way S' contains the items not yet selected, stored contiguously. We point out that S' cannot be a *pure* copy of S but it must be implemented as an *array of pointers* to S's items. The reason is that these items may have variable length (e.g. strings) so their retrieval in constant time could not be obtained via arithmetic operations, as well as the replacement step might be impossible due to difference in length between $S'[p]$ and $S'[n-s]$. Pointers avoid these issues but occupy $\Theta(n \log n)$ bits of space, which might be a non negligible space when n gets large and might turn out even larger than S if the average length of S's objects is shorter than $\log n$.[1] Another drawback of this approach is given by its pattern of memory accesses, which acts over $O(n)$ cells in purely random way, taking $\Theta(m)$ I/Os. This may be slow when $m \approx n$, while in this case we would like to obtain $O(n/B)$ I/Os which is the cost of scanning the whole S.

So let us attack these issues by proposing a series of algorithms that incrementally improve the I/Os and the space resources of the previous solution, up to the final result that will achieve $O(m)$ extra space, $O(m)$ average time and $O(\min\{m, n/B\})$ I/Os. We start by observing that the swap of the items in Step 5 of `Algorithm 5` guarantees that every step generates one distinct item, but forces $\Omega(m)$ I/Os to be executed. The following `Algorithm 6` improves the I/O-complexity by avoiding the item-swapping via the use of an auxiliary data structure that keeps track of the selected positions. However this algorithm may generate *duplicate* positions, which must be discarded and *re-sampled*. Controlling the cost of the re-sampling process is the main drawback of this approach, but we will easily see that this induces a constant-factor slowdown on average, thus making this solution much appealing in practice.

Algorithm 6: Dictionary of sampled positions

1: Initialize the dictionary $\mathcal{D} = \emptyset$;
2: **while** $(|\mathcal{D}| < m)$ **do**
3: $p = \texttt{Rand}(1, n)$;
4: If $p \notin \mathcal{D}$ insert it;
5: **end while**

`Algorithm 6` stops when $\mathcal{D}$ contains m (distinct) integers which constitute the positions of the items to be sampled. According to our observation made at the beginning of the lecture, $\mathcal{D}$ may

[1] This may occur only if S contains duplicate items.

be sorted before S is accessed on disk to reduce the seek time. In any case, the efficiency of the algorithm mainly depends on the implementation of the dictionary $\mathcal{D}$. The literature offers many data structures that efficiently support membership and insert operations, based either on hashing or on trees. Here we consider only an hash-based solution which consists of implementing $\mathcal{D}$ via a hash table of size $\Theta(m)$ with collisions managed via chaining and a universal hash function for table access [2]. This way each membership query and insertion operation over $\mathcal{D}$ takes $O(1)$ time on average (the load factor of this table is $O(1)$), and total space $O(m)$. Time complexity could be forced to be worst case by using more sophisticated data structures, such as dynamic perfect hashing, but the final time bounds would always be *in expectation* because of the underlying re-sampling process. So we are left with the problem of evaluating the re-sampling cost: namely how many times do we need to re-sample a position in order to get a new one to insert in $\mathcal{D}$? This is derived via a simple probabilistic argument which observes that the probability of re-sampling equals the probability of extracting an item which is already present in $\mathcal{D}$. This can be evaluated as $|\mathcal{D}|/n \leq m/n < 1/2$ because, without loss of generality, we can assume that $m < n/2$ otherwise we can solve the *complement* of the current problem and thus randomly select the positions of the items that are *not* sampled from S. So we need an average of $O(1)$ re-samplings in order to obtain a new item for $\mathcal{D}$, and thus advancing in our selection process. Overall we have proved the following:

FACT 3.1 `Algorithm 6` *based on hashing with chaining requires $O(m)$ average time and takes $O(m)$ additional space to select uniformly at random m positions in $[1, n]$. The average depends both on the use of hashing and the cost of re-sampling. An additional sorting-cost is needed if we wish to extract the sampled items of S in a streaming-like fashion, thus taking $O(\min\{m, n/B\})$ I/Os.*

If we substitute hashing with a (balanced) search tree and assume to work in the RAM model (hence we assume $m < M$), then we can avoid the sorting step by performing an *in-visit* of the search tree in $O(m)$ time. However, `Algorithm 6` would still require $O(m \log m)$ time because each insertion/membership operation would take $O(\log m)$ time. We could do better by deploying an *integer*-based dictionary data structure, such as a van Emde-Boas tree, and thus take $O(\log \log n)$ time for each dictionary operation. The two bounds would be incomparable, depending on the relative magnitudes of m and n. Many other trade-offs are possible by changing the underlying dictionary data structure, so we leave to the reader this exercise.

The next step is to avoid a dictionary data structure and use *sorting* as a basic block of our solution. This could be particularly useful in practice because comparison-based sorters, such as `qsort`, are built-in in many programming languages.

Algorithm 7: Sorting

1: $\mathcal{D} = \emptyset$;
2: **while** ($|\mathcal{D}| < m$) **do**
3: $\quad \mathcal{X} = (m - |\mathcal{D}|)$ positions randomly drawn from $[1, n]$;
4: $\quad$ Concatenate to $\mathcal{X}$ the positions in $\mathcal{D}$;
5: $\quad$ Sort $\mathcal{X}$ and eliminate the duplicates;
6: $\quad$ Set $\mathcal{D}$ as the resulting $\mathcal{X}$;
7: **end while**

The cost of `Algorithm 7` depends on the number of times the sorting step is repeated and thus do exist duplicates in the sampled items. We argue that each iteration requires to draw fewer and

fewer random integers, and thus that a small number of re-samplings is needed. Under some reasonable conditions, we will show that a constant number of re-samplings suffices to generate the m distinct samples. But before digging into the math, let us introduce a simple optimization to the pseudo-code above: Steps 4 and 5 can be implemented by first sorting $\mathcal{X}$ and then merging the two sorted sequences of $\mathcal{X}$ and $\mathcal{D}$. In practice this is faster because $\mathcal{X}$ is getting shorter and shorter, but asymptotically this optimization is ineffective because the time complexity of `Algorithm 7` is dominated by the cost of the first iteration which involves m positions.

So let us compute the probability that `Algorithm 7` executes just one iteration: this means that the m sampled items are all distinct. This analysis is well known in the literature and goes under the name of *birthday problem*: how many people do we need in a room in order to have a probability larger than $1/2$ that at least two of them have the same birthday. In our context we have that people = items and birthday = position in S. By mimicking the analysis done for the birthday problem, we can estimate the probability that a duplicate among m randomly-drawn items does not occur as:

$$\frac{m!\binom{n}{m}}{n^m} = \frac{n(n-1)(n-2)\cdots(n-m+1)}{n^m} = 1 \times (1-\frac{1}{n}) \times (1-\frac{2}{n}) \times \cdots (1-\frac{m-1}{n})$$

Given that $e^x \geq 1 + x$, we can re-write the above formula as:

$$\leq e^0 \times e^{-1/n} \times e^{-2/n} \times \cdots e^{-(m-1)/n} = e^{-(1+2+\cdots+(m-1))/n} = e^{-m(m-1)/2n}$$

So the probability that a duplicate *does not* occur is upper bounded by $e^{-m(m-1)/2n}$ and, in the case of the birthday paradox in which $n = 365$, this is smaller than one-half already for $m = 23$. In general we have that about $\sqrt{n}$ elements suffices to make the probability of a duplicate not negligible. If $m \ll \sqrt{n}$ then e^x can be well approximated with $1 + x$ so $e^{-m(m-1)/2n}$ is a reasonable estimate of the collision probability and thus it could be used to estimate the number of re-samplings needed to complete `Algorithm 7`. Here we wish to follow a different argument which computes the average number of collisions, and will be useful when dealing with perfect hashing in a subsequent lecture (see Chapter **??**). The probability that two sampled integers collide is $n/n^2 = 1/n$, because we have n colliding pairs of integers in the range $[1, n]$. Given that we draw m integers, we have $\binom{m}{2}$ potential colliding pairs among them, and thus an average of $\frac{m(m-1)}{2n} < m^2/2n$ collisions. By using the Markov's inequality the probability that this number is larger than m^2/n (i.e. twice the expectation) is smaller than $1/2$, so two re-samplings are enough on average to guarantee less than m^2/n collisions. Actually we can look at the number m^2/n as $m \times m/n < m/2$ by applying the complement-argument above. In general, after k iterations of `Algorithm 7` we will ensure on average that the items to be re-sampled are $m/2^k$, so $O(\log m)$ iterations will be enough. Precisely, we could be more careful in this estimate and keep the factor m/n explicit and thus derive that $O(\log_{n/m} m)$ iterations are enough. Typically $m \ll n$, so that number of iterations is a constant.

FACT 3.2 `Algorithm 7` *requires a constant number of sorting steps on average, and $O(m)$ additional space, to select uniformly at random m items from the sequence $S[1, n]$. This is $O(m \log m)$ average time and m worst-case I/Os if $m \leq M$ is sufficiently small to keep the sampled positions in internal memory. Otherwise an external-memory sorter is needed. The average depends on the re-sampling, integers are returned in sorted order for streaming-like access to the sequence S.*

Sorting could be speeded up by deploying the specialty of our problem, namely, that items to be sorted are m random integers in a fixed range $[1, n]$. Hence we could use either radix-sort or, even better for its simplicity, bucket sort. In the latter case, we can use an array of m slots each identifying a range of n/m positions in $[1, n]$. If item i_j is randomly selected, then it is inserted in slot $\lfloor jn/m \rfloor$.

Since the m items are randomly sampled, each slot will contain $O(1)$ items on average, so that we can sort them in constant time per bucket by using insertion sort or the built-in `qsort`.

FACT 3.3 `Algorithm 7` *based on bucket-sort and* `qsort` *requires $O(m)$ average time and $O(m)$ additional space, whenever $m \leq M$. The average depends on the re-sampling. Integers are returned in sorted order for streaming-like access to the sequence S.*

We conclude this section by noticing that all the proposed algorithms, except `Algorithm 5`, generate the set of sampled positions using $O(m)$ space. If $m < M$ the random generation can occur within main memory without incurring in any I/Os. Sometimes this is useful because the randomized algorithm that invokes the random-sampling subroutine does not need the corresponding items, but rather their positions.

3.2 Stream model and known sequence length

We next turn to the case in which S is flowing through a channel and the input size n is known. We will turn to the more general case in which n is unknown at the end of the lecture, in the next section. This stream-based model imposes that every item of S is considered once and the algorithm must immediately and irrevocably take a decision whether or not that item must be included or not in the set of sampled items. Possibly future items may kick out that one from the sampled set, but no item can be re-considered again in the future. This scenario is particularly useful when the sequence S is very very long that we cannot store it or it could be too much expensive to process several times (e.g. Internet traffic or query logs).

Even in this case the algorithms are simple in their design but their probabilistic analysis is a little bit more involved than before. The algorithms of the previous section offer an *average* time complexity because they are faced with the re-sampling problem: possibly some samples have to be eliminated because duplicated. In order to avoid re-sampling, we need to ensure that each item is not considered more than once. So the algorithms that follow implement this idea is the simplest possible way, namely, they scan the input sequence S and consider each item once for all. This approach brings with itself two main difficulties which are related with the guarantee of both conditions: uniform sample from the range $[1, n]$ and sample of size m.

We start by designing an algorithm that draws just one item from S (hence $m = 1$), and then we generalize it to the case of a subset of $m > 1$ items. This algorithm proceeds by selecting the item $S[j]$ with probability $\mathcal{P}(j)$ which is properly defined in order to guarantee both two properties above.[2] In particular we set $\mathcal{P}(1) = 1/n$, $\mathcal{P}(2) = 1/(n-1)$, $\mathcal{P}(3) = 1/(n-2)$ etc. etc., so that the algorithm stops whenever one item is selected. Eventually item $S[n]$ is selected because its drawing probability is $\mathcal{P}(n) = 1$. So the proposed algorithm guarantees the condition on the sample size $m = 1$, but more subtle is to prove that the probability of sampling $S[j]$ is $1/n$, independently of j, given that we defined $\mathcal{P}(j) = 1/(n-j+1)$. The reason derives from a simple probabilistic argument because $n - j + 1$ is the number of remaining elements in the sequence and all of them have to be drawn uniformly at random.

The pseudo-code above details the algorithm for the case of an arbitrarily large sample $m > 1$. The difference resides in the probability of sampling $S[j]$ which is now set to $\mathcal{P}(j) = \frac{m-s}{n-j+1}$ where s is the number of items already selected before $S[j]$. Notice that if we already got all samples, it is

[2] In order to draw an item with probability p, it suffices to draw a random real $r \in [0, 1]$ and then compare it against p. If $r \leq p$ then the item is selected, otherwise no.

Algorithm 8: Scanning and selecting

```
1: s = 0;
2: for (j = 1; j ≤ n; j++) do
3:     p = Rand(0, 1);
4:     if (p ≤ (m−s)/(n−j+1)) then
5:         select S[j];
6:         s++;
7:     end if
8: end for
```

$s = m$ and thus $\mathcal{P}(j) = 0$, which correctly means that `Algorithm 8` does not generate more than m samples. On the other hand, it is easy to convince ourselves that `Algorithm 8` cannot generate less than m items, say y, given that the last y items of S would have probability 1 to be selected and thus they would be surely included in the final sample (according to Step 4). As far as the uniformity of the sample is concerned, we show that $\mathcal{P}(j)$ equals the probability that $S[j]$ is included in a random sample of size m given that s samples lie within $S[1, j-1]$. We can rephrase this as the probability that $S[j]$ is included in a random sample of size $m - s$ taken from $S[j, n]$, and thus from $n - j + 1$ items. This probability is obtained by counting how many such combinations include $S[j]$, i.e. $\binom{m-s(j)-1}{n-j}$, and dividing by the number of such combinations that do not include $S[j]$, i.e. $\binom{m-s(j)}{n-j}$. This ratio leads to the formula for $\mathcal{P}(j)$.

FACT 3.4 `Algorithm 8` *takes $O(n/B)$ I/Os, $O(n)$ time, n random samples, and $O(m)$ additional space to draw uniformly at random m items from the sequence $S[1, n]$ in a streaming-like way.*

We conclude this section by pointing out a sophisticated solution proposed by Jeff Vitter [3] that reduces the amount of randomly-generated numbers from n to m, and thus speeds up the solution to $O(m)$ time and I/Os. This solution could be also fit into the framework of the previous section (random access to input data), and in that case its specialty would be the avoidance of re-sampling. Its key idea is not to generate random *indicators*, which specify whether or not an item $S[j]$ has to be selected, but rather generate random *jumps* that count the number of items to skip over before selecting the next item of S. Vitter introduces a random variable $G(v, V)$ where v is the number of items remaining to be selected, and V is the total number of items left to be examined in S. According to our previous notation, we have that $v = m - s$ and $V = n - j + 1$. The item $S[G(v, V) + 1]$ is the next one selected to form the uniform sample. It goes without saying that this approach avoids the generation of duplicate samples, but yet it incurs in an average bound because of the cost of generating the jumps according to the following distribution:

$$\mathcal{P}(G = g) = \begin{pmatrix} V - g - 1 \\ v - 1 \end{pmatrix} / \begin{pmatrix} V \\ v \end{pmatrix}$$

In fact the key problem here is that we cannot tabulate (and store) the values of all binomial coefficients in advance, because this would need space exponential in $V = \Theta(n)$. Surprisingly Vitter solved this problem in $O(1)$ average time, by adapting in an elegant way the von Neumann's rejection-acceptance method to the discrete case induced by G's jumps. We refer the reader to [3] for further details.

3.3 Stream model and unknown sequence length

It goes without saying that the knowledge of n was crucial to compute $\mathcal{P}(j)$ in `Algorithm 8`. If n is unknown we need to proceed differently, and indeed the rest of this lecture is dedicated to detail two possible approaches to solve this problem in the streaming model.

The first one is pretty much simple and deploys a min-heap $\mathcal{H}$ of size m plus a real-number random generator, say `Rand(0,1)`. The key idea underlying this algorithm is to associate a random key to each item of S and then use the heap $\mathcal{H}$ to select the items corresponding to the top-m keys. The pseudo-code below implements this idea, we notice that $\mathcal{H}$ is a min-heap so it takes $O(1)$ time to detect the minimum key among the current top-m ones. This is the key compared with r_j in order to establish whether or not $S[j]$ must enter the top-m set.

Algorithm 9: Heap and random keys

```
1: Initialize the heap H with m dummy pairs ⟨−∞, ∅⟩;
2: for each item S[j] do
3:     r_j = Rand(0, 1);
4:     m = the minimum key in H;
5:     if (r_j > m) then
6:         insert ⟨r_j, S[j]⟩ in H;
7:     end if
8: end for
9: return H
```

Since the heap has size m, the final sample will consists of m items. Each item takes $O(\log m)$ time to be inserted in the heap. So we have proved the following:

FACT 3.5 `Algorithm 9` *takes $O(n/B)$ I/Os, $O(n \log m)$ time, generates n random numbers, and uses $O(m)$ additional space to sample uniformly at random m items from the sequence $S[1,n]$ in a streaming-like way and without the knowledge of n.*

A note is in order at this point. The reader could think to apply this algorithm in the context of the previous section, with the help of a sorting procedure. Namely, one could think to first generate pairs for all n items of S, and then sort them by means of their first (key-)field. The m-size sample could be finally obtained by taking any sub-array of size m of this sorted sequence, for example, the first m items. The limitation of this approach would be the application of the sort-routine on n pairs, rather than the m ones of `Algorithm 7` or `3`, which is unacceptable in the context of massive datasets.

We conclude the lecture by introducing the elegant *reservoir sampling* algorithm, introduced by Knuth in 1997, which improves `Algorithm 9` both in time and space complexity. The idea is similar to the one adopted for `Algorithm 8` and consists of properly defining the probability with which an item is selected. The key issue here is that we cannot take an irrevocable decision on $S[j]$ because we do not know how long the sequence S is, so we need some freedom to *change* what we have decided so far as the scanning of S goes on.

The pseudo-code above uses a "reservoir" array $R[1,m]$ to keep the candidate samples. Initially R is set to contain the first m items of the input sequence. At any subsequent step j, the algorithm makes a choice whether $S[j]$ has to be included or not in the current sample. This choice occurs with probability $\mathcal{P}(j) = m/j$, in which case some previously selected item has to be kicked out from

Algorithm 10: Reservoir sampling

```
1: Initialize array R[1, m] = S[1, m];
2: for each next item S[j] do
3:       h = Rand(1, j);
4:       if j ≤ m then
5:             set R[h] = S[j];
6:       end if
7: end for
8: return array R;
```

R. This item is chosen at random, hence with probability $1/m$. This double-choice is implemented in `Algorithm 10` by choosing an integer h in the range $[1, j]$, and making the substitution only if $h \leq j$. This event has probability m/j: exactly what we wished to set for $\mathcal{P}(j)$.

For the correctness, it is clear that `Algorithm 10` selects m items, it is less clear that these items are drawn uniformly at random from S, which actually means with probability m/n. Let's see why by assuming inductively that this property holds for a sequence of length $n-1$. The base case in which $n = m$ is obvious, every item has to be selected with probability $m/n = 1$, and indeed this is what Step 1 does by selecting all $S[1, m]$ items. To prove the inductive step (from $n-1$ to n items), we notice that the uniform-sampling property holds for $S[n]$ since by definition that item is inserted in R with probability $\mathcal{P}(n) = m/n$ (Step 4). Computing the probability of being sampled for the other items in $S[1, n-1]$ is more difficult to see. Each of these items has probability $m/(n-1)$ of being in the reservoir R, by the inductive hypothesis. This item remains in the reservoir if either $S[n]$ is not picked (which occurs with probability $1 - \frac{m}{n}$) or if it is not kicked out by the picked $S[n]$ (which occurs with probability $\frac{m}{n} \times \frac{m-1}{m}$). Summing up these terms we get that $n-1/n$ is the probability that an item is not kicked out from the reservoir. Overall an item belongs to the reservoir R at the n-th step of `Algorithm 10` iff it was in the reservoir at the $(n-1)$-th step and it is not kicked out at the n-th step: namely, $m/(n-1) \times (n-1)/n = m/n$. To understand this formula assume that we have a reservoir of 1000 items, so the first 1000 items of S are inserted in R by Step 1. Then the item 1001 is inserted in the reservoir with probability $1000/1001$, the item 1002 with probability $1000/1002$, and so on. Each time an item is inserted in the reservoir, a random element is kicked out from it, hence with probability $1/1000$. After n steps the reservoir R contains 1000 items, each sampled from S with probability $1000/n$.

FACT 3.6 `Algorithm 10` *takes $O(n/B)$ I/Os, $O(n)$ time, n random numbers, and $O(m)$ additional space to sample uniformly at random m items from the sequence $S[1, n]$ in a streaming-like way and without the knowledge of n. Hence it is time, space and I/O-optimal in this model of computation.*

References

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