A Appendix: Decision Tree

In this section, we introduce the connection between optimal question selection problem and optimal decision tree problem, and thus complete the proofs of the computation complexity of OQS and approximation ratio of *minimax branch* given in Section 2.

A.1 Definitions

Definition A.1. (Decision tree) Given a set of m tests T, a set of n items X, and a set of test results R, where each pair of $t \in T$ and $x \in X$ is associated with a test result $r \in R$, denoted as t(x). A *decision tree DT* on T, X is a rooted tree that satisfies the following properties:

- Each internal node is labeled by a test in *T*.
- Each internal node has at least two children.
- Each outgoing edge of each internal node is labeled by a value in *R*.
- For any internal node, the labels of its outgoing edges are different from each other.
- Each leaf node is labeled by a non-empty subset of *X*.
- Given a path from the root to a leaf $(t_1, r_1, \dots, t_n, r_n, X_0)$, we have $t_i(x) = r_i$ for any $1 \le i \le n$ and $x \in X_0$.
- For any two $x_1, x_2 \in X$, x_1 and x_2 are labeled on the same leaf iff for any $t \in T$, $t(x_1) = t(x_2)$.

Example A.2. Figure 5 shows an example of decision trees. The items are eight integers $\{0,1,6,11,12,15,16,21\}$, and the tests are calculating the remainder of dividing 2,3,5 respectively. The left tabular lists the corresponding test results. A decision tree of these tests and items is shown on the right side. Each internal node is marked with its label and each leaf is marked with its corresponding item.

		T_1	T_2	T_3
		mod 2	mod 3	mod 5
X_1	0	0	0	0
X_2	1	1	1	1
X_3	6	0	0	1
X_4	11	1	2	1
X_5	12	0	0	2
X_6	15	1	0	0
X_7	16	0	1	1
X_8	21	1	0	1

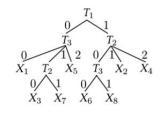


Figure 5. An example of decision trees. The right tree is a decision tree constructing from the items and tests which are listed in the left tabular.

Given a decision tree DT, we define the $\cos c(X_i)$ of an item X_i be the depth of its corresponding leaf (the depth of the root is defined as 0). This definition has an explicit realistic correspondence: it is equal to the number of the tests used by DT to identify X_i . For instance, on the decision

tree shown in Figure 5, $c(X_1) = c(X_2) = c(X_4) = C(X_5) = 2$, $c(X_3) = c(X_6) = c(X_7) = c(X_8) = 3$.

Based on the definitions of decision trees and the costs of items, we now describe the problem of constructing an optimal decision tree.

Definition A.3. (\mathfrak{DT} Problem) Given a set of tests T, a set of items X, a set of test results R, and a probability distribution φ on X, which assigns a probability to each item in X and all probabilities sum up to 1, the goal of *optimal decision tree problem* \mathfrak{DT} is to construct a decision tree in which the expected cost of a random item is minimized, i.e., find a decision tree that minimizes $\sum_{x \in X} \varphi(x)c(x)$. This expected cost is called as the *cost of a decision tree*.

Specially, when φ is fixed to a uniform distribution on X, the problem is named as \mathcal{UDT} . When the tests are all binary, i.e., the results are always Boolean values, the problem is named as $2 - \mathcal{DT}$. Besides, when the two conditions are satisfied at the same time, the name is $2 - \mathcal{UDT}$.

Example A.4. In Example A.2, when φ is a uniform distribution on X, the cost of the decision tree in Figure 5 is $\frac{5}{2}$. When φ is a uniform distribution on $\{X_1, X_5, X_6\}$ and other items have no chance to occur, the cost of the decision tree is $\frac{7}{3}$. We show the corresponding optimal decision trees in Figure 6. The left tree is the answer of \mathbb{UDT} with the minimum cost $\frac{19}{8}$, and the right tree is the answer of \mathbb{DT} with the minimum cost $\frac{5}{3}$ when q is a uniform distribution on $\{X_1, X_5, X_6\}$.

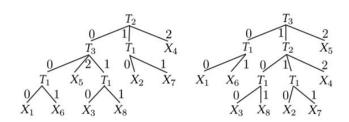


Figure 6. The left tree and the right tree are the optimal decision tree when q is a uniform distribution on X and on $\{X_1, X_5, X_6\}$ respectively.

A.2 Some results on constructing optimal decision trees

Complexity of Optimal Decision Tree. As decision trees are used in many fields, constructing an optimal decision tree has become an important and fascinating subject. Over the past decades, there have been a lot of theoretical results and algorithms published. As many other optimization problems, $2 - \mathcal{UDT}$ was proved as an NP-complete problem in very early days [28], which implies \mathcal{UDT} , $2-\mathcal{DT}$, \mathcal{DT} are all NP-hard. After realizing the hardness of finding an optimal

polynomial-time algorithm, most of subsequent works focus on finding efficient approximation algorithms and proving the hardness of approximating \mathfrak{DT} .

An Approximation Algorithm. As the background, we first give the definitions of approximation algorithms, approximation ratios and the hardness of approximation. Intuitively, the approximation ratio measures the distance between the optimal solution and the solution given by a approximation algorithm, and the hardness of approximation shows how hard to find an approximation algorithm within a given approximation ratio.

Definition A.5. (Approximation Algorithm) For an optimization problem \mathcal{P} of which the goal is to minimize an objective function c, an algorithm A is an approximation algorithm with approximation ratio k iff it satisfies the following two conditions:

- For any instance of \mathcal{P} , the result of A is always valid.
- For any instance of \mathcal{P} , the inequality $c(S) \leq kc(S')$ holds for any valid solution S', where S is the solution given by A.

Definition A.6. (Hardness of Approximation) An optimization problem \mathcal{P} is hard to be approximated within approximation ratio k iff there is no polynomial-time algorithm that approximates \mathcal{P} within ratio k unless P = NP.

With these definitions, we show how *minimax branch* works for \mathfrak{DT} . For each node, *minimax branch* always choose the test which partition the items represented by this node as equally as possible. More concretely, we assume there is a function par that partitions a set of items S based on a test $t_i \in T$, i.e., $par(S,t_i) = \{S'_1,\ldots,S'_k\}$ where each S_i corresponds to a possible result of the test. We further define the cost of test t_i on item set S as $cost(t_i,S) = \max_{S'_j \in par(S,t_i)} \sum_{x \in S'_j} \varphi(x)$, i.e., the largest sum of probabilities among all subsets in this partition. Then $minimax\ branch$ always chooses the test with the smallest cost to partition the items.

Many research results indicate that *minimax branch* is an efficient approximation algorithm. We introduce them below.

Approximation Ratios of *minimax branch.* Table 3 summaries the state-of-the-art results in different branches of \mathcal{DT} problem. As we can see from the table, *minimax branch* is the state-of-the-art algorithm for the first three problems. The only exception is \mathcal{DT} , of which a polynomial time algorithm with an ratio $O(\log m)$ is found [21]. However, that algorithm is much more complex than *minimax branch*.

On the other hand, under the assumption that $P \neq NP$, $2 - \mathcal{UDT}$ and \mathcal{UDT} are hard to be approximated within any factors less than 2 and 4 respectively, and there is an approximation ratio $r(m) = \Omega(\log m)$ within which both $2 - \mathcal{DT}$ and \mathcal{DT} are hard to be approximated. Especially, for $2 - \mathcal{DT}$,

the approximation ratio $O(\log m)$ of *minimax branch* has already reached the lower bound $\Omega(\log m)$. Therefore, *minimax branch* is an optimal polynomial time algorithm to approximate $2 - \mathcal{DT}$ unless P = NP.

Problem	Hardness	Ref.	minimax branch	Ref.
2 - UDT	$2 - \epsilon, \forall \epsilon > 0$		$1 + \ln m$ *	[1]
UDT	$4 - \epsilon, \forall \epsilon > 0$	[10]	$O(\log m)$ *	[11]
$2 - \mathfrak{DT}$	$\Omega(\log m)$	[10]	$O(\log m)$ *	[10]
DT	$\Omega(\log m)$		$O(\log^2 m)$	[10]

* The best approximation ratio found in polynomial time so far. **Table 3.** The summary of related results. The second column shows the hardness of approximation and the fourth column shows the proved approximation ratio of the *minimax branch* strategy. Parameter m represents the number of items, i.e., |X|.

A.3 Relationship between Question Selection and Decision Tree

In this subsection, we discuss the relationship between optimal question selection problem and optimal decision tree problem. Intuitively, each program in the program space corresponds to an item to be distinguished by the decision tree, each question corresponds to a test, and each answer corresponds to a test result.

From optimal decision tree to question selection. We first consider how to reduce optimal decision tree problem to optimal question selection problem. We start by defining a mapping from instances of \mathcal{DT} to instances of \mathcal{OQS} . More concretely, we have the following mapping.

$$\pi(X, T, R, \varphi) = (\mathbb{P}, \mathbb{Q}, \mathbb{A}, \varphi')$$

where

- *X* is a set of items.
- *T* is a set of tests.
- *R* is a set of test results.
- φ is a distribution over items in X.
- $\mathbb{P} = \{\pi_x(t) \mid x \in X\}$ is a set of programs with if-else structures. Let t_1, t_2, \dots, t_n be items in T. The program $\pi_x(t)$ for item x is defines as follows.

// program for x if input $== t_1$ then return test result of t_1 on x else if input $== t_2$ then return test result of t_2 on x

else if input $==t_{n-1}$ then return test result of t_{n-1} on x else return test result of t_n on x

- \mathbb{Q} is a question domain and is equal to T.
- \mathbb{A} is a answer domain and is equal to R.
- φ' is a distribution over programs in \mathbb{P} and $\varphi'(\pi_x(t))$ is defined as $\varphi(x)$.

It is easy to see that π can be implemented as a polynomial-time algorithm.

We then present Algorithm 4 which constructs a decision tree from a question selection function QS. The algorithm calls Construct with an empty question-answer sequence (line 14). The function Construct first calls the question selection function QS (line 3) and creates either a leaf node (line 4) or an internal node (lines 6-9) based on whether the return value is \top or not. When creating an internal node, the children are created by recursively calling Construct with the chosen question and the corresponding question-answer sequence.

Algorithm 4 Constructing a decision tree using a question selection function

Input: A set of tests T, a set of items X, a set of results R, a probability distribution φ on X and a question selection function QS.

Output: The root node of a decision tree. 1: **function** Construct($\mathbb{P}, \mathbb{Q}, \mathbb{A}, \varphi', C$) $node \leftarrow NewNode$ 2: if $QS(C) = \top$ then 3: 4: The label of $node \leftarrow \mathbb{P}|_{C}$ 5: $q^* \leftarrow QS[\mathbb{P}, \mathbb{Q}, \mathbb{A}, \varphi'](C)$ 6: The label of $node \leftarrow q^*$ 7: $A \leftarrow \{\mathbb{D}[p](q^*) \mid p \in \mathbb{P}|_C\}$ 8: 9: Construct($\mathbb{P}, \mathbb{Q}, \mathbb{A}, \varphi', C \cup \{(q^*, a)\})$) | $a \in A$ } 10: end if 11: return node 12: 13: end function 14: $(\mathbb{P}, \mathbb{Q}, \mathbb{A}, \varphi') \leftarrow \pi(X, T, R, \varphi)$ 15: **return** Construct($\mathbb{P}, \mathbb{Q}, \mathbb{A}, \varphi', ()$)

Lemma A.7. Algorithm 4 returns a decision tree.

Proof. Obviously, Algorithm 4 returns a tree. To show it is a decision tree, we need to check whether the properties of a decision tree are satisfied or not. First, it is easy to see the internal nodes, the edges, and the leaf nodes are labeled correctly, and the outgoing edges of the same node have different labels. Second, because QS returns a non- \top value only when some question can further distinguish remaining programs, each internal node must have at least two children. Third, since the label of a leaf node is the set of valid programs with respect to C, items labeled on the leaf node must be consistent with previous tests. Fourth, since QS returns \top only when the remaining programs cannot be distinguished by any question-answer pairs, we know that items on the same leaf cannot be further distinguished by any tests. Fifth, since the tree construction process considers all items and any two leaves have different paths from the root, any two indistinguishable items must be labeled on the same leaf node.

Lemma A.8. Given an item $x \in X$, the path from the root to x on the decision tree returned by Algorithm 4 has the length of len(QS, x).

Proof. Given an item x, iteratively calling QS generates a sequence of questions. It is easy to see len returns the length of this sequence. By induction on the first n questions in the sequence, we can see that (1) there is always a path corresponding to the first n questions; (2) when QS returns \top , the path reaches a leaf node whose labeled set must contains x. Putting them together, we know the lemma holds.

Lemma A.9. Algorithm 4 has polynomial time complexity if QS has polynomial time complexity.

Proof. First, each call to Construct creates a new node, so the number of calls to Construct is equal to the size of the decision tree, which is a polynomial of the number of items in X. Second, when $QS[\mathbb{P}, \mathbb{Q}, \mathbb{A}, \varphi']$ is polynomial-time, each statement in Construct costs polynomial time with respect to the size of X and the size of T. As a result, the whole algorithm is polynomial-time.

Based on these lemmas, we know that DT is polynomialtime reducible to OQS, and thus we can adapt several results from previous research works on DT.

Theorem A.10. The problem of approximating DT with approximation ratio k is polynomial-time reducible to the problem of approximating OQS with approximation ratio k.

Proof. This is a direct result of Lemma A.8, Lemma A.9, and Lemma A.7. □

Corollary A.11. DT is polynomial-time reducible to OQS.

Proof. Let k be 1. Theorem A.10 reduces to this corollary. \Box

Corollary A.12 (Theorem 2.6). OQS is NP-hard.

Proof. By contradiction, if OQS is not NP-hard, DT cannot be NP-hard by Theorem A.10.

Let 2-0QS be the subproblem of 0QS when all questions are boolean, i.e., $|\mathbb{A}=2|$, UOQS be the subprogram when φ is a uniform distribution and 2-UOQS be the subprogram when both two conditions are met.

Corollary A.13. OQS and 2 - OQS are hard to be approximated with a ratio of $\Omega(\log |\mathbb{P}|)$; UOQS is hard to be approximated with a ratio of $4 - \epsilon$ for any $\epsilon > 0$; 2 - UOQS is hard to be approximated with a ratio of $2 - \epsilon$ for any $\epsilon > 0$.

Proof. Similar to previous corollaries, this corollary can be proved by contradiction. \Box

From question selection to optimal decision tree. Now we show the other direction is also polynomial-time reducible. Similarly, we first define a mapping from instances of OQS

to instances of $\mathcal{D}T$. More concretely, we construct the following mapping.

$$\rho(\mathbb{P},\mathbb{Q},\mathbb{A},\varphi')=(X,T,R,\varphi)$$

where

- \mathbb{P} is a domain of programs.
- \mathbb{Q} is the question domain \mathbb{P} defined on.
- \mathbb{A} is the answer domain \mathbb{P} defined on.
- φ' is the distribution over programs in \mathbb{P} .
- X is a set of items to be distinguished by the decision and is equal to P.
- *T* is a set of tests and is equal to \mathbb{Q} , where the test result of $q \in \mathbb{Q}$ on $x \in X$ is equal to $\mathbb{D}[x](q)$.
- R is a set of test results and is equal to A.
- φ is a distribution over items in X and is equal to φ' .

It is easy to see that ρ can be implemented as a polynomial-time algorithm if programs in $\mathbb P$ are all polynomial-time. To better discuss the complexity of OQS, we ignore the time complexities of programs in $\mathbb P$ and assume $\mathbb D$ can always be calculated within constant time.

Based on ρ , we present Algorithm 5, which solves the question selection problem with a decision tree constructor Construct. This algorithm directly constructs a decision tree, and returns the label of the corresponding path. We have the following three lemmas for this algorithm.

Algorithm 5 Constructing a question selection function using a decision tree constructor

Input: A program space \mathbb{P} , a question domain \mathbb{Q} , an answer domain \mathbb{A} , a probability distribution φ of \mathbb{P} , and a sequence of question-answer pairs C

Output: the next question .

- 1: $(X, T, R, \varphi') \leftarrow \rho(\mathbb{P}, \mathbb{Q}, \mathbb{A}, \varphi)$
- 2: $d \leftarrow \text{Construct}(X, T, R, \varphi')$
- 3: **if** there is a path from the root in *d* corresponding to *C* **then**
- 4: $path \leftarrow \text{the path in } d \text{ corresponding to } C$
- 5: **else**
- 6: **return** ⊤
- 7: end if
- 8: $node \leftarrow the end of path$
- 9: **if** *node* is a leaf node **then**
- 10: return ⊤
- 11: **else**
- 12: **return** the label of node
- 13: **end if**

Lemma A.14. Algorithm 5 defines a question selection function.

Proof. We need to show two properties of an input selection function hold. The first one is a direct result of the last property of a decision tree. The second one is ensured since each internal node has at least two children.

Lemma A.15. Let the question selection function defined by Algorithm 5 be QS. Given a program $p \in \mathbb{P}$, the path from the root to p in the decision tree returned by Construct has the length of len(inSel, p).

Proof. This can be proved by showing that the algorithm always traverses exactly this path during each invocation. \Box

Lemma A.16. Algorithm 5 is polynomial-time if both Construct and all programs in \mathbb{P} are polynomial-time.

Proof. It is easy to see there is no loop in the algorithm and each statement costs polynomial time if the preconditions are satisfied.

Theorem A.17. The problem of approximating OQS with approximation ratio k is polynomial-time reducible to the problem of approximating DT with approximation ratio k.

Proof. This is a direct result from Lemma A.16, Lemma A.14, and Lemma A.15. □

Corollary A.18. OQS is polynomial-time reducible to DT.

Proof. Let k be 1. Theorem A.17 reduces to this corollary. \Box

Now, we can apply above results to show that minimax branch is an efficient approximation algorithm for OQS and its subproblems.

Theorem A.19 (Theorem 2.8). The minimax branch strategy for OQS problem has the approximation ratio $1 + \ln m$ for 2 - UOQS, $O(\log m)$ for UOQS and 2 - OQS, and $O(\log^2 m)$ for OQS, where $m = |\mathbb{P}|$.

Proof. This corollary can be proved as follows. We first implement a question selection function by converting *minimax branch* on \mathfrak{DT} through Algorithm 5. Clearly, this converted algorithm has the same approximation ratios on \mathfrak{OQS} as on \mathfrak{DT} . Furthermore, by the definition of *minimax branch* on \mathfrak{OQS} , it always chooses the same input as the above converted question selection function. Therefore, we obtain the approximation ratios of *minimax branch* on \mathfrak{OQS} and its subproblems.

B Appendix: Proofs

In this section, we complete the proofs of the theorems in Section 3, 4 and 5.

Lemma B.1 (Lemma 3.1). For any OQS instance $(\mathbb{P}, \mathbb{Q}, \mathbb{A}, \varphi)$ and any $P \subseteq \mathbb{P}$, let q_0 and q_1 be the questions selected by MINIMAX0 and MINIMAX, respectively, then q_0 and q_1 have the same efficiency on P, i.e.:

$$\max_{a \in \mathbb{A}} \left| P|_{(q_0, a)} \right| = \max_{a \in \mathbb{A}} \left| P|_{(q_1, a)} \right|$$

Proof. By the definition of $P|_{(i,o)}$, we have:

$$\forall q \in \mathbb{Q}, \ \max_{a \in \mathbb{A}} \left| P|_{(q,a)} \right| = \max_{j} \left(\sum_{k=j+1}^{n} [\mathbb{D}[p_j](q) = \mathbb{D}[p_k](q)] \right)$$

Apply this equality to MINIMAX, and then we obtain this lemma. $\hfill\Box$

Theorem B.2 (Theorem 3.2). For any OQS instance $(\mathbb{P}, \mathbb{Q}, \mathbb{A}, \varphi)$ and any sequence of examples $C \in (\mathbb{Q} \times \mathbb{A})^*$, define the cost of a question cost(q) to be $\max_{a \in \mathbb{A}} w\left(\mathbb{P}|_{C \cup \{(q,a)\}}\right)$. Let P be a set of independent samples from distribution $\varphi|_C$, q_1 and q_0 be the questions chosen by SampleSy and minimax branch respectively, then $\forall \epsilon > 0$:

$$\Pr\left[\cos t(q_1) > (1+\epsilon)\cos t(q_0)\right] \le 2d|\mathbb{Q}|\exp\left(-\frac{|P|\epsilon^2}{2d^2}\right)$$

where $d = \max_{q \in \mathbb{Q}} |\{\mathbb{D}[p](q) \mid p \in \mathbb{P}\}|$ which represents the maximum number of different answers on a single question.

Proof. Let n be the number of samples and $P = \{p_1, \ldots, p_n\}$ be the samples. By the definition of the sampler, p_1, \ldots, p_n are independent samples from distribution $\varphi|_C$. For a question $q \in \mathbb{Q}$, answer $a \in \mathbb{A}$, let $f(q,a) = \Pr_{p \sim (\varphi|_C)}[\mathbb{D}[p](q) = a]$, i.e., the probability for a sample p to be consistent with question-answer example (q,a).

Then, by Chernoff bound:

$$\forall \epsilon' > 0, q \in \mathbb{Q}, a \in \mathbb{A}, \Pr\left[\left|\frac{\left|P\right|_{(q,a)}\right|}{n} - f(q,a)\right| > \epsilon'\right] < 2e^{-2n\epsilon'^2}$$

Take union bound on all possible inputs and corresponding outputs, we obtain:

$$\forall \epsilon' > 0, \Pr \left[\exists q \in \mathbb{Q}, \exists a \in \mathbb{A}, \left| \frac{\left| P|_{(q,a)} \right|}{n} - f(q,a) \right| > \epsilon' \right] < 2d |\mathbb{Q}| e^{-2n\epsilon'^2}$$

For a question $q \in \mathbb{Q}$, we define two cost functions:

- $c_1(q) = \max_{a \in \mathbb{A}} \frac{|P|_{(q,a)}|}{n}$, which represents the cost on the samples.
- $c_2(q) = \max_{a \in \mathbb{A}} f(q, a)$, which represents the cost on $\mathbb{P}|_C$. Note that $c_2(q) \times w(\mathbb{P}|_C) = cost(q)$

By the definitions of q_0 and q_1 , we know that q_0 and q_1 are $\arg\min_{q\in\mathbb{Q}}c_2(q)$ and $\arg\min_{q\in\mathbb{Q}}c_1(q)$, respectively.

Notice that:

$$\forall q \in \mathbb{Q}, \forall a \in \mathbb{A}, \left| \frac{\left| P|_{(q,a)} \right|}{n} - f(q,a) \right| \le \epsilon'$$

$$\implies \forall q \in Q, |c_1(q) - c_2(q)| \le \epsilon'$$

$$\implies c_2(q_1) - c_2(q_0) \le 2\epsilon'$$

The last inequality holds because:

$$c_2(q_1) - c_2(q_0)$$

$$\leq (c_1(q_1) - c_1(q_0)) + |c_1(q_1) - c_2(q_1)| + |c_1(q_0) - c_2(q_0)|$$

Consider the three terms on the right side: Since q_1 is the best input with respect to P, the first term is non-positive. With the precondition that for all inputs, the difference between c_1 and c_2 are bounded, the second and the third term are both no more than ϵ' . Therefore the sum is at most $2\epsilon'$.

Take ϵ' as $\frac{1}{2}\epsilon$, we obtain:

$$\forall \epsilon > 0, \Pr\left[c_2(q_1) - c_2(q_0) > \epsilon\right] \le 2|\mathbb{Q}||\mathbb{A}|e^{-\frac{1}{2}n\epsilon^2}$$

The definition of $c_2(q) = \max_{a \in \mathbb{A}} f(q, a)$ implies $c_2(q) \ge \frac{1}{d}$. Substitute ϵ with $\epsilon c_2(q_0)$:

$$\Pr\left[c_2(q_1) > c_2(q_0)(1+\epsilon)\right] \le 2d|\mathbb{Q}| \exp\left(-\frac{|P|\epsilon^2 c_2(q_0)^2}{2}\right)$$
$$\le 2d|\mathbb{Q}| \exp\left(-\frac{|P|\epsilon^2}{2d^2}\right)$$

Because $c_2(q)$ is proportional to the value of cost(q), this inequality is equivalent to the theorem

Lemma B.3 (Lemma 4.5). For any program set P and constant w, define $B(P) \subseteq P$ as the set of programs which makes $\psi_{good}[p](q,w)$ unsatisfiable, then:

- $w \le 1/2 \Longrightarrow \forall P$, programs in B(P) are indistinguishable from each other.
- $w > 1/2 \Longrightarrow \forall t > 0, \exists P \text{ s.t. } B(P) \text{ contains at least } t$ programs which are distinguishable from each other.

Proof. For the first part, let p_1, p_2 be any two programs in B(P) and q be a question in \mathbb{Q} , let $P_1(q), P_2(q)$ be the set of programs in P which have the same answer as p_1 and p_2 on q, respectively.

By the definition of B(P), $|P_1(q)| > \frac{|P/p_1|}{2} + n(p_1)$, $|P_2(q)| > \frac{|P/p_2|}{2} + n(p_2)$ where n(p) represents the number of p in set P. Therefore $|P_1(q)|$, $|P_2(q)| > \frac{|P|}{2}$, which implies $|P_1(q) \cap P_2(q)| > 0$. By the definition of $P_1(q)$ and $P_2(q)$, we have $\mathbb{D}[p_1](q) = \mathbb{D}[p_2](q)$. Since p_1, p_2, q are chosen arbitrarily, we obtain that all programs in B(P) are indistinguishable.

For the second part, we can construct such a *P* in the following way:

- let *m* be a large enough integer which satisfies $2^m \ge t$ and $\frac{2^{m-1}}{2^m-1} < w$.
- P contains 2^m programs, \mathbb{Q} contains m questions, and the answer for the ith program on the jth question is equal to the jth digit in the binary representation of i.

Then, for any $p \in P$, $q \in \mathbb{Q}$, $|P/p| = 2^m - 1$ and there are 2^{m-1} programs performing differently with p. Since $\frac{2^{m-1}}{2^m-1} < w$, B(P) contains all the programs in P, which are all distinguishable from each other.

Theorem B.4 (Theorem 4.6). For an OQS instance $(\mathbb{P}, \mathbb{Q}, \mathbb{A}, \varphi, \epsilon)$, let n be a lower bound of the number of samples in each turn, β be an upper bound of questions required by EpsSy, then:

$$\forall n > \max\left(18\ln\left(\frac{2\beta|\mathbb{Q}|}{\epsilon}\right), \frac{16\ln 2}{\epsilon^2} + \frac{8}{\epsilon^2}\ln\left(\frac{1}{\epsilon}\right)\right),$$
$$\forall f_{\epsilon} > \log_{3/2}\left(\frac{2\beta}{\epsilon}\right), e(EpsSy, p) \le \epsilon$$

Proof. There are two termination conditions in *EpsSy*. Let $e_1(EpsSy, \varphi)$ be the error rate when *EpsSy* returns through condition one (Line 5 in Algorithm 2) and $e_2(EpsSy, \varphi)$ be

that for condition two (Line 16 in Algorithm 2). The theorem is equivalent to both e_1 and e_2 are bounded.

For $e_1(\textit{EpsSy}, \varphi)$, let C be the final question-answer sequence, m be the number of samples which are indistinguishable from p^* , $ind(p^*)$ be the probability for a random program from distribution $\varphi|_C$ to be indistinguishable from p^* . By Chernoff bound:

$$\forall \epsilon' > 0, \Pr\left[\frac{m}{n} - ind(p^*) > \epsilon'\right] \le \exp(-2n\epsilon'^2)$$

Since $\frac{m}{n} > 1 - \frac{\epsilon}{2}$, take ϵ' as $\frac{\epsilon}{4}$, then:

$$\Pr\left[ind(p^*) < 1 - \frac{3}{4}\epsilon\right] \le \exp(-n\epsilon^2/8)$$

Since the target program also follows the conditional distribution $\varphi|_C$, the error rate at this time should be $1-ind(p^*)$. Combining with above inequality, we obtain:

$$\begin{split} e_1(\textit{EpsSy}, \varphi) & \leq \frac{3}{4} \epsilon \Pr[\textit{ind}(p^*) \geq 1 - \frac{3}{4} \epsilon] + \Pr[\textit{ind}(p^*) < 1 - \frac{3}{4} \epsilon] \\ & \leq \frac{3}{4} \epsilon + \exp(-n\epsilon^2/8) \end{split}$$

Then for $e_2(EpsSy, \varphi)$, let r_j , q_j be the recommendation and the question of the jth round, C_j be the question-answer sequence before the jth round, and r^* be the target program. Note that r^* is a random variable which is subject to φ , and its distribution conditional on C_j is $\varphi|_{C_j}$. For convenience, we involve two properties of interaction rounds:

- The *j*th round is *good* iff the question q_j is challengeable.
- The *j*th round is *effective* iff the following inequality holds:

$$\Pr_{r \sim \varphi|_{C_j}} \left[\mathbb{D}[r^*](q_j) \neq \mathbb{D}[r_j](q_j) \middle| \ r^* \text{ and } r \text{ are distinguishable} \right] \geq \frac{1}{3}$$

In an effective round, if the recommendation is incorrect, it will be excluded with a probability of at least $\frac{1}{3}$. We start by proving that with a high probability, every good round is effective, i.e., the following inequality holds:

Pr
$$[\exists j \in [\beta]$$
, round j is good but not effective $] \le \beta |\mathbb{Q}| \exp(-\frac{1}{18}n)$ (5)

Suppose round j is a good round, and r_j , r^* are distinguishable, let $P = \{p_1, \ldots, p_n\}$ be the set of samples. For a question $q \in \mathbb{Q}$, let g(q) be the probability for a random program to differ with r_j on q, i.e., $g(q) = \Pr_{x \sim \varphi|_{C_j}}[\mathbb{D}[x](q) \neq \mathbb{D}[r_j](q)]$. Since r^* is subject to $\varphi|_{C_j}$, for any $q \in \mathbb{Q}$, we have:

$$\Pr\left[\mathbb{D}[r^*](q) \neq \mathbb{D}[r_j](q)\middle| r^* \text{ and } r \text{ are distinguishable}\right] \geq g(q)$$

Let h(q) be the number of samples which differs with r_j on q. Then, by Chernoff bound:

$$\forall \epsilon' > 0, q \in \mathbb{Q}, \Pr\left[\frac{h(q)}{n} - g(q) > \epsilon'\right] \le \exp(-2n\epsilon'^2)$$

Take a union bound on all possible questions, we obtain:

$$\begin{split} \forall \epsilon' > 0, \Pr \left[\forall q \in \mathbb{Q}, \frac{h(q)}{n} - g(q) > \epsilon' \right] &\leq |\mathbb{Q}| \exp(-2n\epsilon'^2) \\ \Longrightarrow &\forall \epsilon' > 0, \Pr \left[\frac{h(q_j)}{n} - g(q_j) > \epsilon' \right] \leq |\mathbb{Q}| \exp(-2n\epsilon'^2) \end{split}$$

Take $\epsilon' = \frac{1}{6}$. Since $h(q_j) \ge \frac{1}{2}n$ (guaranteed by the definition of good rounds), we have:

$$\Pr\left[g(q_j) < \frac{1}{3} \middle| \text{ round } j \text{ is good}\right] \le |\mathbb{Q}| \exp(-\frac{1}{18}n)$$

$$\Longrightarrow \Pr\left[\text{round } j \text{ is good but not effective}\right] \le |\mathbb{Q}| \exp(-\frac{1}{18}n)$$

Take a union bound on all possible rounds, we obtain Inequality 5.

Now we bound $e_2(EpsSy, \varphi)$ with the help of Inequality 5. Let Δ be the event that every good round is effective, let ξ_j be the event that EpsSy returns a wrong recommendation in the jth round though condition two (Line 16 in Algorithm 2). Since ξ_j happens only when a wrong recommendation survives for f_ϵ good rounds, $\Pr[x_j|\Delta]$ is no larger than $\left(\frac{2}{3}\right)^{f_\epsilon}$. Take union bound on all possible rounds, we obtain:

$$\Pr\left[\exists j \in [\beta], \xi_j \middle| \Delta\right] \le \beta \left(\frac{2}{3}\right)^{f_{\epsilon}}$$

Therefore, we can bound $e_2(EpsSy, \varphi)$ by n and f_{ϵ} :

$$\begin{split} e_2(\textit{EpsSy}, \varphi) &\leq \Pr[\neg \Delta] + \Pr\left[\exists j \in [\beta], \xi_j \middle| \Delta\right] \\ &\leq \beta |\mathbb{Q}| \exp(-\frac{1}{18}n) + \beta \left(\frac{2}{3}\right)^{f_\epsilon} \end{split}$$

The target theorem can be obtained by setting n and f_{ϵ} to proper values on which both e_1 and e_2 are bounded:

$$\begin{split} \forall n > \max\left(18\ln\left(\frac{2\beta|\mathbb{Q}|}{\epsilon}\right), \frac{16\ln 2}{\epsilon^2} + \frac{8}{\epsilon^2}\ln\left(\frac{1}{\epsilon}\right)\right), \\ \forall f_\epsilon > \log_{3/2}\left(\frac{2\beta}{\epsilon}\right), e(\textit{EpsSy}, p) \leq \epsilon \end{split}$$

Theorem B.5 (Theorem 5.7). For a program domain \mathbb{P} , an example sequence C and a distribution φ defined by a PCFG, let G be an acyclic VSA that represents $\mathbb{P}|_C$, then SAMPLE(S) is subject to the conditional distribution $\varphi|_C$, where S is the start symbol of V.

Proof. First, we prove that function GetPr(s) is well behaved, i.e., it returns the sum of probabilities of all subprograms which are expanded from s. Formally, for each non-terminal symbol s in G, let SP(s) be the set of subprograms expanded from s; for each subprogram sp, let w(sp) be the probability of sp given by the PCFG. We firstly show that GetPr(s) always returns $\sum_{sp \in SP(s)} w(sp)$.

We prove it by induction on the acyclic structure of *G*. By the definition of VSA, there are three possible forms of the rule expanding from non-terminal symbol *s*.

Form $s:=p_1|\dots|p_k$ is the initial case of the induction. At this time, $SP(s)=\{p_1,\dots,p_k\}$ and $w(p_i)=\gamma(\sigma(s,p_i))$. Therefore $\operatorname{GetPr}(s)=\sum_{i=1}^k\gamma(\sigma(s,p_i))=\sum_{sp\in SP(s)}w(sp)$. For form $s:=s_1|\dots|s_k$, there is a bijection between SP(s)

For form $s := s_1 | \dots | s_k$, there is a bijection between SP(s) and $\bigcup_{i=1}^k SP(s_i)$. For subprogram sp in SP(s), let sp' be the corresponding subprogram which is expanded from s_i , then w(sp) is equal to $w(sp') \times \gamma(\sigma(s, s_i))$. By these facts, we have:

$$\sum_{sp \in SP(s)} w(sp) = \sum_{i=1}^{k} \left(\sum_{sp' \in SP(s_i)} w(sp') \right) \times \gamma(\sigma(s, s_i))$$

By the induction hypothesis, $\sum_{sp' \in SP(s_i)} w(sp')$ is equal to GetPr(s_i). Therefore:

$$\sum_{sp \in SP(s)} w(sp) = \sum_{i=1}^k \operatorname{GetPr}(s_i) \times \gamma(\sigma(s,s_i)) = \operatorname{GetPr}(s)$$

For form $s := F(s_1, \ldots, s_k)$, there is also a bijection between SP(s) and $SP(s_1) \times SP(s_2) \times \cdots \times SP(s_k)$. For subprogram sp in SP(s), let sp_1, \ldots, sp_k be the corresponding subprograms, then w(sp) is equal to $\gamma(\sigma(s,F)) \prod_{i=1}^k w(sp_i)$. By these facts, we have:

$$\sum_{sp \in SP(s)} w(sp) = \gamma(\sigma(s, F)) \left(\sum_{sp_1 \in SP(s_1)} \cdots \sum_{sp_k \in SP(s_k)} \prod_{i=1}^k w(sp_i) \right)$$
$$= \gamma(\sigma(s, F)) \prod_{i=1}^k \left(\sum_{sp_i \in SP(s_i)} w(sp_i) \right)$$

By the induction hypothesis, $\sum_{sp_i \in SP(s_i)} w(sp_i)$ is equal to GetPr(s_i). Therefore:

$$\sum_{sp \in SP(s)} w(sp) = \gamma(\sigma(s, F)) \prod_{i=1}^{k} GetPr(s_i) = GetPr(s)$$

So far, we have proven that GetPr is well behaved. To prove Theorem B.5, we discuss a stronger property instead: for each subprogram sp which is expanded from symbol s in G, the probability for Sample(s) to return sp is proportional to w(sp). Obviously, the target theorem is the special case when s = S.

We prove this property by induction on the acyclic structure of G, too. For convenience, we use $\phi_s(sp)$ to denote the probability of choosing sp from symbol s.

For form $s := p_1 | \dots | p_k$, according to the definition of Sample, Sample(s) picks p_i with the probability proportional to $w(p_i)$. This forms the initial case of the induction.

For form $s := s_1 | \dots | s_k$, let sp_1, sp_2 be any two subprograms expanded from non-terminal symbol s, there are two possible cases:

• Both sp_1, sp_2 correspond to the same sub-symbol s_i . The induction hypothesis shows $\phi_s(sp_1) : \phi_s(sp_2) = w(sp_1) : w(sp_2)$ directly.

• sp_1 and sp_2 correspond to two different sub-symbols s_i and s_i . Then by the induction hypothesis:

$$\phi_{s_i}(sp_1) = w(sp_1)/\gamma(\sigma(s,s_i)) \text{GetPr}(s_i)$$

$$\phi_{s_j}(sp_2) = w(sp_2)/\gamma(\sigma(s,s_j)) \text{GetPr}(s_j)$$

Since the probability for Sample(s) to choose s_i is proportional to $\gamma(\sigma(s,s_i))$ GetPr(s_i), we obtain $\phi_s(sp_1)$: $\phi_s(sp_2) = w(sp_1)$: $w(sp_2)$.

For form $s:=F(s_1,\ldots,s_k)$, let $x=F(x_1,\ldots,x_k),y=F(y_1,\ldots,y_k)$ be two subprograms rooted at s. By the induction hypothesis, $\forall i\in[k], \phi_{s_i}(x_i):\phi_{s_i}(y_i)=w(x_i):w(x_j)$. Therefore:

$$\frac{\phi_s(x)}{\phi_s(y)} = \frac{\prod_{i=1}^k \phi_{s_i}(x_i)}{\prod_{i=1}^k \phi_{s_i}(y_i)} = \frac{\prod_{i=1}^k w(x_i)}{\prod_{i=1}^k w(y_i)} = \frac{w(x)}{w(y)}$$

So far, we show that the induction holds on all three forms. Therefore the target theorem has been proven. \Box

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