Statistically Model Checking PCTL Specifications on Markov Decision Processes via Reinforcement Learning

Yu Wang, Nima Roohi, Matthew West, Mahesh Viswanathan, and Geir E. Dullerud

Abstract—Probabilistic Computation Tree Logic (PCTL) is frequently used to formally specify control objectives such as probabilistic reachability and safety. In this work, we focus on model checking PCTL specifications statistically on Markov Decision Processes (MDPs) by sampling, e.g., checking whether there exists a feasible policy such that the probability of reaching certain goal states is greater than a threshold. We use reinforcement learning to search for such a feasible policy for PCTL specifications, and then develop a statistical model checking (SMC) method with provable guarantees on its error. Specifically, we first use upper-confidence-bound (UCB) based Q-learning to design an SMC algorithm for bounded-time PCTL specifications, and then extend this algorithm to unbounded-time specifications by identifying a proper truncation time by checking the PCTL specification and its negation at the same time. Finally, we evaluate the proposed method on case studies.

I. INTRODUCTION

Probabilistic Computation Tree Logic (PCTL) is frequently used to formally specify control objectives such as reachability and safety on probabilistic systems [1]. To check the correctness of PCTL specifications on these systems, model checking methods are required [2]. Although model checking PCTL by model-based analysis is theoretically possible [1], it is not preferable in practice when the system model is unknown or large. In these cases, model checking by sampling, i.e. statistical model checking (SMC), is needed [3], [4].

The statistical model checking of PCTL specifications on Markov Decision Processes (MDPs) is frequently encountered in many decision problems — e.g., for a robot in a grid world under probabilistic disturbance, checking whether there exists a feasible control policy such that the probability of reaching certain goal states is greater than a probability threshold [5]–[7]. In these problems, the main challenge is to search for such a feasible policy for the PCTL specification of interest.

To search for feasible policies for temporal logics specifications, such as PCTL, on MDPs, one approach is model-based reinforcement learning [8]–[11] — i.e., first inferring the transition probabilities of the MDP by sampling over each state-action pair, and then searching for the feasible policy via model-based analysis. This approach is often inefficient, since not all transition probabilities are relevant to the PCTL specification of interest. Here instead, we adopt a model-free reinforcement learning approach [12].

Common model-free reinforcement learning techniques cannot directly handle temporal logic specifications. One solution is to find a surrogate reward function such that the policy learned for this surrogate reward function is the one needed for checking the temporal logic specification of interest. For certain temporal logics interpreted under special semantics (usually involving a metric), the surrogate reward can be found based on that semantics [13]–[15]. For temporal logics under the standard semantics [16], the surrogate reward functions can be derived via constructing the product MDP [7], [17], [18] of the initial MDP and the automaton realizing the temporal logic specification. However, the complexity of constructing the automaton from a general linear temporal logic (LTL) specification is double exponential [16], [19]. For a fraction of LTL, namely LTL/GU, the complexity is exponential [20], [21]. In addition, the size of the product MDP is usually much larger than the initial MDP, although the produce MDP may be constructed on-the-fly to reduce the extra computation cost, as it did in [18].

In this work, we propose a new statistical model checking method for PCTL specifications on MDPs. For a lucid discussion, we only consider non-nested PCTL specifications. PCTL formulas in general form with nested probabilistic operators can be handled in the standard manner using the approach proposed in [22], [23]. Our method uses upper-confidence-bound (UCB) based Q-learning to directly learn the feasible policy of PCTL specifications, without constructing the product MDP. The effectiveness of UCB-based Q-learning has been proven for the $K$-bandit problem, and has been numerically demonstrated on many decision-learning problems on MDPs (see [24]).

For bounded-time PCTL specifications, we treat the statistical model checking problem as a finite sequence of $K$-bandit problems and use the UCB-based Q-learning to learn the desirable decision at each time step. For unbounded-time PCTL specifications, we look for a truncation time to reduce it to a bounded-time problem by checking the PCTL specification and its negation at the same time. Our statistical model checking algorithm is online; it terminates with probability 1, and only when the statistical error of the learning result is smaller than a user-specified value.

The rest of the paper is organized as follows. The preliminaries on labeled MDPs and PCTL are given in Section III. In Section III, using the principle of optimism in the face of uncertainty, we design Q-learning algorithms to solve
finite-time and infinite-time probabilistic satisfaction, and give finite sample probabilistic guarantees for the correctness of the algorithms. We implement and evaluate the proposed algorithms on several case studies in Section V. Finally, we conclude this work in Section V.

II. PRELIMINARIES AND PROBLEM FORMULATION

The set of integers and real numbers are denoted by \( \mathbb{N} \) and \( \mathbb{R} \), respectively. For \( n \in \mathbb{N} \), let \( [n] = \{1, \ldots, n\} \). The cardinality of a set is denoted by \(|\cdot|\). The set of finite-length sequences taken from a finite set \( S \) is denoted by \( S^* \).

A. Markov Decision Process

A Markov decision process (MDP) is a finite-state probabilistic system, where the transition probabilities between the states are determined by the control action taken from a given finite set. Each state of the MDP is labeled by a set of atomic propositions indicating the properties holding on it, e.g., whether the state is a safe/goal state.

Definition 1: A labeled Markov decision process (MDP) is a tuple \( M = (S, A, T, AP, L) \) where

- \( S \) is a finite set of states.
- \( A \) is a finite set of actions.
- \( T : S \times A \times S \rightarrow [0,1] \) is a partial transition probability function. For any state \( s \in S \) and any action \( a \in A \),
  \[
  \sum_{s' \in S} T(s, a, s') = \begin{cases} 0, & \text{if } a \text{ is not allowed on } s \\ 1, & \text{otherwise.} \end{cases}
  \]

With a slight abuse of notation, let \( A(s) \) be the set of allowed actions on the state \( s \).
- \( AP \) is a finite set of labels.
- \( L : S \rightarrow 2^{AP} \) is a labeling function.

Definition 2: A policy \( \Pi : S^* \rightarrow A \) decides the action to take from the sequence of states visited so far. Given a policy \( \Pi \) and an initial state \( s \in S \), the MDP \( M \) becomes purely probabilistic, denoted by \( M_{\Pi,s} \). The system \( M_{\Pi,s} \) is not necessarily Markovian.

B. Probabilistic Computation Tree Logic

The probabilistic computation tree logic (PCTL) is defined inductively from atomic propositions, temporal operators and probability operators. It reasons about the probabilities of time-dependent properties.

Definition 3 (Syntax): Let AP be a set of atomic propositions. A PCTL state formula is defined by

\[
\phi ::= a | \neg \phi | \phi_1 \land \phi_2 | \mathbf{P}_{\min}^\phi(X\phi) | \mathbf{P}_{\max}^\phi(X\phi) \\
| \mathbf{P}_{\min}^\phi(\phi_1 U_T \phi_2) | \mathbf{P}_{\max}^\phi(\phi_1 U_T \phi_2) \\
| \mathbf{P}_{\min}^\phi(\phi_1 R_T \phi_2) | \mathbf{P}_{\max}^\phi(\phi_1 R_T \phi_2)
\]

where \( a \in AP, \in \{<, >, =, \geq\} \), \( T \in \mathbb{N} \cup \{\infty\} \) is a (possibly infinite) time horizon, and \( p \in [0,1] \) is a threshold. The operators \( \mathbf{P}_{\min}^\phi \) and \( \mathbf{P}_{\max}^\phi \) are called probability operators, and the “next”, “until” and “release” operators \( X, U_T, R_T \) are called temporal operators.

More temporal operators can be derived by composition: for example, “or” is \( \phi_1 \lor \phi_2 ::= \neg(\neg\phi_1 \land \neg\phi_2) \); “true” is \( \text{True} = a \lor (\neg a) \); “finally” is \( \text{F}_T \phi ::= \text{True} U_T \phi \); and “always” is \( \text{G}_T \phi ::= \text{F}_T \phi \) \( \land \text{G}_T \phi \). For simplicity, we write \( U_\infty, R_\infty, F_\infty \) and \( G_\infty \) as \( U, R, F \) and \( G \), respectively.

Definition 4 (Semantics): For an MDP \( M = (S, A, T, s_{\text{init}}, AP, L) \), the satisfaction relation \( \models \) is defined by for a state \( s \) or path \( \sigma \) by

\[
s \models a \text{ iff } a \in L(s), \\
s \models \neg \phi \text{ iff } s \not\models \phi, \\
s \models \phi_1 \land \phi_2 \text{ iff } s \models \phi_1 \text{ and } s \models \phi_2, \\
s \models \mathbf{P}_{\min}^\phi(X\phi) \text{ iff } \min_{\Pi} \mathbb{P}_{\sigma_{\sim\text{Min}},\Pi}[\sigma = X\phi] \geq p, \\
s \models \mathbf{P}_{\max}^\phi(X\phi) \text{ iff } \max_{\Pi} \mathbb{P}_{\sigma_{\sim\text{Min}},\Pi}[\sigma = X\phi] \geq p, \\
s \models \mathbf{P}_{\min}^\phi(\phi_1 U_T \phi_2) \text{ iff } \min_{\Pi} \mathbb{P}_{\sigma_{\sim\text{Min}},\Pi}[\sigma = \phi_1 U_T \phi_2] \geq p, \\
s \models \mathbf{P}_{\max}^\phi(\phi_1 U_T \phi_2) \text{ iff } \max_{\Pi} \mathbb{P}_{\sigma_{\sim\text{Min}},\Pi}[\sigma = \phi_1 U_T \phi_2] \geq p, \\
s \models \mathbf{P}_{\min}^\phi(\phi_1 R_T \phi_2) \text{ iff } \min_{\Pi} \mathbb{P}_{\sigma_{\sim\text{Min}},\Pi}[\sigma = \phi_1 R_T \phi_2] \geq p, \\
s \models \mathbf{P}_{\max}^\phi(\phi_1 R_T \phi_2) \text{ iff } \max_{\Pi} \mathbb{P}_{\sigma_{\sim\text{Min}},\Pi}[\sigma = \phi_1 R_T \phi_2] \geq p, \\
s \models X\phi \text{ iff } \sigma(1) \models \phi, \\
s \models \phi_1 U_T \phi_2 \text{ iff } \exists i < T. \sigma(i) \models \phi_2 \land (\forall j < i. \sigma(i) \models \phi_1), \\
s \models \phi_1 R_T \phi_2 \text{ iff } \sigma \models \neg \phi_1 U_T \neg \phi_2
\]

where \( \in \{<, >, =, \geq\} \). And \( \sigma \sim M_{\Pi,s} \) means the path \( \sigma \) is drawn from the MDP \( M \) under the policy \( \Pi \), starting from the state \( s \) from.

The PCTL formulas \( s \models \mathbf{P}_{\max}^\phi(X\phi) \) (or \( s \models \mathbf{P}_{\min}^\phi(X\phi) \)) mean that the maximal (or minimal) satisfaction probability of “next” \( \phi \) is \( \geq p \). The PCTL formulas \( s \models \mathbf{P}_{\min}^\phi(\phi_1 U_T \phi_2) \) (or \( s \models \mathbf{P}_{\max}^\phi(\phi_1 U_T \phi_2) \)) mean that the maximal (or minimal) satisfaction probability that \( \phi_1 \) holds “until” \( \phi_2 \) holds is \( \geq p \).

III. NON-NESTED PCTL SPECIFICATIONS

In this section, we consider the statistical model checking of non-nested PCTL specifications using an upper-confidence-bound based Q-learning. For simplicity, we focus on \( \mathbf{P}_{\min}^\phi(a_1 U_T a_2) \) and \( \mathbf{P}_{\max}^\phi(a_1 R_T a_2) \) where \( a_1 \) and \( a_2 \) are atomic propositions. Other cases can be handled in the same way. We discuss the case of \( T = 1 \) in Section III-A, the case of \( T > 1 \) in Section III-B and the case of \( T = \infty \) in Section III-C. Similar to other works on statistical model checking [3], [4], we make the following assumption.

Assumption 1: For \( s \models \mathbf{P}_{\max}^\phi(a_1 U_T a_2) \) and \( s \models \mathbf{P}_{\max}^\phi(a_1 R_T a_2) \) with \( T \in \mathbb{N} \cup \{\infty\} \) and \( \in \{<, >, =, \geq\} \), we assume that \( \max_{\Pi} \mathbb{P}_{\sigma_{\sim\text{Min}},\Pi}[\sigma = \phi_1 U_T \phi_2] \neq p \) and \( \max_{\Pi} \mathbb{P}_{\sigma_{\sim\text{Min}},\Pi}[\sigma = \phi_1 R_T \phi_2] \neq p \), respectively.

When it holds, as the number of samples increases, the samples will be increasingly concentrated on one side of the threshold \( p \) by the Central Limit Theorem. Therefore, a statistical analysis based on the majority of the samples has increasing accuracy. When it is violated, the samples would be evenly distributed between the two sides of the boundary \( p \), regardless of the sample size. Thus, no matter
how the sample size increases, the accuracy of any statistical test would not increase. Compared to statistical model checking algorithms based on sequential probability ratio tests (SPRT) [25], [26], no assumption on the indifference region is required here. Finally, by Assumption [1], we have the additional semantic equivalence between the PCTL specifications: \( P_{\leq p}^\text{max} \equiv P_{\leq p}^\text{max,sp} \) and \( P_{\geq p}^\text{max,sp} \equiv P_{\leq p}^\text{max} \); thus, we will not distinguish between them below.

For further discussion, we first identify a few trivial cases. For \( s \models P_{\leq p}^\text{max}(a_1 U T a_2) \), let

\[
S_0 = \{ s \mid a_1 \notin L(s), a_2 \notin L(s) \}
\]

\[
S_1 = \{ s \mid a_2 \in L(s) \}.
\]

(1)

Then for any policy \( \Pi \models P_{\sigma \sim M_{T \Phi}}[\sigma = \phi_1 U T \phi_2] = 0 \) if \( s \in S_0 \); and \( P_{\sigma \sim M_{T \Phi}}[\sigma = \phi_1 U T \phi_2] = 1 \) if \( s \in S_1 \). The same holds for \( s \models P_{\leq p}^\text{max}(a_1 R T a_2) \) by defining \( S_1 \) to be the union of end components of the MDP \( M \) labeled by \( a_2 \) (this only requires knowing the topology of \( M \)) [16]. In the rest of this section, we focus on handling the nontrivial case \( s \in S \setminus (S_0 \cup S_1) \).

### A. Single Time Horizon

When \( T = 1 \), for any \( s \in S \setminus (S_0 \cup S_1) \), the PCTL specification \( a_1 U T a_2 \) (or \( a_1 R T a_2 \)) holds on a random path \( \sigma \) starting from the state \( s \) if and only if \( \sigma(1) \in S_1 \), where \( S_0 \) and \( S_1 \) are from [1]. Thus, it suffices to learn from samples whether

\[
\max_{a \in A(s)} Q_1(s, a) > p,
\]

(2)

where

\[
Q_1(s, a) = P_{\sigma(1) \sim T(s, a, \cdot)}[\sigma = \phi_1 U_1 \phi_2]_{\sigma(0) = s}
\]

and \( \sigma(1) \sim T(s, a, \cdot) \) means \( \sigma(1) \) is drawn from the transition probability \( T(s, a, \cdot) \) for state \( s \) and action \( a \). This is an \( |A(s)| \)-arm bandit problem; we solve this problem by upper-confidence-bound strategies [27], [28].

Specifically, for the iteration \( k \), let \( N(k)(s, a, s') \) be the number samples for the one-step path \( (s, a, s') \), and with a slight abuse of notation, let

\[
N(k)(s, a, s') = \sum_{s' \in S} N(k)(s, a, s').
\]

(3)

The unknown transition probability function \( T(s, a, s') \) is estimated by the empirical transition probability function

\[
\hat{T}(k)(s, a, s') = \begin{cases} 
\frac{N(k)(s, a, s')}{N(k)(s, a)}, & \text{if } N(k)(s, a) > 0, \\
\frac{1}{|A|}, & \text{if } N(k)(s, a) = 0.
\end{cases}
\]

(4)

And the estimation of \( Q_1(s, a) \) from the existing \( k \) samples is

\[
\hat{Q}_1(k)(s, a) = \sum_{s' \in S_1} \hat{T}(k)(s, a, s').
\]

(5)

Since the value of the Q-function \( Q_1(s, a) \in [0, 1] \) is bounded, we can construct a confidence interval for the estimate \( \hat{Q}_1(k)(s, a) \) with statistical error at most \( \delta \) using Hoeffding’s inequality by

\[
\hat{Q}_1(k)(s, a) = \max \left\{ \hat{Q}_1(k)(s, a) - \sqrt{\frac{\ln(\delta/2)}{2N(k)(s, a)}}, 0 \right\},
\]

\[
\hat{Q}_1(k)(s, a) = \min \left\{ \hat{Q}_1(k)(s, a) + \sqrt{\frac{\ln(\delta/2)}{2N(k)(s, a)}}, 1 \right\},
\]

where we set the value of the division to be \( \infty \) for \( N(k)(s, a) = 0 \).

Remark 1: We use Hoeffding’s bounds to yield hard guarantees on the statistical error of the model checking algorithms. Tighter bounds like Bernstein’s bounds [29] can also be used, but they only yield asymptotic guarantees on the statistical error.

The sample efficiency for learning for the bandit problem [2] depends on the choice of sampling policy, decided from the existing samples. A provably best solution is to use the Q-learning from [27], [28]. Specifically, an upper confidence bound (UCB) is constructed for each state-action pair using the number of samples and the observed reward, and the best action is chosen with the highest possible reward, namely the UCB. The sampling policy is chosen by maximizing the possible reward greedily:

\[
\pi_1^*(s) = \argmax_{a \in A(s)} \hat{Q}_1(k)(s, a).
\]

(7)

The action is chosen arbitrarily when there are multiple candidates. The choice of \( \pi_1^*(s) \) in (7) ensures that the policy giving the upper bound of the value function gets most frequently sampled in the long run.

To initialize the iteration, the Q-function is set to

\[
\hat{Q}_1^0(s, a) = \begin{cases} 
1, & \text{if } s \notin S_0, \\
0, & \text{otherwise},
\end{cases}
\]

(8)

where

\[
\hat{Q}_1^0(s, a) = \begin{cases} 
1, & \text{if } s \in S_1, \\
0, & \text{otherwise},
\end{cases}
\]

(8)

to ensure that every state-action is sampled at least once. The termination condition of the above algorithm is

\[
\begin{cases} 
\text{true}, & \text{if } \max_{a \in A(s)} \hat{Q}_1^k(s, a) > p, \\
\text{false}, & \text{if } \max_{a \in A(s)} \hat{Q}_1^k(s, a) < p, \\
\text{continue}, & \text{otherwise},
\end{cases}
\]

(9)

where \( p \) is the probability threshold in the non-nested PCTL formula.

Remark 2: For \( s \models P_{\leq p}^\text{max}(a_1 U T a_2) \) or \( s \models P_{\geq p}^\text{max}(a_1 R T a_2) \), it suffices to change the termination condition (9) by returning true if \( \hat{Q}_1^k(s, a) < p \), and returning false if \( \hat{Q}_1^k(s, a) > p \). The same statements hold for general PCTL specifications, as discussed in Sections III-B and III-C.

Now, we summarize the above discussion by Algorithm [1] and Theorem [1] below.

**Theorem 1:** The return value of Algorithm [1] is correct with probability at least \( 1 - |A| \delta \).

**Proof:** We provide the proof of a more general statement in Theorem [2].
Algorithm 1 SMC of $s \models P_{\geq p}^\text{max}(a_1 U a_2)$ or $s \models P_{\geq p}^\text{max}(a_1 R a_2)$

Require: MDP $\mathcal{M}$, parameter $\delta$.
1: Initialize the Q-function, and the policy by (3)(4).
2: Obtain $S_0$ and $S_1$ by (1).
3: while True do
4: Sample from $\mathcal{M}$, and update the transition probability function by (3)(4).
5: Update the bounds on the Q-function and the policies by (6)(7).
6: Check termination condition (9).
7: end while

Remark 3: The Hoeffding bounds in (6) are conservative. Consequently, as shown in the simulations in Section IV, the actual statistical error of the our algorithms can be smaller than the given value. However, as the MDP is unknown, finding tighter bounds is challenging. One possible solution is to use asymptotic bounds, such as Bernstein’s bounds [29]. Accordingly, the algorithm will only give asymptotic probabilistic guarantees.

B. Finite Time Horizon

When $T \in \mathbb{N}$, for any $s \in S \setminus (S_0 \cup S_1)$, let

\[ V_h(s) = \max_{\hat{A}} \mathbb{P}_{\sigma \sim \mathcal{M}_{1,n}, \{\sigma \models a_1 U_1 a_2\}}, \]
\[ Q_h(s, a) = \max_{\Pi(h) = a} \mathbb{P}_{\sigma \sim \mathcal{M}_{1,n}, \{\sigma \models a_1 U_1 a_2\}}, \quad h \in [T], \]

i.e., $V_h(s)$ and $Q_h(s, a)$ are the maximal satisfaction probability of $a_1 U_1 a_2$ for a random path starting from $s$ for any policy and any policy with first action being $a$, respectively. By definition, $V_h(s)$ and $Q_h(s, a)$ satisfy the Bellman equation

\[ V_h(s) = \max_{a \in A} Q_h(s, a), \]
\[ Q_{h+1}(s, a) = \sum_{s' \in S} T(s, a, s') V_h(s') + \sum_{s' \in S_1} T(s, a, s'). \]

The second equality of the second equation is derived from

\[ V_h(s) = \begin{cases} 
0, & \text{if } s \in S_0, \\
1, & \text{if } s \in S_1, 
\end{cases} \]

by the semantics of PCTL.

From (11), we check $P_{\geq p}^\text{max}(a_1 U_1 a_2)$ by induction on the time horizon $T$. For $h \in T$, the lower and upper bounds for $Q_h(s, a)$ can be derived using the bounds on the value function for the previous step — for $h = 1$ from (6) and for $h > 0$ by the following lemma.

\[ Q_{h+1}^{(k)}(s, a) = \max \left\{ 0, \sum_{s' \in S \setminus (S_0 \cup S_1)} T^{(k)}(s, a, s') V_h(s') + \sum_{s' \in S_1} T^{(k)}(s, a, s') - \sqrt{\frac{\ln(\delta_h/2)}{2N^{(k)}(s, a)}}, \right\}, \]

\[ \overline{Q}_{h+1}^{(k)}(s, a) = \max \left\{ 1, \sum_{s' \in S \setminus (S_0 \cup S_1)} T^{(k)}(s, a, s') V_h(s') + \sum_{s' \in S_1} T^{(k)}(s, a, s') + \sqrt{\frac{\ln(\delta_h/2)}{2N^{(k)}(s, a)}}, \right\}, \]

where $\delta_h$ is a parameter such that $Q_h(s, a) \in [\underline{Q}_h^{(k)}(s, a), \overline{Q}_h^{(k)}(s, a)]$ with probability at least $1 - \delta_h$. The bounds in (12) are derived from (11) by applying Hoeffding’s inequality, using the fact that $\mathbb{E}[T^{(k)}(s, a, s')] = T(s, a, s')$ and the Q-functions are bounded within $[0, 1]$.

From the boundedness of $Q_h(s, a) \in [0, 1]$, we note that this confidence interval encompasses the statistical error in both the estimated transition probability function $T^{(k)}(s, a, s')$ and the bounds $\overline{V}_h^{(k)}(s, a)$ and $\underline{V}_h^{(k)}(s, a)$ of the value function. Accordingly, the policy $\pi_h^{(k)}$ chosen by the OFU principle at the $h$ step is

\[ \pi_h^{(k)}(s) = \arg\max_{a \in A(s)} \overline{Q}_h^{(k)}(s, a), \]

with an optimal action chosen arbitrarily when there are multiple candidates, to ensure that the policy giving the upper bound of the value function is sampled the most in the long run. To initialize the iteration, the Q-function is set to

\[ \underline{Q}_0^{(0)}(s, a) = \begin{cases} 
1, & \text{if } s \not\in S_0, \\
0, & \text{otherwise,} 
\end{cases} \quad \overline{Q}_0^{(0)}(s, a) = \begin{cases} 
1, & \text{if } s \in S_1, \\
0, & \text{otherwise,} 
\end{cases} \]

for all $h \in [T]$, to ensure that every state-action is sampled at least once.

Sampling by the updated policy $\pi_h^{(k)}(s)$ can be performed in either episodic or non-episodic ways [24]. The only requirement is that the state-action pair $(s, \pi_h^{(k)}(s))$ should be performed frequently for each $h \in [T]$ and for each state $s$ satisfying $s \in S \setminus (S_0 \cup S_1)$. In addition, batch samples may be drawn, namely sampling over the state-action pairs multiple times before updating the policy. In this work, for simplicity, we use a non-episodic, non-batch sampling method, by drawing

\[ s' \sim T(s, \pi_h^{(k)}(s), \cdot), \]

for all $h \in [T]$ and state $s$ such that $a_1 \in L(s), a_2 \not\in L(s)$. The Q-function and the value function are set and initialized
Algorithm 2 SMC of $s \models P_{>p}(a_1 U_T a_2)$ or $s \models P_{>p}(a_1 R_T a_2)$

Require: MDP $M$, parameters $\delta_h$ for $h \in [T]$
1: Initialize the Q-function and the policy by (15) (14).
2: Obtain $S_0$ and $S_1$ by (I).
3: while true do
4: Sample by (16), and update the transition probability function by (3) (4).
5: Update the bounds by (12) (13) and the policy by (14).
6: Check the termination condition (17).
7: end while

by (13) and (15). The termination condition is give by

$$P_{>p} \phi : \begin{cases} \text{false, if } V_H^{(k)}(s_0) < p, \\ \text{true, if } V_H^{(k)}(s_0) > p, \\ \text{continue, otherwise}, \end{cases}$$

where $p$ is the probability threshold in the non-nested PCTL formula. The above discussion is summarized by Algorithm 2 and Theorem 2.

Theorem 2: Algorithm 2 terminates with probability 1 and its return value is correct with probability at least $1 - N |A| \sum_{h \in [T]} \delta_h$, where $N = |S \setminus (S_0 \cup S_1)|$.

Proof: By construction, as the number of iterations $k \to \infty$, $V_T^{(k)} - V^{(k)} \to 0$. Thus, by Assumption 1 the termination condition (17) will be satisfied with probability 1. Now, let $E$ be the event that the return value of Algorithm 2 is correct, and let $F_k$ be the event that Algorithm 2 terminates at the iteration $k$, then we have $P(E) = \sum_{k \in \mathbb{N}} P(E|F_k)P(F_k)$. For any $k$, the event $E$ happens given that $F_k$ holds, if the Hoeffding confidence intervals hold by (12) hold for any actions $a \in A$, $h \in [T]$, and state $s$ with $s \in S \setminus (S_0 \cup S_1)$. Thus, we have $P(E|F_k) \geq 1 - N |A| \sum_{h \in [T]} \delta_h$, where $N = |S \setminus (S_0 \cup S_1)|$, implying that the return value of Algorithm 2 is correct with probability $P(E) \geq 1 - N |A| \sum_{h \in [T]} \delta_h$.

By Theorem 2, the desired overall statistical error splits into the statistical errors for each state-action pair through the time horizon. For implementation, we can split it equally by replacing argmax with argmin in (14), and max with min in (13). The termination condition is the same as (17).

Remark 4: Due to the semantics in Definition 4, running Algorithm 2 proving $P_{>p}(\phi)$ or disproving $P_{<p}(\phi)$ is easier than disproving $P_{>p}(\phi)$ or proving $P_{<p}(\phi)$; and the difference increases with the number of actions $|A|$ and the time horizon $T$. This is because proving $P_{>p}(\phi)$ or disproving $P_{<p}(\phi)$ requires only finding and evaluating some policy $\Pi$ with $P_{M_0}[s \models \phi] > p$, while disproving it requires evaluating all possible policies with sufficient accuracy. This is illustrated by the simulation results presented in Section IV.

C. Infinite Time Horizon

Infinite-step satisfaction probability can be estimated from finite-step satisfaction probabilities, using the monotone convergence of the value function in the time step $H$.

$$V_0(s) \leq \ldots \leq V_H(s) \leq \ldots \leq V(s) = \lim_{H \to \infty} V_H(s).$$

Therefore, if the satisfaction probability is larger than $p$ for some step $H$, then the statistical model checking algorithm should terminate, namely,

$$\begin{cases} \text{false, if } V_H^{(k)}(s_0) > p, \\ \text{continue, otherwise}, \end{cases}$$

where $p$ is the probability threshold in the non-nested PCTL formula.

The general idea in using the monotonicity to check infinite horizon satisfaction probability in finite time is that if we check both $P_{>p}(a_1 U a_2)$ and its negation $P_{<p}(\neg a_1 R \neg a_2)$ at the same time, one of them should terminate in finite time. Here $\neg a_1$ and $\neg a_2$ are treated as atomic propositions. We can use Algorithm 2 to check their satisfaction probabilities for any time horizon $T$ simultaneously. The termination in finite time is guaranteed, if the time horizon for both computations increase with the iterations. The simplest choice is to increase $H$ by 1 for every $K$ iterations; however, this brings the problem of tuning $K$.

Here, we use the convergence of the best policy as the criterion for increasing $H$ for each satisfaction computation. Specifically, for all the steps $h$ in each iteration, in addition to finding the optimal policy $\pi_h^{(k)}(s)$ with respect to the upper confidence bounds of the Q-functions $Q_h^{(k)}(s, a)$ by (14), we also consider the the optimal policy with respect to the lower confidence bounds of the Q-functions $Q_h^{(k)}(s, a)$. Obviously, when $\pi_h^{(k)}(s) \in \arg\max_{a \in A} Q_h^{(k)}(s, a)$, we know that the policy $\pi_h^{(k)}(s)$ is optimal for all possible Q-functions within $[Q_h^{(k)}, \overline{Q_h^{(k)}}]$. This implies that these bounds are fine enough for estimating $Q_H$; thus, if the algorithm does not terminate by the condition (19), we let

$$H \leftarrow \begin{cases} 1, & \text{initially}, \\ H + 1, & \text{if } \pi_h^{(k)}(s) \in \arg\max_{a \in A} Q_h^{(k)}(s, a) \text{ for all } s \in S, \\ \text{Continue}, & \text{otherwise}, \end{cases}$$

Combining the above procedure, we derive Algorithm 3 and Theorem 3 below for statistically model checking PCTL formula $P_{>p}(a_1 U a_2)$.

Theorem 5: Algorithm 3 terminates with probability 1 and its return value is correct with probability $1 - \max\{|N_1, N_2| \sum_{h \in [T]} \delta_h, H = \text{the largest time horizon when the algorithm stops}, N_1 = |S \setminus (S_0^H \cup S_0^\phi)| \text{ and } N_2 = |S \setminus (S_0^\psi \cup S_1^\psi)| \text{ where } S_0^\phi, S_0^\psi \text{ and } S_1^\psi \text{ derived from (I) for } \phi = a_1 U a_2 \text{ and } \psi = a_1 R a_2$, respectively.

Proof: Terminates with probability 1 follows easily from (18). Following the proof of Theorem 2 if the procedure of checking either $P_{>p}(\phi)$ or its negation $P_{<p}(\neg \phi)$
Algorithm 3 SMC of $s \models P_{\text{max}}^*(a_1Ua_2)$

Require: MDP $\mathcal{M}$, parameters $\delta_h$ for $h \in \mathbb{N}$.
1: Initialize two sets of Q-function and the policy by (15) for (i) $P_{\text{max}}^*(a_1Ua_2)$ and (ii) $P_{\text{max}}^*\sim\mathcal{P}(\sim a_1R\sim a_2)$, respectively.
2: Obtain $S_0$ and $S_1$ for (i) and (ii) respectively by 1.
3: while True do
4: Sample by (16), and update $\mathcal{T}^{(k)}(s,a,s')$ by (3) (4).
5: Update the bounds on the Q-function, the policies, the value function, and the time horizon by (12)-(14) respectively for (i) and (ii).
6: Check the termination condition (19).
7: end while

Algorithm 3 stops and the largest time horizon is $H$, then the return value is correct with probability at least $1 - |A| \max\{N_1,N_2\}$ $\sum_{h \in \mathcal{T}} \delta_h$, Thus, the theorem holds.

Remark 5: By Theorem 3 given the desired overall confidence level $\delta$, we can split it geometrically by $\delta_h = (1 - \lambda)\lambda^{h-1}\delta$, where $\lambda \in (0,1)$.

Remark 6: Similar to Section III-B checking $P_{\text{min}}^*(\phi)$ for $\sim \in \{\leq,\geq\}$ is derived by replacing argmax with argmin in (14), and max with min in (13). The termination condition is the same as (19).

Remark 7: Finally, we note that the exact savings of sample costs for Algorithms 2 and 3 depend on the structure of the MDP. Specifically, the proposed method is more efficient than [9], [10], [30], when the satisfaction probabilities differ significantly among actions, as it can quickly detect sub-optimal actions without over-sampling on them. On the other hand, if all the state-action pairs yield the same Q-value, then an equal number of samples will be spent on each of them — in this case, the sample cost of Algorithms 2 and 3 is the same as [9], [10], [30].

IV. Simulation

To evaluate the performance of the proposed algorithms, we ran them on two different sets of examples. In all the simulations, the transition probabilities are unknown to the MDPs, we considered the formula $P_{\sim \mathcal{P}}(\sim a_1R\sim a_2)$ for the infinite horizon, and $P_{\sim \mathcal{P}}(\sim F\alpha)$ for the finite horizon. In both cases $\alpha$ encodes the atomic predicate that is true iff values of both dice are chosen and their sum is less than an arbitrarily chosen constant. Also, in the finite case, $H = 5$ in the smallest example and 10 everywhere else.

For each MDP, we first numerically estimate the values of $\max H_{\mathcal{M}_H}[1_{a_1Ua_2}]$ and $\max H_{\mathcal{M}_H}[1_{a_1Ua_2}]$, for the randomly generated MDPs, and $\max H_{\mathcal{M}_H}[1_{a_1Ua_2}]$, for the variants of the two-dice examples, using the known models on PRISM [32]. Then, we use Algorithms 2 and 3 on the example models with only knowledge of the topology of the MDPs and without knowing the exact transition probabilities. For every MDP, we tested each algorithm with two different thresholds $p$, one smaller and the other larger than the estimated probability, to test the proposed algorithms, with $\delta$ set to 5%. We ran each randomly generated test 100 times and each two-dice variant test 10 times. Here we only report average running time and average number of iterations. All tests returned the correct answers — this suggests that the Hoeffding’s bounds used in the proposed algorithms are conservative (see Remark 5).

The algorithms are implemented in Scala and ran on Ubuntu 18.04 with 17-8700 CPU 3.2GHz and 16GB memory.

Table I shows the results for finite horizon reachability. An interesting observation in these tables is that in all examples, disproving the formula is 3 to 100 times faster. We believe this is mainly because, to disprove $P_{\sim \mathcal{P}}(\sim a_1R\sim a_2)$, all we need is one policy $P$ for which $P_{\sim \mathcal{P}}(\sim a_1R\sim a_2)$ holds. However, to prove $P_{\sim \mathcal{P}}(\sim a_1R\sim a_2)$, one needs to show that every policy $P$ satisfies $P_{\sim \mathcal{P}}(\sim a_1R\sim a_2)$ (see Remark 4).

Tables II and III show the results for infinite horizon reachability. Note that Algorithm 3 considers both the formula and its negation, and contrary to the finite horizon reachability, disproving a formula is not always faster for the infinite case. In most of the larger examples that are randomly generated, $H_1$ and $H_2$ are very small on average. This shows that in these examples, the algorithm was smart enough to learn there is no need to increase $H$ in order to
solve the problem. However, this is not the case for two-dice examples. We believe this is because in the current implementation, the decision to increase $H$ does not consider the underlying graph of the MDP. For example, during the execution, if the policy forces the state to enter a self-loop with only one enabled action, which is the case in two-dice examples, then after every iteration the value of $H$ will be decreased by 1.

V. CONCLUSION

We proposed a statistical model checking method for Probabilistic Computation Tree Logic on Markov decision processes using reinforcement learning. We first checked PCTL formulas with bounded time horizon, using upper-confidence-bounds based Q-learning, and then extended the technique to unbounded-time specifications by finding a proper truncation time by checking the specification of interest and its negation at the same time. Finally, we demonstrated the efficiency of our method on several case studies.

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