A Note on Enumeration by Fair Sampling

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April 6, 2021

Abstract

This note describes an algorithm for enumerating all the elements in a finite set based on uniformly random sampling from the set. This algorithm can be used for enumeration by fair sampling with quantum annealing. Our algorithm is based on a lemma of the coupon collector’s problem and is an improved version of the algorithm described in arXiv:2007.08487 (2020). We provide a mathematical analysis and a numerical demonstration of our algorithm.

1 Enumeration by fair sampling

The objective of the algorithm described in this note is to enumerate all the elements of a finite set by repeating uniformly random sampling from the set. This is mathematically formulated as follows.

Problem 1. Suppose there exists a sampler that samples an element of a finite set $X$ with equal probability, that is, the probability that the sampler returns $x \in X$ is $1/|X|$, where $|X|$ is the number of all the elements of $X$ and is unknown. Then, using the sampler repeatedly, enumerate all the elements of $X$ with success probability greater than or equal to $1 - \epsilon$, where $\epsilon \in (0, 1]$ is a failure tolerance.

This kind of problem appears in the application of quantum annealing to enumeration problems [1]. Quantum annealing is a procedure to find ground states of an Ising Hamiltonian. By designing a Hamiltonian so that the ground state(s) of the spin configuration corresponds to desired combinations, such as cost minimum or constraint satisfactory combinations, one can sample them by quantum annealing. If the Hamiltonian system has multiple ground states corresponding to elements of a finite set, one can take advantage of the sampling ability of quantum annealing to enumerate all the elements of the set.

Although current versions of quantum annealing do not always sample ground states with equal probability [2] and the research on how to achieve the fair sampling in quantum annealing is still one of the most interesting subjects on quantum annealing [1][3], as the first step toward the application of quantum annealing to enumeration problems, we address a framework for enumeration by fair sampling assuming that we have a fair sampler. The same topic was addressed in the appendix of Ref. [1], in which an algorithm for enumeration by fair sampling was proposed based on a well-known lemma in the coupon collector’s problem. The coupon collector’s problem is a classic problem in probability theory, which is described as follows: If there are $n$ different types of coupons and we can get one of the types of coupons with equal probability at each trial, how many trial do we need to collect all $n$ types of coupons? The evaluation of the probability distribution of the number of trials needed to collect all types of coupons derives a termination condition of samplings in the enumeration. In this note, we derive an improved version of the algorithm in Ref. [1] based on an extension of the lemma in the coupon collector’s problem used in Ref. [1].

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Algorithm 1 Enumeration by Uniformly Random Sampling

Input: Sampling method Sample(), failure tolerance $\epsilon \in (0, \frac{1}{e}]$, checkpoints $C = [m_1, \ldots, m_M] \in \mathbb{N}^M$ s.t. $m_i < m_j$ for any $i < j$ and $m_M \geq |X|$

Output: Collection of samples $S$

1: $S \leftarrow \{\}$
2: $t \leftarrow 0$
3: for $i = 1, \ldots, M$ do
4: while $t \leq \lceil m_i \log(m_i M/\epsilon) \rceil$ do
5: $s \leftarrow \text{Sample}()$
6: $S \leftarrow S \cup \{s\}$
7: $t \leftarrow t + 1$
8: end while
9: if $|S| < m_i$ then
10: break
11: end if
12: end for
13: return $S$

2.1 Algorithm description

An algorithm for Problem 1 can be derived based on the following lemma (See Sec. 2.2 for the proof).

Lemma 1. Let $T_m$ be the random variable representing the number of samplings necessary to collect $m$ different elements of $X$. If the true value of the number of all the elements of $X$ is $n$, for any positive integer $m (\leq n)$ and any positive real number $\epsilon (\leq 1/e)$, the tail distribution of $T_m$ is bounded from above as

$$P \left( T_m > \lceil m \log\frac{m}{\epsilon} \rceil \bigg| |X| = n \right) \leq \epsilon. \quad (1)$$

This implies that, if the number of collected elements after $\lceil m \log(m/\epsilon) \rceil$ samplings is less than $m$, we can judge that no more different element exists in $X$ with failure probability less than or equal to $\epsilon$. In other words, we can use the condition $T_m > \lceil m \log(m/\epsilon) \rceil$ as a termination condition of samplings.

Algorithm 1 is an algorithm based on Lemma 1. In this algorithm, there are $M$ checkpoints for checking the termination condition $T_{m_i} > \lceil m_i \log(m_i M/\epsilon) \rceil$. The maximum integer of the checkpoints, $m_M$, should be larger than the unknown value of $|X|$ in order to ensure success in the enumeration. Thus, one needs to estimate a (rough) upper bound of $|X|$ before applying the algorithm. Note that the number of checkpoints, $M$, is contained in the logarithm of the termination conditions so that the failure probability of the judgement at each checkpoint is less than or equal to $\epsilon/M$ rather than $\epsilon$. This ensures that the total failure probability is less than or equal to $\epsilon$.

The success probability and the number of times of sampling for Algorithm 1 to collect all the elements of $X$ is formally stated as follows.

Theorem 1. Algorithm 1 outputs the collection of all the elements of $X$ with success probability greater than or equal to $1 - \epsilon$, if the input satisfies the requirements $\epsilon \in (0, 1/e]$, $m_i < m_j$ for any $1 \leq i < j \leq M$, and $m_M \geq |X|$. In success cases, the number of times of sampling the algorithm calls is $\lceil m_k \log(m_k M/\epsilon) \rceil$, where index $k$ $(1 \leq k \leq M)$ satisfies $m_{k-1} < |X| \leq m_k$ (let $m_{k-1}$ be 0 for $k = 1$).

Proof. Let $k$ be the index of the checkpoint that satisfies $m_{k-1} < |X| \leq m_k$, which always exists if $|X| \leq m_M$. In the cases of success in the enumeration, the algorithm does not break out of the loop at all checkpoints before the $k$-th checkpoint, and collects all the elements of $X$ before breaking out at the $k$-th checkpoint. Because the number of samplings the algorithm has done up to the $k$-th checkpoint is $\lceil m_k \log(m_k M/\epsilon) \rceil$, the second statement of the theorem is true.

To prove the first statement, we evaluate the success probability under the condition $|X| = n$. From the above discussion, we can express the success probability as

$$P(\text{success}) = P \left( \bigwedge_{i=1}^{k-1} \left\{ T_{m_i} \leq \lceil m_i \log\frac{m_i M}{\epsilon} \rceil \right\} \land \left\{ T_n \leq \lceil m_k \log\frac{m_k M}{\epsilon} \rceil \right\} \bigg| |X| = n \right).$$

\(^1\text{See the proof of Theorem 1 below for the detailed discussion.}\)
Taking the negation, the failure probability can be expressed as
\[
P(\text{failure}) = P \left( \bigvee_{i=1}^{k-1} \left\{ T_{m_i} > \left\lceil m_i \log \frac{m_i M}{\epsilon} \right\rceil \right\} \lor \left\{ T_n > \left\lceil m_k \log \frac{m_k M}{\epsilon} \right\rceil \right\} \bigg| X = n \right).
\]

Due to the subadditivity of probabilities, we obtain
\[
P(\text{failure}) \leq \sum_{i=1}^{k-1} P \left( T_{m_i} > \left\lceil m_i \log \frac{m_i M}{\epsilon} \right\rceil \bigg| X = n \right) + P \left( T_n > \left\lceil m_k \log \frac{m_k M}{\epsilon} \right\rceil \bigg| X = n \right).
\]

Since \( m_k \geq n \), we get
\[
P \left( T_n > \left\lceil n \log \frac{n M}{\epsilon} \right\rceil \bigg| X = n \right)
= P \left( \left\lceil m_k \log \frac{m_k M}{\epsilon} \right\rceil \bigg| X = n \right) + P \left( \left\lceil m_k \log \frac{m_k M}{\epsilon} \right\rceil \geq T_n > \left\lceil n \log \frac{n M}{\epsilon} \right\rceil \bigg| X = n \right)
\geq P \left( T_n > \left\lceil m_k \log \frac{m_k M}{\epsilon} \right\rceil \bigg| X = n \right) + P \left( T_n > \left\lceil n \log \frac{n M}{\epsilon} \right\rceil \bigg| X = n \right),
\]

which gives
\[
P(\text{failure}) \leq \sum_{i=1}^{k-1} P \left( T_{m_i} > \left\lceil m_i \log \frac{m_i M}{\epsilon} \right\rceil \bigg| X = n \right) + P \left( T_n > \left\lceil n \log \frac{n M}{\epsilon} \right\rceil \bigg| X = n \right).
\]

According to Lemma 1, all of \( k \) terms in the right hand side of the above inequality are less than or equal to \( \epsilon/M \). Therefore, the failure probability is less than or equal to \( \epsilon \), under the condition \( X = n \). Because the above discussion is valid for any \( n \), the first statement of the theorem is proven.

2.2 Proof of Lemma 1

In this subsection, we prove Lemma 1. Before giving a proof of Lemma 1, we prove the special case for \( m = n \):

**Lemma 2.** Suppose \( X \) is a finite set with size \( n \). Let \( T \) be the random variable representing the number of times of samplings necessary to collect all \( n \) different elements of \( X \). Then, for any positive real number \( \epsilon \), the tail distribution of \( T \) is bounded from above as

\[
P \left( T > \left\lceil n \log \frac{n}{\epsilon} \right\rceil \bigg| X = n \right) \leq \epsilon.
\]

The expectation value of \( T_{m_{k-1}+1} \) given \( |X| = n \) is greater than \( n \log[(n + 1)/(n - m_{k-1} + 2)] \). The proof is as follows. Let \( t_i \) be the random variable representing the number of times of sampling necessary to obtain a new (uncollected) element after \( i - 1 \) elements are collected. The probability distribution of \( t_i \) is the geometric distribution with expectation \( n/(n - i + 1) \). Thus, for \( m \leq n \), we get

\[
E( T_m | |X| = n ) = E \left( \sum_{i=1}^{m} t_i \bigg| |X| = n \right) = \sum_{i=1}^{m} E( t_i | |X| = n ) = n \sum_{k=n-m+1}^{n} \frac{1}{k} > n \int_{n-m+1}^{n+1} \frac{dx}{x} = n \log \frac{n+1}{n-m+1}.
\]

Substituting \( m_{k-1} + 1 \) for \( m \) completes the proof.
Proof. Let $S_\tau$ be the set of elements that have been already collected until time $\tau$. The probability that an element $x \in X$ has not been sampled yet up to the moment $\tau$ is
\[
P (x \notin S_\tau | |X| = n) = \left( 1 - \frac{1}{n} \right)^\tau \leq e^{-\frac{\tau}{n}}.
\]
Thus, the probability that $T > \tau$ can be evaluated as
\[
P (T > \tau | |X| = n) = \mathbb{P} \left( \bigvee_{x \in X} \{ x \notin S_\tau \} | |X| = n \right)
\leq \sum_{x \in X} P (x \notin S_\tau | |X| = n)
\leq ne^{-\frac{\tau}{n}}.
\]
Substituting $\tau = \lceil n \log(n/\epsilon) \rceil$, we obtain
\[
P \left( T > \left\lceil n \log \frac{n}{\epsilon} \right\rceil | |X| = n \right) \leq \epsilon.
\]

Now, let us prove Lemma 2 as an extension of Lemma 1.

**Proof.** Let $t_i$ be the random variable representing the number of times of sampling necessary to obtain a new (uncollected) element after $i - 1$ elements are collected. This can be expressed as

\[
t_i = T_i - T_{i-1}.
\]

In the case that $t_i = l$ under the condition $|X| = n$, after $i - 1$ elements are collected, the sampler returns any of the $i - 1$ collected elements until the $(l - 1)$-th trial and returns one of the $n - (i - 1)$ uncollected elements at the $l$-th trial. Thus, the probability distribution of $t_i$ is the geometric distribution
\[
P (t_i = l | |X| = n) = \frac{n - (i - 1) - 1}{n} \left( \frac{i - 1}{n} \right)^{l - 1}.
\]
Here, note that $t_1, \ldots, t_m$ are independent of each other.

The random variable $T_m$ can be expressed as
\[
T_m = t_1 + t_2 + \cdots + t_m,
\]
and the tail distribution of $T_m$ can be written as
\[
P (T_m > \bar{\tau} | |X| = n) = \sum_{\tau > \bar{\tau}} \sum_{\sum_{i=1}^m \tau_i = \tau} \mathbb{P} (t_1 = \tau_1, \ldots, t_m = \tau_m | |X| = n)
\leq \sum_{\tau > \bar{\tau}} \sum_{\sum_{i=1}^m \tau_i = \tau} n^{-\bar{\tau}} \prod_{i=1}^m [n - (i - 1)] (i - 1)^{\tau_i - 1},
\]
where $\bar{\tau}, \tau$, and $\tau_i$ for $1 \leq i \leq m$ are positive integers and $\sum_{i=1}^m \tau_i = \tau$ means the summation with respect to all possible combinations of $\tau_1, \tau_2, \ldots, \tau_m$ such that $\sum_{i=1}^m \tau_i = \tau$.

We will prove the inequality
\[
P (T_m > \bar{\tau} | |X| = n) \leq P (T_m > \bar{\tau} | |X| = m),
\]
under the condition
\[
m \leq n, \quad 0 < \epsilon \leq \frac{1}{e}, \quad \bar{\tau} \geq \left\lceil m \log \frac{m}{\epsilon} \right\rceil,
\]
\footnote{This condition implies the random variable $T_m$ equals to the integer $\tau$.}
so that the tail distribution of $T_m$ given $|X| = n$ is bounded from above by a probability that can be bounded using Lemma 2. To examine the dependence with respect to $n (\geq m)$ of the probability $P(T_m > \bar{\tau} \mid |X| = n)$, let us define functions $f : \mathbb{R} \to \mathbb{R}$ and $g_\tau : \mathbb{R} \to \mathbb{R}$ as
\[
    f(x) = \prod_{i=1}^{m} [x - (i - 1)],
\]
\[
    g_\tau(x) = x^{-\tau} f(x).
\]
If the function $g_\tau$ monotonically decreases with respect to $x (\geq m)$, Eq. (3) is true as shown below. The first derivative of $g_\tau$ is
\[
    g'_\tau(x) = -\tau x^{-\tau - 1} f(x) + x^{-\tau} \sum_{i=1}^{m} \frac{f(x)}{x - (i - 1)}
    = x^{-\tau - 1} f(x) \left[ \sum_{i=1}^{m} \frac{x}{x - (i - 1) - \tau} \right].
\]
Because $f(x) > 0$ for $x \geq m$, if the condition
\[
    \tau \geq \sum_{i=1}^{m} \frac{x}{x - (i - 1)}
\]
is satisfied for all $x \geq m$, the function $g_\tau$ decreases monotonically with respect to $x (\geq m)$. The right hand side of the above condition is bounded from above in the range $x \geq m$ as
\[
    \sum_{i=1}^{m} \frac{x}{x - (i - 1)} \leq \sum_{i=1}^{m} \frac{m}{m - (i - 1)}
    = m \left( 1 + \sum_{k=2}^{m} \frac{1}{k} \right)
    = m \left( 1 + \int_{1}^{m} \frac{dy}{[y]} \right)
    \leq m \left( 1 + \int_{1}^{m} \frac{dy}{y} \right)
    = m \log m + m
    = m \log \frac{m}{\epsilon}
    \leq m \log \frac{m}{\epsilon} \quad (\because \epsilon \leq 1/e).
\]
Thus, the condition
\[
    m \leq n, \quad 0 < \epsilon \leq \frac{1}{e}, \quad \tau \geq \left\lceil m \log \frac{m}{\epsilon} \right\rceil
\]
is a sufficient condition for the monotonical decreasing of $g_\tau$. Under the condition (4), the above sufficient condition for the monotonical decreasing of $g_\tau$ is satisfied for any $\tau > \bar{\tau}$. Thus, we obtain the inequality
\[
    P(T_m > \bar{\tau} \mid |X| = n) = \sum_{\tau > \bar{\tau}} \sum_{\sum_{i=1}^{m} \tau_i = \tau} g_\tau(n) \prod_{i=1}^{m} (i - 1)^{\tau_i - 1}
    \leq \sum_{\tau > \bar{\tau}} \sum_{\sum_{i=1}^{m} \tau_i = \tau} g_\tau(m) \prod_{i=1}^{m} (i - 1)^{\tau_i - 1}
    = P(T_m > \bar{\tau} \mid |X| = m),
\]
under the condition (4).

Substituting $\bar{\tau} = \lceil m \log(m/\epsilon) \rceil$, we get the inequality we want to prove:
\[
    P \left( T_m > \lceil m \log \frac{m}{\epsilon} \rceil \mid |X| = n \right) \leq P \left( T_m > \lceil m \log \frac{m}{\epsilon} \rceil \mid |X| = m \right) \leq \epsilon,
\]
where the second inequality is due to Lemma 2.
3 Numerical tests and discussions

Results of numerical tests are shown in Fig. 1. In the numerical tests, the checkpoints were $C = [2^1, 2^2, \cdots, 2^{10}]$ (the same as those in the algorithm in Ref. [1]), the failure tolerance $\epsilon$ was 0.01, the numbers of all the elements $|X|$ for test cases were 50, 100, 150, $\cdots$, 1000, and the number of times of test runs for each case was $10^5$.

The left panel shows the numbers of times of sampling in success cases. The numerical results (circle) and the theoretical result (solid line) are in good agreement with each other as expected.

The right panel shows the failure rates of the algorithm. For all test cases, the failure rates were less than the failure tolerance $\epsilon$, which demonstrates the validity of Algorithm 1. Moreover, the failure rates were much smaller than the failure tolerance and for most cases they were almost zero. This is because the inequality in Lemma 1 is not tight. In the proof of Lemma 1, we proved the inequality

$$g_\tau(n) \leq g_\tau(m).$$

The tightness of the inequality is represented by the ratio of $g_\tau(n)$ and $g_\tau(m)$,

$$\rho_\tau \equiv \frac{g_\tau(n)}{g_\tau(m)} = \left( \frac{n}{m} \right)^{\tau},$$

which can be extremely smaller than 1 as shown in Fig. 2. This figure additionally shows that the inequality is tight when $m \simeq n$. This may be the reason why the failure rates in some test cases where $m_k \simeq n$ are relatively large.

The looseness of the inequality implies that we can derive more efficient algorithms for Problem 1 based on a tighter inequality evaluation. Further improvements of the efficiency (the number of times of sampling) and the adaptation for non-uniform samplings of the sampling-based enumeration algorithm remains as future works.

Acknowledgements

This work is supported by JST, PRESTO Grant Number JPMJPR2018.
Figure 2: The tightness of the inequality which is the basis of Algorithm 1. The tightness is represented by $\rho_\tau$, that is, the ratio of $g_\tau(n)$ and $g_\tau(m)$. In this figure, $n = 100$ and $\tau = \lceil m \log(m/\epsilon) \rceil$ with $\epsilon = 0.01$. Note that the vertical axis is log-scaled.

References

[1] V. Kumar, C. Tomlin, C. Nehrkorn, D. O’Malley, and J. Dulny III, “Achieving fair sampling in quantum annealing”, arXiv:2007.08487 (2020).

[2] M. S. Kötz, G. Mazzola, A. J. Ochoa, H. G. Katzgraber, and M. Troyer, “Uncertain fate of fair sampling in quantum annealing”, Phys. Rev. A 100, 030303 (2019).

[3] M. Yamamoto, M. Ohzeki, and K. Tanaka, “Fair Sampling by Simulated Annealing on Quantum Annealer”, J. Phys. Soc. Jpn. 89, 025002 (2020).