

\section*{1 Introduction}

Automata learning automatically generates models from system observations such as test logs. Hence, it enables model-based verification for black-box software systems \cite{231}, e.g., via model checking. Automata learning techniques generally fall into two categories: passive and active learning. Passive algorithms

\* This work is an extended version of the conference paper “$L^*$-Based Learning of Markov Decision Processes” accepted for presentation at FM 2019, the 23rd International Symposium on Formal Methods in Porto, Portugal.
take a given sample of system traces as input and generate models consistent with the sample. The quality and comprehensiveness of learned models therefore largely depend on the given sample. In contrast, active algorithms actively query the system under learning (SUL) to sample system traces. This enables to steer the trace generation towards parts of the SUL’s state space that have not been thoroughly covered, potentially finding yet unknown aspects of the SUL.

Many active automata learning algorithms are based on Angluin’s L∗ algorithm [4]. It was originally proposed for learning deterministic finite automata (DFA) accepting regular languages and later applied to learn models of reactive systems, by considering system traces to form regular languages [24]. L∗ has been extended to formalisms better suited for modelling reactive systems such as Mealy machines [31,36] and extended finite state-machines [13]. Most L∗-based work, however, targets deterministic models, with the exceptions of algorithms for non-deterministic Mealy machines [20] and non-deterministic input-output transition systems [43]. Both techniques are based on testing, but abstract away the observed frequency of events, thus they do not use all available information.

Here, we present an L∗-based approach for learning models of stochastic systems with transitions that happen with some probability depending on non-deterministically chosen inputs. More concretely, we learn deterministic Markov decision processes (MDPs), like IoAlergia [29,30], a state-of-the-art passive learning algorithm. Such models are commonly used to model randomised distributed algorithms [9], e.g. in protocol verification [27,33]. We present two learning algorithms: the first takes an ideal view assuming perfect knowledge about the exact distribution of system traces. The second algorithm relaxes this assumption, by sampling system traces to estimate their distribution. We refer to the former as exact learning algorithm L∗_{mdp} and to the latter as sampling-based learning algorithm L∗_{mdp}. We implemented L∗_{mdp} and evaluated it by comparing it to IoAlergia [29,30]. Experiments showed favourable performance of L∗_{mdp}, i.e. it produced more accurate models than IoAlergia given approximately the same amount of data. Apart from the empirical evaluation, we show that the model learned by L∗_{mdp} converges in the limit to an MDP isomorphic to the canonical MDP representing the SUL. To the best of our knowledge, L∗_{mdp} is the first L∗-based learning algorithm for MDPs that can be implemented via testing. Our contributions span the algorithmic development of learning algorithms, their analysis with respect to convergence and the implementation as well as the evaluation of learning algorithms.

This work is an extended version of the conference paper “L∗-Based Learning of Markov Decision Processes” accepted for presentation at FM 2019, the 23rd International Symposium on Formal Methods in Porto, Portugal. It provides additional details on the implementation of L∗_{mdp}, the convergence analysis of both learning algorithms and an extended evaluation.

The rest of this paper is structured as follows. We introduce notational conventions, preliminaries on MDPs and active automata learning in Sect. 2. Sect. 3 provides a characterisation of MDPs and presents the exact learning algorithm L∗_{mdp}. Sect. 4 describes the sampling-based L∗_{mdp} and analyses it with respect to
In Sect. 4, we apply a pseudo-random function \( \text{randSel} \). Hence, according to a uniform distribution, i.e. \( \forall \) input and returning a single element of the set, whereby the element is chosen from the indicator function of \( A \). In the remainder of this paper, distributions \( \mu \) may be partial functions, in which case we implicitly set \( \mu(e) = 0 \) if \( e \) is not defined for \( e \). For \( A \subseteq S \), \( 1_A \) denotes the indicator function of \( A \), i.e. \( 1_A(e) = 1 \) if \( e \in A \) and \( 1_A(e) = 0 \) otherwise. Hence, \( 1_{\{e\}} \) for \( e \in S \) is the probability distribution assigning probability 1 to \( e \).

In Sect. 5 we apply a pseudo-random function \( \text{randSel} \) taking taking a set \( S \) as input and returning a single element of the set, whereby the element is chosen according to a uniform distribution, i.e. \( \forall e \in S : \mathbb{P}(\text{randSel}(S) = e) = \frac{1}{|S|} \). In addition to that, we use the function \( \text{coinFlip}(p) \) returning \( \text{true} \) with probability \( p \) and \( \text{false} \) otherwise.

Markov Decision Processes.

**Definition 1 (Markov decision process (MDP)).** A labelled Markov decision process (MDP) is a tuple \( \mathcal{M} = (Q, \Sigma^I, \Sigma^O, q_0, \delta, L) \) where

- \( Q \) is a finite non-empty set of states,
- \( \Sigma^I \) and \( \Sigma^O \) are finite sets of input and output symbols respectively,
- \( q_0 \in Q \) is the initial state,
- \( \delta : Q \times \Sigma^I \rightarrow \text{Dist}(Q) \) is the probabilistic transition function, and
- \( L : Q \rightarrow \Sigma^O \) is the labelling function.

An MDP is deterministic if \( \forall q \in Q, \forall i : \delta(q, i)(q') > 0 \wedge \delta(q, i)(q'') > 0 \rightarrow q' = q'' \vee L(q') \neq L(q'') \).

We learn deterministic labelled MDPs as learned by passive learning techniques like IOALER-GIA [20]. Such MDPs define at most one successor state for each source state and input-output pair.

**Fig. 1.** MDP model of a faulty coffee machine.
In the following, we refer to these models uniformly as MDPs. We use \( \Delta : Q \times \Sigma^* \times \Sigma^O \rightarrow Q \cup \{ \bot \} \) to compute successor states. The function is defined by \( \Delta(q, i, o) = q' \in Q \) with \( L(q') = o \) and \( \delta(q, i)(q') > 0 \) if there exists such a \( q' \), otherwise \( \Delta \) returns \( \bot \). Fig. 1 shows an MDP model of a faulty coffee machine [3]. Outputs in curly braces label states and inputs with corresponding probabilities.

Definition 2 (Scheduler). Given an MDP \( \mathcal{M} = \langle Q, \Sigma^I, \Sigma^O, q_0, \delta, L \rangle \), a scheduler for \( \mathcal{M} \) is a function \( s : \text{Path}_\mathcal{M} \rightarrow \text{Dist}(\Sigma^n) \).

The composition of an MDP \( \mathcal{M} \) and a scheduler \( s \) induces a deterministic Markov chain, i.e., a fully probabilistic system allowing to define a probability measure over paths. Additionally to \( \mathcal{M} \) and \( s \), we also need a probability distribution \( p_t \in \text{Dist}(\mathbb{N}_0) \) over the path lengths. An MDP \( \mathcal{M} \), a scheduler \( s \), and a path length probability distribution \( p_t \) induce a probability distribution \( P^{l}_{\mathcal{M}, s} \) on finite paths \( \text{Path}_\mathcal{M} \), defined by:

\[
P^{l}_{\mathcal{M}, s}(q_0 i_1 q_1 \cdots i_n q_n) = p_t(n) \cdot \left( \prod_{j=1}^{n} s(q_0 \cdots i_{j-1} q_{j-1})(i_j) \cdot \delta(q_{j-1}, i_j)(q_j) \right)
\]

Sequences of Observations. During the execution of a finite path \( \rho \), we observe a trace \( L(\rho) = t \), i.e., an alternating sequence of inputs and outputs starting with an output, with \( t = o_0 i_1 o_1 \cdots i_{n-1} o_{n-1} i_n o_n \) and \( L(q_i) = o_i \). Since we consider deterministic MDPs, \( L \) is invertible, thus each trace in \( \Sigma^O \times (\Sigma^I \times \Sigma^O)^* \) corresponds to at most one path and \( P^{l}_{\mathcal{M}, s} \) can be adapted to traces \( t \) by defining:

\[
P^{l}_{\mathcal{M}, s}(t) = \begin{cases} P^{l}_{\mathcal{M}, s}(\rho) & \text{if there is a } \rho \text{ with } L(\rho) = t \\ 0 & \text{otherwise} \end{cases}
\]

We say that a trace \( t \) is observable if there exists a \( \rho \) with \( L(\rho) = t \), thus there is a scheduler \( s \) and a \( p_t \) such that \( P^{l}_{\mathcal{M}, s}(t) > 0 \). In a deterministic MDP \( \mathcal{M} \),
each observable trace \( t \) uniquely defines a state of \( \mathcal{M} \) reached by executing \( t \) from the initial state \( q_0 \). We compute this state by \( \delta^*(t) = \delta^*(q_0, t) \) defined by

\[
\delta^*(q, L(q)) = q \quad \text{and}
\delta^*(q, o_0 i_1 o_1 \cdots i_{n-1} o_{n-1} i_n o_n) = \Delta(\delta^*(q, o_0 i_1 o_1 \cdots i_{n-1} o_{n-1}), i_n, o_n).
\]

If \( t \) is not observable, then there is no path \( \rho \) with \( t = L(\rho) \), denoted by \( \delta^*(t) = \perp \). We denote the last output \( o_n \) of a trace \( t = o_0 \cdots i_n o_n \), by \( \text{last}(t) \).

We use three types of observation sequences with short-hand notations:
- **Traces**: abbreviated by \( \mathcal{T} \mathcal{R} = \Sigma^O \times (\Sigma^1 \times \Sigma^O)^* \)
- **Test sequences**: abbreviated by \( \mathcal{T} \mathcal{S} = (\Sigma^O \times \Sigma^1)^* \)
- **Continuation sequences**: abbreviated by \( \mathcal{C} \mathcal{S} = \Sigma^1 \times \mathcal{T} \mathcal{S} \)

These sequence types alternate between inputs and outputs, thus they are related among each other. In slight abuse of notation, we use \( A \times B \) and \( A \cdot B \) interchangeably for the remainder of this paper. Furthermore, we extend the sequence notations and the notion of prefixes to \( \Sigma^O, \Sigma^1, \mathcal{T} \mathcal{R}, \mathcal{T} \mathcal{S} \) and \( \mathcal{C} \mathcal{S} \), e.g., test sequences and traces are related by \( \mathcal{T} \mathcal{R} = \mathcal{T} \mathcal{S} \cdot \Sigma^O \).

As noted, a trace in \( \mathcal{T} \mathcal{R} \) leads to a unique state of an MDP \( \mathcal{M} \). A test sequence in \( s \in \mathcal{T} \mathcal{S} \) of length \( n+1 \) consists of a trace in \( t \in \mathcal{T} \mathcal{R} \) with \( n \) outputs and an input \( i \in \Sigma^1 \) with \( s = t \cdot i \); thus executing test sequence \( s = t \cdot i \) puts \( \mathcal{M} \) into the state reached by \( t \) and tests \( \mathcal{M} \)'s reaction to \( i \). Extending the notion of observability, we say that the test sequence \( s \) is observable if \( t \) is observable. A continuation sequence \( c \in \mathcal{C} \mathcal{S} \) begins and ends with an input, i.e. concatenating a trace \( t \in \mathcal{T} \mathcal{R} \) and \( c \) creates a test sequence \( t \cdot c \) in \( \mathcal{T} \mathcal{S} \). Informally, continuation sequences test \( \mathcal{M} \)'s reaction in response to multiple consecutive inputs.

**Lemma 1.** If trace \( t \in \mathcal{T} \mathcal{R} \) is not observable, then any \( t' \in \mathcal{T} \mathcal{R} \) such that \( t \ll t' \) is not observable as well.

Lemma 1 follows directly from (1). For a non-observable \( t \), we have \( \forall s, p_i : P_{\mathcal{M},1}(t) = 0 \) and extending \( t \) to create \( t' \) only adds further factors. The same property holds for test sequences.

**Active Automata Learning.** We consider active automata learning in the minimally adequate teacher (MAT) framework [4], introduced by Angluin for the \( L^* \) algorithm. It assumes the existence of a MAT, which is able to answer queries. \( L^* \) learns a DFA representing an unknown regular language \( L \) over some alphabet \( A \) and therefore requires two types of queries: **membership** and **equivalence** queries. First, \( L^* \) repeatedly selects strings in \( A^* \) and checks if they are in \( L \) via **membership** queries. Once the algorithm has gained sufficient information, it forms a hypothesis DFA consistent with the membership query results. It then poses an **equivalence** query checking for equivalence between \( L \) and the language accepted by the hypothesis. The teacher responds either with **yes** signaling equivalence; or with a counterexample to equivalence, i.e. a string in the symmetric difference between \( L \) and the language accepted by the hypothesis. After processing a counterexample, \( L^* \) starts a new round of learning, consisting
of membership queries and a concluding equivalence query. Once an equivalence query returns yes, learning stops with the final hypothesis as output.

$L^*$ has been extended to learn models of reactive systems such as Mealy machines [36]. In practice, queries for learning models of black-box systems are usually implemented via testing [2]. Therefore, equivalence queries are generally only approximated as complete testing for black-box systems is impossible unless there is an upper bound on the number of system states. We cover the ideal setting in Sect. 3 by presenting an $L^*$-based exact learning algorithm for MDPs. In Sect. 4, we discuss an implementation in a sampling-based setting that approximates queries by testing the SUL.

### 3 Exact Learning of MDPs

This section presents $L^*_{mdp}$, an exact active learning algorithm for MDPs, the basis for the sampling-based algorithm presented in Sect. 4. In contrast to sampling, $L^*_{mdp}$ assumes the existence of a teacher with perfect knowledge about the SUL that is able to answer two types of queries: output distribution queries and equivalence queries. The former asks for the exact distribution of outputs following a test sequence in the SUL. The latter takes a hypothesis MDP as input and responds either with yes iff the hypothesis is observationally equivalent to the SUL or with a counterexample to equivalence. A counterexample is a test sequence leading to different output distributions in hypothesis and SUL. First, we describe how we capture the semantics of MDPs.

**Semantics of MDPs.** We can interpret an MDP as a function $M : TS \rightarrow \text{Dist}(\Sigma^O) \cup \{\bot\}$, mapping test sequences $s$ to output distributions or undefined behaviour for non-observable $s$. This follows the interpretation of Mealy machines as functions from input sequences to outputs [37]. Likewise, we will define which functions $M$ capture the semantics of MDPs by adapting the Myhill-Nerode theorem for regular languages [32]. We denote the set of sequences $s$ where $M(s) \neq \bot$ as defined domain $\text{dd}(M)$ of $M$.

**Definition 3 (MDP Semantics).** Given an MDP $\langle Q, \Sigma^I, \Sigma^O, q_0, \delta, L \rangle$, its semantics is a function $M$, defined for $i \in \Sigma^I$, $o \in \Sigma^O$, $t \in TR$ as follows:

- $M(\epsilon)(L(q_0)) = 1$
- $M(t \cdot i) = \bot$ if $\delta^*(t) = \bot$
- $M(t \cdot i)(o) = p$ otherwise if $\delta(\delta^*(t), i)(q) = p > 0 \land L(q) = o$

**Definition 4 (M-Equivalence of Traces).** Two traces $t_1, t_2 \in TR$ are equivalent with respect to $M : TS \rightarrow \text{Dist}(\Sigma^O) \cup \{\bot\}$, denoted $t_1 \equiv_M t_2$, iff $\text{last}(t_1) = \text{last}(t_2)$ and for all continuations $v \in CS$ it holds that $M(t_1 \cdot v) = M(t_2 \cdot v)$.

A function $M$ defines an equivalence relation on traces, like the Myhill-Nerode equivalence for formal languages [32]. Two traces are $M$-equivalent if they end
in the same output and if their behaviour in response to future inputs is the same. Two traces leading to the same MDP state are in the same equivalence class of \( \equiv_M \), as in Mealy machines [37].

We can now state which functions characterise MDPs, as an adaptation of the Myhill-Nerode theorem for regular languages [32], like for Mealy machines [37].

**Theorem 1 (Characterisation).** A function \( M : TS \rightarrow \text{Dist}(\Sigma^O) \cup \{\bot\} \) represents the semantics of an MDP iff

- \( \equiv_M \) has finite index,
- finite number of states
- \( M(\epsilon) = 1_{\{o\}} \) for an \( o \in \Sigma^O \),
- initial output
- \( \text{dd}(M) \) is prefix-closed, and
- \( \forall t \in TR : \text{either } \forall i \in \Sigma^1 : M(t \cdot i) \neq \bot \text{ or } \) input enabledness
- \( \forall i \in \Sigma^1 : M(t \cdot i) = \bot \)

**Proof.** Direction \( \Rightarrow \): first we show that the semantics \( M \) of an MDP \( \mathcal{M} = \langle Q, \Sigma^I, \Sigma^O, q_0, \delta, L \rangle \) fulfils the conditions of Theorem 1. According to Def. 3, \( M(\epsilon)(L(q_0)) = 1 \), thus the second condition is fulfilled.

Let \( t \in TR \) be an observable trace, then we have for \( i \in \Sigma^1, o \in \Sigma^O \):
\[
M(t \cdot i)(o) = \delta(q', i)(q) = p
\]
where \( q' = \delta^*(t) \), if \( p > 0 \) and \( L(q) = o \). Since \( M \) contains finitely many states \( q' \), \( \delta(q', i) \) and therefore also \( M(t \cdot i) \) take only finitely many values. \( M \)-equivalence of traces \( t \) depends on the outcomes of \( M \) and on their last outputs \( \text{last}(t_i) \), which are both finite, therefore \( M \)-equivalence defines finitely many equivalence classes for observable traces. For non-observable \( t \in TR \) we have \( \delta^*(t) = \bot \) which implies \( M(t \cdot i) = \bot \). As a consequence of Lemma 1 we also have \( M(t \cdot c) = \bot \) for any \( c \in CS \). Hence, non-observable traces are equivalent with respect to \( M \) if they end in the same output, therefore \( M \) defines finitely many equivalence classes for non-observable traces. In summary, \( \equiv_M \) has finite index, i.e. the first condition is fulfilled. Prefix-closeness of the defined domain \( \text{dd}(M) \) of \( M \) follows from Lemma 1. Any extension of a non-observable test sequence is also non-observable, thus \( M \) fulfils the third condition.

For the fourth condition, we again distinguish two cases. If \( t \) is a non-observable trace, i.e. \( \delta^*(t) = \bot \), then \( M(t \cdot i) = \bot \) for all \( i \in \Sigma^1 \) according to Def. 3 which fulfils the second sub-condition. For observable \( t \), the distribution \( M(t \cdot i) \) depends on \( \delta(\delta^*(t), i) \), which is defined for all \( i \) due to input-enabledness of \( M \), satisfying the first subcondition.

Direction \( \Leftarrow \): from an \( M \) satisfying the conditions given in Theorem 1 we can construct an MDP \( \mathcal{M}_c = \langle Q, \Sigma^I, \Sigma^O, q_0, \delta, L \rangle \) by:

- \( Q = (TR/\equiv_M) \setminus \{[t]|t \in TR, \exists i \in I : M(t \cdot i) = \bot\} \)
- \( q_0 = [o_0] \), where \( o_0 \in \Sigma^O \) such that \( M(\epsilon) = 1_{\{o_0\}} \)
- \( L([s \cdot o]) = o \) (by Def. 4 all traces in the same equivalence class end with the same output)
- for \( [t] \in Q \):
  \[ \delta([t], i)((t \cdot i \cdot o)) = M(t \cdot i)(o) \] (defined by fourth condition of Theorem 1)

Each equivalence class of \( \equiv_M \) gives rise to exactly one state in \( Q \), except for the equivalence classes of non-observable traces \( Q \).
The MDP $\mathcal{M}_c$ in the above construction is minimal with respect to the number of states and unique, up to isomorphism. Therefore, we refer such an MDP as canonical MDP $\text{can}(M)$ for MDPs semantics $M$.

Viewing MDPs as reactive systems, we consider two MDPs to be equivalent, if we make the same observations on both.

**Definition 5 (Output-Distribution Equivalence).** MDPs $\mathcal{M}_1$ and $\mathcal{M}_2$ over $\Sigma^I$ and $\Sigma^O$ with semantics $M_1$ and $M_2$ are output-distribution equivalent, denoted $\mathcal{M}_1 \equiv_{\text{od}} \mathcal{M}_2$, iff

$$\forall s \in TS : M_1(s) = M_2(s)$$

**Queries.** We are now able to define queries focusing on the observable behaviour of MDPs. Assume that we want to learn a model of a black-box deterministic MDP $\mathcal{M}$, with semantics $M$. Output distribution queries (odq) and equivalence queries (eq) are then defined as follows:

- **output distribution (odq):** an odq query takes a sequence $s \in TS$ as input and returns $M(s)$.
- **equivalence (eq):** an eq query takes a hypothesis Mealy machine $\mathcal{H}$ with semantics $H$ as input and returns yes if $\mathcal{H} \equiv_{\text{od}} \mathcal{M}$; otherwise it returns an $s \in TS$ such that $H(s) \neq M(s)$ and $M(s) \neq \bot$.

**Remark 1.** For any counterexample $s$ to $\mathcal{H} \equiv_{\text{od}} \mathcal{M}$ such that $M(s) = \bot$, there is a prefix $s'$ of $s$ with $H(s') \neq M(s')$ and $M(s) \neq \bot$, i.e. $s'$ is also a counterexample but observable on the SUL with semantics $M$. Hence, we can restrict potential counterexamples to be observable test sequences.

**Proof.** Since $s$ is a counterexample and $M(s) = \bot$, we have $H(s) \neq \bot$. Let $s''$ be the the longest prefix of $s$ such that $M(s'') = \bot$, thus $s''$ is of the form $s'' = s' \cdot o \cdot i$ with $M(s')(o) = 0$. Due to prefix-closedness of $dd(H)$, $H(s) \neq \bot$ implies $H(s'') \neq \bot$, therefore $H(s')(o) > 0$. Hence, $s'$ with $M(s') \neq \bot$ is also a counterexample because $H(s') \neq M(s')$.

**Observation Tables.** Like $L^*$, we store information in observation table triples $(S, E, T)$, where:

- $S \subseteq TR$ is a prefix-closed set of traces, initialised to $\{o_0\}$, a singleton set containing the trace consisting of the initial output $o_0$ of the SUL, given by $\text{odq}(o)(o_0) = 1$.
- $E \subseteq CS$ is a suffix-closed set of continuation sequences, initialised to $\Sigma^I$,
- $T : (S \cup Lt(S)) \cdot E \rightarrow \text{Dist}(\Sigma^O) \cup \{\bot\}$ is a mapping from test sequences to output distributions or $\bot$ denoting undefined behaviour. This mapping basically stores a finite subset of $M$. The set $Lt(S) \subseteq S \cdot \Sigma^I \cdot \Sigma^O$ is given by $Lt(S) = \{s \cdot i \cdot o | s \in S, i \in \Sigma^I, o \in \Sigma^O, \text{odq}(s \cdot i)(o) > 0\}$.

We can view an observation table as a two-dimensional array with rows labelled by traces in $S \cup Lt(S)$ and columns labelled by $E$. We refer to traces in $S$ as short traces and to their extensions in $Lt(S)$ as long traces. An extension $s \cdot i \cdot o$
of a short trace \(s\) is in \(Lt(S)\) if \(s \cdot i \cdot o\) is observable. Analogously to traces, we refer to rows labelled by \(S\) as short rows and we refer to rows labelled by \(Lt(S)\) as long rows. The table cells store the mapping defined by \(T\). To represent rows labelled by traces \(s\) we use functions \(row(s) : E \rightarrow \text{Dist}(\Sigma^O) \cup \{\bot\}\) for \(s \in S \cup Lt(S)\) with \(row(s)(e) = T(s \cdot e)\). Equivalence of rows labelled by traces \(s_1, s_2\), denoted \(\text{eqRow}_E(s_1, s_2)\), holds iff \(row(s_1) = row(s_2)\) and approximates \(M\)-equivalence \(s_1 \equiv_M s_2\), by considering only continuations in \(E\), i.e. \(s_1 \equiv_M s_2\) implies \(\text{eqRow}_E(s_1, s_2)\). The observation table content defines the structure of hypothesis MDPs based on the following principle: we create one state per equivalence class of \(S/\text{eqRow}_E\), thus we identify states with traces in \(S\) reaching them and we distinguish states by their future behaviour in response to sequences in \(E\) (as is common in active automata learning \([37]\)). The long traces \(Lt(S)\) serve to define transitions. Transition probabilities are given by the distributions in the mapping \(T\).

Table 1 shows a part of the observation table created during learning of the coffee machine shown in Fig. 1. The set \(S\) has a trace for each state of the MDP. Note that these traces are pairwise inequivalent with respect to \(\text{eqRow}_E\), where \(E = \Sigma^1 = \{\text{but}, \text{coin}\}\). We only show one element of \(Lt(S)\), which gives rise to the self-loop in the initial state with the input \text{but} and probability 1.

**Definition 6 (Closedness).** An observation table \(\langle S, E, T \rangle\) is closed if for all \(l \in Lt(S)\) there is an \(s \in S\) such that \(\text{eqRow}_E(l, s)\).

**Definition 7 (Consistency).** An observation table \(\langle S, E, T \rangle\) is consistent if for all \(s_1, s_2 \in S, i \in \Sigma^1, o \in \Sigma^O\) such that \(\text{eqRow}_E(s_1, s_2)\) it holds either that (1) \(T(s_1 \cdot i)(o) = 0 \land T(s_2 \cdot i)(o) = 0\) or (2) \(\text{eqRow}_E(s_1 \cdot i \cdot o, s_2 \cdot i \cdot o)\).

Closedness and consistency are required to derive well-formed hypotheses, analogously to \(L^*\) \([4]\). We require closedness to create transitions for all inputs in all states and we require consistency to be able to derive deterministic hypotheses. During learning, we apply Algorithm 1 repeatedly to establish closedness and consistency of observation tables. The algorithm adds a new short trace if the table is not closed and adds a new column if the table is not consistent.

We derive a hypothesis \(H = \langle Q_h, \Sigma^1, \Sigma^O, q_{0h}, \delta_h, L_h \rangle\) from a closed and consistent observation table \(\langle S, E, T \rangle\), denoted \(H = \text{hyp}(S, E, T)\), as follows:

\[\text{Table 1. Parts of observation table for learning the faulty coffee machine (Fig. 1).}\]

| \(S\) | \(Lt(S)\) |
|------|----------|
| \(\text{init} \cdot \text{coin} \cdot \text{beep}\) | \(\text{init} \cdot \text{key} \cdot \text{coffee}\) |
| \(\text{init} \cdot \text{coin} \cdot \text{beep}\) | \(\text{init} \cdot \text{coffee}\) |
| \(\text{init} \cdot \text{coin} \cdot \text{beep} \cdot \text{but} \cdot \text{coffee}\) | \(\text{init} \cdot \text{coffee}\) |
| \(\text{init} \cdot \text{but} \cdot \text{init}\) | \(\text{init} \cdot \text{coffee}\) |
| \(\text{but} \cdot \text{coffee}\) | \(\text{beep} \cdot 1\) |

Note that \(s_1 \in S\) implies that \(T(s_1 \cdot i) \neq \bot\) such that \(T(s_1 \cdot i)(o) = 0\) follows from \(\text{eqRow}_E(s_1, s_2)\) and \(T(s_1 \cdot i)(o) = 0\).
Algorithm 1 Making an observation table closed and consistent

1: function MakeClosedAndConsistent(S, E, T)
2: if (S, E, T) is not closed then
3:   \( i \leftarrow i' \in L(S) \) such that \( \forall s \in S : \text{row}(s) \neq \text{row}(i') \lor \text{last}(s) \neq \text{last}(i') \)
4:   \( S \leftarrow S \cup \{i\} \)
5: else if (S, E, T) is not consistent then
6:   for all \( s_1, s_2 \in S \) such that eqRow\(_E\)(\( s_1, s_2 \)) do
7:     for all \( i \in \Sigma^1, o \in \Sigma^O \) do
8:       if \( T(s_1 \cdot i)(o) > 0 \) and \( \neg \text{eqRow}\(_E\)(s_1 \cdot i \cdot o, s_2 \cdot i \cdot o) \) then
9:         \( E \leftarrow E \cup \{i \cdot o\} \)
10:    return (S, E, T)
11: return \( \text{eqResult} \)

Algorithm 2 The main algorithm implementing \( L_{\text{MDP}}^* \)

Input: \( \Sigma^E \), exact teacher capable of answering \( \text{odq} \) and \( \text{eq} \)
Output: learned model \( \mathcal{H} \) (final hypothesis)

1: \( o_0 \leftarrow o \) such that \( \text{odq}(o) = 1 \)
2: \( S \leftarrow \{o_0\}, E \leftarrow \Sigma^E \)
3: procedure \text{Fill}(S, E, T)
4: repeat
5:   while (S, E, T) not closed or not consistent do
6:     \( (S, E, T) \leftarrow \text{MakeClosedAndConsistent}(S, E, T) \)
7:     \( \text{Fill}(S, E, T) \)
8:     \( \mathcal{H} \leftarrow \text{hyp}(S, E, T) \)
9:     \( \text{eqResult} \leftarrow \text{eq} \mathcal{H} \)
10: if \( \text{eqResult} \neq \text{yes} \) then
11:     \( \text{cex} \leftarrow \text{eqResult} \)
12:     for all \( i \in \text{prefixes}(\text{cex}) \) do
13:       \( S \leftarrow S \cup \{i\} \)
14:     \( \text{Fill}(S, E, T) \)
15: until \( \text{eqResult} = \text{yes} \)
16: return \( \text{hyp}(S, E, T) \)
17: procedure \text{Fill}(S, E, T)
18: for all \( s \in S \cup L(S), e \in E \) do
19: if \( T(s \cdot e) \) undefined then \( \triangleright \) we have no information about \( T(s \cdot e) \) yet
20: \( T(s \cdot e) \leftarrow \text{odq}(s \cdot e) \)

Learning Algorithm. Algorithm 2 implements \( L_{\text{MDP}}^* \) using queries \text{odq} and \text{eq}. First, the algorithm initialises the observation tables and fills the table cells with output distribution queries (Lines 1 to 3). The main loop in Lines 4 to 15 makes the observation table closed and consistent, derives a hypothesis \( \mathcal{H} \) and performs an equivalence query \text{eq} \( \mathcal{H} \). If a counterexample \text{cex} is found, all its prefix traces are added as short traces to \( S \), otherwise the final hypothesis is returned, as it is output-distribution equivalent to the SUL. Whenever the table contains empty cells, the \text{Fill} procedure assigns values to these cells via \text{odq}. 

- \( Q_h = \{ (\text{last}(s), \text{row}(s)) | s \in S \} \)
- \( Q_{h_0} = \{ o_0, \text{row}(o_0) \}, o_0 \in S \) is the trace consisting of the initial SUL output
- for \( s \in S, i \in \Sigma^1 \) and \( o \in \Sigma^O \) :
  - \( \delta_h((\text{last}(s), \text{row}(s)), (o, \text{row}(s \cdot i \cdot o))) = p \) if \( T(s \cdot i)(o) = p > 0 \)
- for \( s \in S, L_h((\text{last}(s), \text{row}(s))) = \text{last}(s) \)
Correctness & Termination. In the following, we will show that $L_{\text{mdp}}$ terminates and learns correct models, i.e. models that are output-distribution equivalent to the SUL. Like Angluin [4], we will show that derived hypotheses are consistent with queried information and that they are minimal with respect to the number of states. For the remainder of this section, let $M$ be the semantics of the MDP underlying the SUL and let $M = \text{can}(M)$ be the corresponding canonical MDP and let $\mathcal{H} = \langle Q, \Sigma^L, \Sigma^O, q_0, \delta, L \rangle$ denote hypotheses. The first two lemmas relate to observability of traces.

**Lemma 2.** For all $s \in \mathcal{T}S, o \in \Sigma^O, e \in \mathcal{CS} : M(s)(o) = 0 \Rightarrow M(s \cdot o \cdot e) = \bot$.

**Proof.** Let $\delta_M$ be the probabilistic transition relation of $M$. $M(s)(o) = 0$ with $s = t \cdot i$, for $i \in \Sigma^L$ implies that there is no state labelled $o$ reachable by executing $i$ in the state $\delta_M^L(t)$ (Def. 3), thus $\delta_M^L(t \cdot i \cdot o) = \delta_M^L(s \cdot o) = \bot$. By Def. 3, $M(s \cdot o \cdot i') = \bot$ for any $i'$. Due to prefix-closedness of $\text{dd}(M)$, we have $M(s \cdot o \cdot e) = \bot$ for all $e \in \mathcal{CS}$.

**Lemma 3.** Let $\langle S, E, T \rangle$ be a closed and consistent observation table. Then for $s \in S$ and $s \cdot o \in S \cup Lt(S)$ we have $T(s \cdot i)(o) > 0$.

**Proof.** The lemma states that traces labelling rows are observable. Algorithm 2 adds elements to $S$ and consequently $Lt(S)$ in two cases: (1) if an equivalence query returns a counterexample and (2) to make observation tables closed.

**Case 1.** Counterexamples $c \in \mathcal{T}S$ returned by equivalence queries $\text{eq}(\mathcal{H})$ satisfy $M(c) \neq \bot$ (see also Remark 1). In Sect. 3 of Algorithm 2 we add $t_p$ to $S$ for each $t_p \cdot i_p \in \text{prefixes}(c)$. Due to prefix-closedness of $\text{dd}(M)$, $M(t_p \cdot i_p) \neq \bot$ for all $t_p \cdot i_p \in \text{prefixes}(c)$, and therefore $M(s \cdot i)(o) = T(s \cdot i)(o) > 0$ for each added trace $t_p$ of the form $t_p = s \cdot i \cdot o$ with $i \in \Sigma^L$ and $o \in \Sigma^O$. The set $Lt(S)$ is implicitly extended by all observable extensions of added $t_p$. By this definition, $Lt(S)$ contains only traces $t = s \cdot i \cdot o$ such that $T(s \cdot i)(o) > 0$.

**Case 2.** If an observation table is not closed, we add traces from $Lt(S)$ to $S$. As noted above, all traces $t = s \cdot i \cdot o$ in $Lt(S)$ satisfy $T(s \cdot i)(o) > 0$. Consequently, all traces added to $S$ satisfy this property as well.

**Theorem 2 (Minimality).** Let $\langle S, E, T \rangle$ be a closed and consistent observation table and let $\mathcal{H} = \text{hyp}(S, E, T)$ be a hypothesis derived from that table with semantics $H$. Then $\mathcal{H}$ is consistent with $T$, that is, $\forall s \in (S \cup Lt(s)) \cdot E : T(s) = H(s)$, and any other MDP consistent with $T$ but inequivalent to $\mathcal{H}$ must have more states.

**Lemma 4.** Let $\langle S, E, T \rangle$ be a closed and consistent observation table. For $\mathcal{H} = \text{hyp}(S, E, T)$ and every $s \in S \cup Lt(S)$, we have $\delta^*(q_0, s) = \langle \text{last}(s), \text{row}(s) \rangle$.

**Proof.** Similarly to [4], we prove this by induction on the trace length $k$, i.e. the number of outputs in $s$. For $k = 1$, i.e. $s = o$, where $o$ is the initial output, we have $\delta^*(q_0, o) = \delta^*(\langle o, \text{row}(o) \rangle, o) = \langle o, \text{row}(o) \rangle$. 
Assume that for every \( s \in S \cup Lt(S) \) of length at most \( k \), \( \delta^*(q_0, s) = \langle \text{last}(s), \text{row}(s) \rangle \). Let \( t \in S \cup Lt(S) \) of length \( k + 1 \), i.e. \( t = s \cdot i \cdot o_t \), for \( s \in T R, i \in \Sigma^1, o_t \in \Sigma^0 \). If \( t \in Lt(S) \) then \( s \) must be in \( S \), and if \( t \in S \), then \( s \in S \) because \( S \) is prefix-closed.

\[
\delta^*(q_0, s \cdot i \cdot o_t) = \Delta(\delta^*(q_0, s), i, o_t)
\]

\[
= \Delta(\langle \text{last}(s), \text{row}(s) \rangle, i, o_t) \quad \text{(by induction hypothesis)}
\]

\[
= \langle q_t, \text{row}(s \cdot i \cdot o_t) \rangle \quad \text{(definition of } \Delta \text{)}
\]

if \( \delta(\langle \text{last}(s), \text{row}(s) \rangle, i)(\langle q_t, \text{row}(s \cdot i \cdot o_t) \rangle) > 0 \)

and \( L(\langle q_t, \text{row}(s \cdot i \cdot o_t) \rangle) = o_t \)

\( \delta(\langle \text{last}(s), \text{row}(s) \rangle, i)(\langle q_t, \text{row}(s \cdot i \cdot o_t) \rangle) > 0 \)

\( \iff T(s \cdot i)(o_t) > 0 \quad \text{(construction of } \delta \text{)} \)

\( \iff \text{true} \quad \text{(Lemma 3)} \)

\( L(\langle q_t, \text{row}(s \cdot i \cdot o_t) \rangle) = o_t \)

\( \iff \text{true} \quad \text{(construction of } L \text{)} \)

**Lemma 5.** Let \((S, E, T)\) be a closed and consistent observation table. Then \( \text{hyp}(S, E, T) \) is consistent with \( T \), i.e. for every \( s \in S \cup Lt(S) \) and \( e \in E \) we have \( T(s \cdot e) = H(s \cdot e) \).

**Proof.** We will prove this by induction on the length of \( e \), i.e. the number of inputs of \( e \). As induction hypothesis, we assume \( T(s \cdot e) = H(s \cdot e) \) for all \( s \in S \cup Lt(S) \) and \( e \in E \) of length at most \( k \). For the base case, we consider \( e \) consisting of a single input, i.e. \( e \in \Sigma^1 \). From Def. 3 we can derive that \( H(s \cdot i) \neq \bot \) if \( \delta^*(s) \neq \bot \), then we have:

\[
H(s \cdot i)(o) = \delta(\delta^*(s), i)(q) \text{ with } L(q) = o
\]

\[
= \delta(\langle \text{last}(s), \text{row}(s) \rangle, i)(q) \text{ with } L(q) = o
\]

\[
= \delta(\langle \text{last}(s), \text{row}(s) \rangle, i)(\langle o, \text{row}(s \cdot i \cdot o) \rangle) \quad \text{(hypothesis construction)}
\]

\[
= T(s \cdot i)(o) \quad \text{(hypothesis construction)}
\]

For the induction step, let \( e \in E \) be of length \( k + 1 \), thus it is of the form \( e = i \cdot o \cdot e_k \) for \( i \in \Sigma^1 \), \( o \in \Sigma^0 \), and due to suffix-closedness of \( E \), \( e_k \in E \). We have to show that \( T(s \cdot e) = H(s \cdot e) \) for \( s \in S \cup Lt(S) \). Let \( s' \in S \) such that \( \text{eqRow}_E(s, s') \), which exists due to observation table closedness. Traces \( s \) and \( s' \) lead to the same hypothesis state because:

\[
\delta^*(q_0, s) = \langle \text{last}(s), \text{row}(s) \rangle = \langle \text{last}(s'), \text{row}(s') \rangle = \delta^*(q_0, s')
\]

Thus, \( s \) and \( s' \) are \( H \)-equivalent and therefore \( H(s \cdot e) = H(s' \cdot e) \). Due to \( \text{eqRow}_E(s, s') \), \( T(s \cdot e) = T(s' \cdot e) \) and in combination:

\[
T(s \cdot e) = H(s \cdot e) \iff T(s' \cdot e) = H(s' \cdot e) \iff T(s' \cdot i \cdot o \cdot e_k) = H(s' \cdot i \cdot o \cdot e_k)
\]
Case 1. Suppose that $s' \cdot i \cdot o \in S \cup Lt(S)$. Then, $T(s' \cdot i \cdot o \cdot e_k) = H(s' \cdot i \cdot o \cdot e_k)$ holds by the induction hypothesis, as $e_k$ has length $k$.

Case 2. Suppose that $s' \cdot i \cdot o \notin S \cup Lt(S)$. Since $s' \in S$ and by the definition of $Lt(S)$, we have $odq(s' \cdot i)(o) = M(s' \cdot i)(o) = 0$. By Lemma 2, if follows that $M(s' \cdot i \cdot o \cdot e) = \perp$ for any continuation $e \in \mathcal{CS}$. As the observation table is filled via $odq$ we have $T(s' \cdot i \cdot o \cdot e_k) = odq(s' \cdot i \cdot o \cdot e_k) = M(s' \cdot i \cdot o \cdot e_k) = \perp$. By the induction base, we have $H(s' \cdot i) = T(s' \cdot i)$ for $i \in \Sigma$, thus $H(s' \cdot i)(o) = T(s' \cdot i)(o) = 0$. With Lemma 2, we can conclude $H(s' \cdot i \cdot o \cdot e_k) = \perp$.

In both cases, it holds that $H(s' \cdot i \cdot o \cdot e_k) = T(s' \cdot i \cdot o \cdot e_k)$ which is equivalent to $H(s \cdot e) = T(s \cdot e)$.

With Lemma 6, we have shown consistency between derived hypotheses and the queried information. Now, we show that hypotheses are minimal with respect to the number of states.

**Lemma 6.** Let $\langle S, E, T \rangle$ be a closed and consistent observation table and let $n$ be the number of different values for $\langle \text{last}(s), \text{row}(s) \rangle$, i.e. the number of states of hypothesis $\text{hyp}(S, E, T)$. Any MDP consistent with $T$ must have at least $n$ states.

**Proof.** Let $\mathcal{M}' = \langle Q', \Sigma', \Sigma^0, q_0', \delta', L' \rangle$ with semantics $M'$ be an MDP consistent with $T$. Let $s_1, s_2 \in S$ such that $\neg \text{eqRow}_e(s_1, s_2)$, then (1) $\text{last}(s_1) \neq \text{last}(s_2)$ or (2) $\text{row}(s_1) \neq \text{row}(s_2)$. If $\text{last}(s_1) \neq \text{last}(s_2)$, then $s_1$ and $s_2$ cannot reach the same state in $\mathcal{M}'$, because the states reached by $s_1$ and $s_2$ need to be labelled differently. If $\text{row}(s_1) \neq \text{row}(s_2)$, then there exists an $e \in E$ such that $M'(s_1 \cdot e) \neq M'(s_2 \cdot e)$, because $\mathcal{M}'$ is consistent with $T$. In this case $s_1$ and $s_2$ cannot reach the same state, as the observed future behaviour is different. Consequently, $\mathcal{M}'$ has at least $n$ states.

**Lemma 7.** Let $\langle S, E, T \rangle$ be a closed and consistent observation table and $\mathcal{H} = \text{hyp}(S, E, T)$ be a hypothesis with $n$ states derived from it. Any other MDP $\mathcal{M}' = \langle Q', \Sigma', \Sigma^0, q_0', \delta', L' \rangle$ with semantics $M'$ consistent with $T$, initial output $L'(q_0)$, and with $n$ or fewer states is isomorphic to $\text{hyp}(S, E, T)$.

**Proof.** From Lemma 6, it follows that $\mathcal{M}'$ has at least $n$ states, therefore we examine $\mathcal{M}'$ with exactly $n$ states. For each state of $\mathcal{H}$, i.e. each unique row labelled by $s \in S$, exists a unique state in $Q'$. We will now define a mapping $\phi$ from short traces to $Q'$ given by $\phi(\langle \text{last}(s), \text{row}(s) \rangle) = \delta^*(q_0', s)$ for $s$ in $S$. It is bijective and we will now show that it maps $q_0$ to $q_0'$, that it preserve the probabilistic transition relation and that it preserves labelling.

First, we start with the initial state and show $\phi(q_0) = q_0'$:

$$
\phi(q_0) = \phi(\langle o, \text{row}(o) \rangle) \quad \text{where } o \text{ is the initial output of the SUL}
$$

$$
= \delta^*(q_0', o)
$$

$$
= q_0' \quad \text{(definition of } \delta^*)
$$
For each \( s \) in \( S \), \( i \) in \( \Sigma^l \) and \( o \) in \( \Sigma^o \). We have:

\[
\delta((\text{last}(s), \text{row}(s)), i)((\text{last}(s \cdot i \cdot o), \text{row}(s \cdot i \cdot o))) = T(s \cdot i)(o) \quad \text{(hypothesis construction)}
\]

and

\[
\delta'(\phi((\text{last}(s), \text{row}(s))), i)(\phi((\text{last}(s \cdot i \cdot o), \text{row}(s \cdot i \cdot o)))) = \delta'(\delta^*(q^0, s), i)(\delta^*(q^0, s \cdot i \cdot o)) = M'(s \cdot i)(o) \quad \text{(Def. \ref{def:canon})}
\]

\[= T(s \cdot i)(o) \quad (\mathcal{M}' \text{ is consistent with } T)\]

Transition probabilities are preserved.

Finally, we show that labelling is preserved. For all \( s \) in \( S \):

\[
L'(\phi((\text{last}(s), \text{row}(s)))) = L'(\delta^*(q^0, s)) = \text{last}(s) \quad \text{(definition of } \delta^*)
\]

and

\[
L((\text{last}(s), \text{row}(s))) = \text{last}(s) \quad \text{(definition of } L, \text{ thus)}
\]

\[
L'(\phi((\text{last}(s), \text{row}(s)))) = L((\text{last}(s), \text{row}(s)))
\]

Labelling is preserved by the mapping \( \phi \).

**Theorem 3.** The algorithm \( L_{\text{mdp}}^* \) terminates and returns an MDP \( \mathcal{H} \) isomorphic to \( \mathcal{M} \), thus, it is minimal and also satisfies \( \mathcal{M} \equiv_{\text{eq}} \mathcal{H} \).

**Termination.** Let \( \langle S, E, T \rangle \) be a closed and consistent observation table and let \( c \in TS \) be a counterexample to equivalence between \( \mathcal{M} \) and hypothesis \( \text{hypo}(S, E, T) \) with semantics \( H \). Since \( c \) is a counterexample, \( M(c) \neq H(c) \). Now let \( \langle S', E', T' \rangle \) be an observation table extended by adding all prefix traces of \( c \) to \( S \) and (re-)establishing closedness and consistency. For \( \text{hypo}(S', E', T') = \mathcal{H}' \) with semantics \( H' \), we have \( T'(c) = M(c) \) due to output distribution queries. Since \( \mathcal{H}' \) is consistent with \( T' \), we have \( T'(c) = H'(c) = M(c) \). Hence, \( H'(c) \neq H(c) \), which shows that \( \mathcal{H}' \) is not equivalent to \( \mathcal{H} \), with \( c \) being a counterexample to equivalence. We do not remove elements from \( S, E, \) or \( T \), thus \( \mathcal{M}' \) is also consistent with \( T \). Therefore, \( \mathcal{M}' \) must have at least one state more than \( \mathcal{M} \) according to Theorem \ref{thm:canon}. It follows that each round of learning, which finds a counterexample, adds at least one state. Since Algorithm \ref{alg:canon} derives minimal hypotheses and \( \mathcal{M} \) can be modelled with finitely many states, there can only be finitely many rounds that find counterexamples. Hence, we terminate after a finite number of rounds, because Algorithm \ref{alg:canon} returns the final hypothesis as soon as no counterexample can be found via equivalence queries \( \text{eq} \).

**Correctness.** The algorithm terminates when the equivalence query \( \text{eq}(\mathcal{H}) \) does not find any new counterexample between the final hypothesis \( \mathcal{H} \) and \( \mathcal{M} \). Since there is no counterexample, we have \( \mathcal{H} \equiv_{\text{eq}} \mathcal{M} \). Theorem \ref{thm:canon} states that \( \mathcal{H} \) is minimal and \( \mathcal{M} = \text{can}(M) \) is consistent with \( T \), therefore it follows from Lemma \ref{lem:isom} that \( \mathcal{H} \) is isomorphic to \( \mathcal{M} \) the canonical MDP modelling the SUL.
4 Learning MDPs by Sampling

In this section, we introduce $L_{\text{mdp}}^*$, an approximate sampling-based learning method for MDPs based on $L_{\text{mdp}}^*$. In contrast to $L_{\text{mdp}}^*$, which requires exact information, we place weaker assumptions on the teacher. Here, we do not require exact output distribution queries and equivalence queries, but we approximate these queries via sampling, i.e. testing. Since large amounts of data are required to produce accurate models, we also alter the learning algorithm structure in contrast to the previous section. The sampling-based $L_{\text{mdp}}^*$ allows to derive an approximate model at any time, unlike most other $L^*$-based algorithms. Therefore, this section is split into three parts: first, we present a sampling-based interface between teacher and learner, as well as the interface between teacher and SUL. The second and third part describe the adapted learner and the implementation of the teacher, respectively.

Queries. The sampling-based teacher maintains a multiset of traces $S$ for the estimation of output distributions that grows during learning. It offers an equivalence query and three queries relating to output distributions and samples $S$.

- **frequency** ($fq$): given a test sequence $s \in T S$, $fq(s): \Sigma^O \to \mathbb{N}_0$ are output frequencies observed after $s$, where $fq(s)(o) = S(s \cdot o)$ for $o \in \Sigma^O$.
- **complete** ($cq$): given a test sequence $s \in T S$, $cq(s)$ returns true if sufficient information is available to estimate an output distribution from $fq(s)$; returns false otherwise.
- **refine** ($rfq$): instructs the teacher to refine its knowledge of the SUL by testing it directed towards rarely observed samples. Traces sampled by $rfq$ are added to $S$, increasing the accuracy of subsequent probability estimations.
- **equivalence** ($eq$): given a hypothesis $H$, $eq$ tests for output-distribution equivalence between the SUL and $H$; returns a counterexample from $TS$ showing non-equivalence, or returns none if no counterexample was found.

The sampling-based teacher thus needs to implement two different testing strategies, one for increasing accuracy of probability estimations along observed traces (refine) and one for finding discrepancies between a hypothesis and the SUL (equivalence). The frequency query and the complete query are used for hypothesis construction by the learner.

To test the SUL, we require the ability to (1) reset it and to (2) perform an input action and observe the produced output. For the remainder of this section, let $M = (Q, \Sigma^I, \Sigma^O, q_0, \delta, L)$ be the MDP underlying the SUL with semantics $M$. Based on $q \in Q$, the current execution state of $M$, we define two operations available to the teacher:

- **reset** resets $M$ to the initial state, i.e. $q = q_0$, and returns $L(q_0)$.
- **step** takes an input $i \in \Sigma^I$ and selects a new state $q'$ according to $\delta(q, i)(q')$.

The step operation then updates the execution state to $q'$ and returns $L(q')$.

Note that we consider $M$ to be a black box, i.e. its structure and transition probabilities are assumed to be unknown. We are only able to perform inputs
and observe output labels, e.g., we observe the initial SUL output \( L(q_0) \) after performing a reset.

### 4.1 Learner Implementation

**Observation Table.** The sampling-based learner is also based on observation tables, therefore we use the same terminology as in Sect. 3.

**Definition 8 (Sampling-based Observation Table).** An observation table is a tuple \( \langle S, E, \hat{T} \rangle \), consisting of a prefix-closed set of traces \( S \subseteq T^R \), a suffix-closed set of continuation sequences \( E \subseteq CS \), and a mapping \( \hat{T} : (S \cup Lt(S)) \cdot E \rightarrow (\Sigma^O \rightarrow N_0) \), where \( Lt(S) = \{ s \cdot i \cdot o \mid s \in S, i \in \Sigma^I, o \in \Sigma^O \mid f(q)(s) > 0 \} \).

An observation table can be represented by a two-dimensional array, containing rows labelled with elements of \( S \) and \( Lt(S) \) and columns labelled by \( E \). Each table cell corresponds to a sequence \( c = s \cdot e \), where \( s \in S \cup Lt(S) \) is the row label of the cell and \( e \in E \) is the column label. It stores queried output frequency counts \( \hat{T}(c) = f(q)(c) \). To represent the content of rows, we define the function \( row \) on \( S \cup Lt(S) \) by \( row(s)(e) = \hat{T}(s \cdot e) \). The traces in \( Lt(S) \) are input-output-extensions of \( S \) which have been observed so far. We refer to traces in \( S/Lt(S) \) as short/long traces. Analogously, we refer to rows labelled by corresponding traces as short and long rows.

As in Sect. 3, we identify states with traces reaching these states. These traces are stored in the prefix-closed set \( S \). We distinguish states by their future behaviour in response to sequences in \( E \). We initially set \( S = \{ L(q_0) \} \), where \( L(q_0) \) is the initial output of the SUL, and \( E = \Sigma^I \). Long traces, as extensions of access sequences in \( S \), serve to define transitions of hypotheses.

**Hypothesis Construction.** As in Sect. 3 observation tables need to be closed and consistent for a hypothesis to be constructed. Unlike before, we do not have exact information to determine equivalence of rows. We need to statistically test if rows are different. First, we give a condition determining whether two sequences lead to statistically different observations, i.e. the corresponding output frequency samples come from different distributions. This condition is based on Hoeffding bounds which are also used by Carrasco and Oncina [12]. We further apply this condition in a check for approximate equivalence between cells and extend this check to rows. Using similar terminology to [12], we refer to such checks as compatibility checks and we say that two cells/rows are compatible if we determine that they are not statistically different. These notions of compatibility serve as the basis for slightly adapted definitions of closedness and consistency.

**Definition 9 (Different).** Two sequences \( s \) and \( s' \) in \( T^S \) produce statistically different output distributions with respect to \( f : T^S \rightarrow (\Sigma^O \rightarrow N_0) \), denoted \( diff_f(s, s') \), iff (1) \( cq(s) \land cq(s') \land n_1 > 0 \land n_2 > 0 \) where \( n_1 = \sum_{o \in \Sigma^O} f(s)(o) \), \( n_2 = \sum_{o \in \Sigma^O} f(s')(o) \), and (2) one of the following conditions holds:
Algorithm 3 Creating compatibility classes

1: for all \( s \in S \) do
2: \[ \text{rank}(s) \leftarrow \sum_{i \in \Sigma^1} \sum_{o \in \Sigma^O} \hat{T}(s \cdot i)(o) \]
3: unpartitioned \( \leftarrow S \), \( R \leftarrow \emptyset \)
4: while unpartitioned \( \neq \emptyset \) do
5: \[ r \leftarrow m \text{ where } m \in \text{unpartitioned} \text{ with largest rank}(m) \]
6: \[ R \leftarrow R \cup \{r\} \]
7: \[ cg(r) \leftarrow \{s \in \text{unpartitioned} | \text{compatible}_E(s, r)\} \]
8: for all \( s \in cg(r) \) do
9: \[ \text{rep}(s) \leftarrow r \]
10: \[ \text{unpartitioned} \leftarrow \text{unpartitioned} \setminus cg(r) \]

2a. \( \exists \alpha \in \Sigma^O : \neg(f(s)(o) > 0 \Leftrightarrow f(s')(o) > 0) \), or
2b. \( \exists \alpha \in \Sigma^O : \left| \frac{f(s)(o)}{n_1} - \frac{f(s')(o)}{n_2} \right| > \left( \sqrt{\frac{1}{n_1}} + \sqrt{\frac{1}{n_2}} \right) \cdot \sqrt{\frac{1}{2} \ln \frac{2}{\alpha}} \), where \( \alpha \) specifies the confidence level \((1-\alpha)^2\) for testing each \( o \) separately based on a Hoeffding bound \([12,22]\).

Definition 10 (Compatible). Two cells labelled by \( e = s \cdot e \) and \( e' = s' \cdot e' \) are compatible, denoted \( \text{compatible}(c, c') \), iff \( \neg \text{diff}(c, c') \). Two rows labelled by \( s \) and \( s' \) are compatible, denoted \( \text{compatible}_E(s, s') \) iff last(\( s \)) = last(\( s' \)) and the cells corresponding to all \( e \in E \) are compatible, i.e. \( \text{compatible}(s \cdot e, s' \cdot e) \).

Compatibility Classes. In Sect. 3 we formed equivalence classes of traces with respect to \( \text{eqRow}_E \) creating one hypothesis state per equivalence class. Now we partition rows labelled by \( s \) based on compatibility. Compatibility given by Def. 10 however, is not an equivalence relation, as it is not transitive in general. As a result, we cannot simply create equivalence classes. We apply the heuristic implemented by Algorithm 3 to partition \( S \).

First, we assign a rank to each trace in \( S \). Then, we partition \( S \) by iteratively selecting the trace \( r \) with the largest rank and computing a compatibility class \( cg(r) \) for \( r \). The trace \( r \) is the (canonical) representative for \( s \) in \( cg(r) \), which we denote by \( \text{rep}(s) \) (Line 9). Each \( r \) is stored in the set of representative traces \( R \). In contrast to equivalence classes, elements in a compatibility class need not be pairwise compatible and an \( s \) may be compatible to multiple representatives, where the unique representative \( \text{rep}(s) \) of \( s \) has the largest rank. However, in the limit \( \text{compatible}_E \) based on Hoeffding bounds converges to an equivalence relation \([12]\) and therefore compatibility classes are equivalence classes in the limit (see Sect. 4.6).

Definition 11 (Sampling Closedness). An observation table \( \langle S, E, \hat{T} \rangle \) is closed if for all \( l \in Lt(S) \) there is a representative \( s \in R \) with \( \text{compatible}_E(l, s) \).

Definition 12 (Sampling Consistency). An observation table \( \langle S, E, \hat{T} \rangle \) is consistent if for all compatible pairs of short traces \( s, s' \) in \( S \) and all input-output pairs \( i \cdot o \in \Sigma^1 \cdot \Sigma^O \), we have that (1) at least one of their extensions has not been observed yet, i.e. \( \hat{T}(s \cdot i)(o) = 0 \) or \( \hat{T}(s' \cdot i)(o) = 0 \), or (2) both extensions are compatible, i.e. \( \text{compatible}_E(s \cdot i \cdot o, s' \cdot i \cdot o) \).
Note that the first condition of consistency may be satisfied because of incomplete information. Given a closed and consistent observation table \( \langle S, E, \hat{T} \rangle \), we derive hypothesis MDP \( H = \text{hyp}(S, E, \hat{T}) \) through the steps below. Note that extensions \( s \cdot i \cdot o \) of \( s \) in \( S \) define transitions. Some extensions may have few observations, i.e. \( \hat{T}(s \cdot i) \) is low and \( \text{cq}(s \cdot i) = \text{false} \). In case of such uncertainties, we add transitions to a special sink state labelled by chaos, an output not in the original alphabet\(^3\). A hypothesis is \( H = \langle Q_h, \Sigma^I, \Sigma^O \cup \{\text{chaos}\}, q_{0h}, \delta_h, L_h \rangle \) where:

- representatives for long traces \( l \in L(t(S)) \) are given by (see Algorithm\(^3\)):
  \[ 
  \text{rep}(l) = r \text{ where } r \in \{r' \in R \mid \text{compatible}_E(l, r') \} \text{ with largest rank}(r) 
  \]
- \( Q_h = \{ \langle \text{last}(s), \text{row}(s) \rangle \mid s \in R \} \cup \{q_{\text{chaos}}\} \)
  - for \( q = \langle o, \text{row}(s) \rangle \in Q_h \setminus \{q_{\text{chaos}}\} \), \( L_h(q) = o \)
  - for \( q_{\text{chaos}} \): \( L_h(q_{\text{chaos}}) = \text{chaos} \) and for all \( i \in \Sigma^I \): \( \delta_h(q_{\text{chaos}}, i)(q_{\text{chaos}}) = 1 \)
- \( q_{0h} = \langle L(q_0), \text{row}(L(q_0)) \rangle \)
- for \( q = \langle o, \text{row}(s) \rangle \in Q_h \setminus \{q_{\text{chaos}}\} \) and \( i \in \Sigma^I \) (note that \( \Sigma^I \subseteq E \)):
  1. If \( \neg \text{cq}(s \cdot i) \): \( \delta(q, i)(q_{\text{chaos}}) = 1 \), i.e. move to chaos
  2. Otherwise estimate a distribution \( \mu = \delta_h(q, i) \) over the successor states:
    \[
    \text{for } o \in \Sigma^O \text{ with } \hat{T}(s \cdot i)(o) > 0; \mu(\langle o, \text{row}(\text{rep}(s \cdot i \cdot o)) \rangle) = \frac{\hat{T}(s \cdot i)(o)}{\sum_{o' \in \Sigma^O} \hat{T}(s \cdot i)(o')}
    \]

**Updating the Observation Table.** Analogously to Sect.\(^4\) we make observation tables closed by adding new short rows and we establish consistency by adding new columns. While Algorithm\(^2\) needs to fill the observation table after executing \text{MAKECLOSEDANDCONSISTENT}, this is not required in the sampling-based setting due to the adapted notions of closedness and consistency.

**Trimming the Observation Table.** Observation table size greatly affects learning performance, therefore it is common to avoid adding redundant information\(^2\). Due to inexact information, this is hard to apply in a stochastic setting. We instead remove rows via a function \text{TRIM}, once we are certain that this does not change the hypothesis. Given an observation table \( \langle S, E, \hat{T} \rangle \), we remove \( s \) and all \( s' \) such that \( s \ll s' \) from \( S \) if:

1. there is exactly one \( r \in R \) such that \( \text{compatible}_E(s, r) \)
2. \( s \notin R \) and \( \forall r \in R : \neg(s \ll r) \)
3. and \( \forall s' \in S, i \in \Sigma^I, \text{ with } s \ll s' : \text{diff}_{\text{fq}}(s' \cdot i, r \cdot i) = \text{false} \), where \( r \in R \) such that \( \langle \text{last}(r), \text{row}(r) \rangle = \delta_h(r) = \delta_h(s') \), and \( \delta_h \) is the transition relation of \( \text{hyp}(S, E, \hat{T}) \).

The first condition is motivated by the observation that if \( s \) is compatible to exactly one \( r \), then all extensions of \( s \) can be assumed to reach the same states as the extensions of \( r \), i.e. we do not need to store \( s \) in the observation table. The other conditions make sure that we do not remove required rows, because of a spurious compatibility check in the first condition. The third condition is related to the implementation of equivalence queries and basically checks if an extension \( s' \) reveals a difference between observed frequencies (queried via \( \text{fq} \))

\(^3\) This is inspired by the introduction of chaos states in \text{ioco}-based learning\(^4\).
Algorithm 4 The main algorithm implementing $L^*_\text{MDP}$

| Line | Description |
|------|-------------|
| 1:   | $S \leftarrow \{L(q_0)\}$, $E \leftarrow \Sigma^1$, $\hat{T} \leftarrow \{}$ \hspace{1cm} $\triangleright$ initialise observation table |
| 2:   | perform $\text{rfq}(S, E, \hat{T})$ \hspace{1cm} $\triangleright$ sample traces for initial observation table |
| 3:   | for all $s \in S \cup \text{Lt}(S)$, $e \in E$ do $\hat{T}(s \cdot e) \leftarrow \text{fq}(s \cdot e)$ \hspace{1cm} $\triangleright$ update observation table with frequency information |
| 4:   | $\hat{T}(s \cdot e) \leftarrow \text{fq}(s \cdot e)$ \hspace{1cm} $\triangleright$ update observation table with frequency information |
| 5:   | $\text{round} \leftarrow 0$ |
| 6:   | repeat |
| 7:   | $\text{round} \leftarrow \text{round} + 1$ |
| 8:   | while $(S, E, \hat{T})$ not closed or not consistent do |
| 9:   | $(S, E, \hat{T}) \leftarrow \text{MakeClosedAndConsistent}((S, E, \hat{T}))$ \hspace{1cm} $\triangleright$ create hypothesis |
| 10:  | $\text{H} \leftarrow \text{hyp}(S, E, \hat{T})$ \hspace{1cm} $\triangleright$ remove rows that are not needed |
| 11:  | $\text{cex} \leftarrow \text{eq}(\text{H})$ \hspace{1cm} $\triangleright$ we found a counterexample |
| 12:  | if $\text{cex} \neq \text{none}$ then $\triangleright$ we found a counterexample |
| 13:  | for all $t \cdot i \in \text{prefixes(} \text{cex} \text{)}$ with $i \in \Sigma^1$ do $\triangleright$ add all prefixes of the counterexample |
| 14:  | $S \leftarrow S \cup \{t\}$ \hspace{1cm} $\triangleright$ add all prefixes of the counterexample |
| 15:  | perform $\text{rfq}(S, E, \hat{T})$ \hspace{1cm} $\triangleright$ sample traces to refine knowledge about SUL |
| 16:  | for all $s \in \text{S} \cup \text{Lt}(\text{S}), e \in E$ do $\hat{T}(s \cdot e) \leftarrow \text{fq}(s \cdot e)$ \hspace{1cm} $\triangleright$ update observation table with frequency information |
| 17:  | until $\text{stop}((S, E, \hat{T}), \text{H}, \text{round})$ |
| 18:  | $\text{return} \ \text{hyp}(S, E, \hat{T})$ \hspace{1cm} $\triangleright$ output final hypothesis |

and frequencies used for hypothesis construction. Note that removed rows do not affect hypothesis construction.

**Learning Algorithm.** Algorithm 4 implements $L^*_\text{MDP}$. It first initialises an observation table $(S, E, \hat{T})$ with the initial SUL output as first row and with the inputs $\Sigma^1$ as columns (Line 1). Lines 2 to 4 perform a refine query and then update $(S, E, \hat{T})$, which corresponds to output distribution queries in $L^*_\text{MDP}$. Here, the teacher resamples the only known trace $L(q_0)$. Resampling that trace consists of observing $L(q_0)$, performing some input and observing another output.

After that, we perform Lines 6 to 19 until a stopping criterion is reached. We establish closedness and consistency of $(S, E, \hat{T})$ in Line 9 to build a hypothesis $\text{H}$ in Line 10. After that, we remove redundant rows of the observation table via $\text{TRIM}$ in Line 11. Then, we perform an equivalence query, testing for equivalence between $\text{SUL}$ and $\text{H}$. If we find a counterexample, we add all its prefix traces as rows to the observation table like in $L^*_\text{MDP}$. Finally, we sample new system traces via $\text{rfq}$ to gain more accurate information about the SUL (Lines 10 to 18). Once we stop, we output the final hypothesis.

**Stopping.** $L^*_\text{MDP}$ and deterministic automata learning usually stop learning once equivalence between the learned hypothesis and the SUL is achieved, i.e. no counterexample can be found. Here, we employ a different stopping criterion, because equivalence can hardly be achieved via sampling. Furthermore, we may wish to carry on resampling via $\text{rfq}$ although we did not find a counterexample. Resampling may improve accuracy of a hypothesis which is beneficial for the test-case generation in subsequent equivalence queries.
Our stopping criterion takes uncertainty in compatibility checks into account. As previously noted, rows may be compatible to multiple other rows. In particular, a row labelled by $s$ may be compatible to multiple representatives, i.e. we are not certain which state is reached by the trace $s$. We address this issue by stopping based on the ratio $r_{\text{unamb}}$ of unambiguous traces to all traces, which we compute by:

$$r_{\text{unamb}} = \frac{|\{s \in S \cup \mathit{Lt}(S) : \text{compRep}(s) = 1\}|}{|S \cup \mathit{Lt}(S)|}$$

where $\text{compRep}(s) = |\{r \in R : \text{compatible}_E(s, r)\}|$

More concretely, we stop if:

1.a. at least $r_{\text{min}}$ rounds have been executed and
1.b. the chaos state $q_{\text{chaos}}$ is unreachable and
1.c. and $r_{\text{unamb}} \geq t_{\text{unamb}}$, where $t_{\text{unamb}}$ is a user-defined threshold, or
2.a. alternatively we stop after a maximum number of rounds $r_{\text{max}}$.

### 4.2 Teacher Implementation

In the following, we describe the implementation of each of the four queries provided by the teacher. Recall that we interact with the SUL $M$ (see Sect. 3).

**Frequency Query.** The teacher keeps track of a multiset of sampled system traces $S$. Whenever a new a trace is added, all its prefixes are added as well, as they have also been observed. Therefore, we have for $t \in T_R, t' \in \text{prefixes}(t) : S(t) \leq S(t')$. The frequency query $\text{fq}(s) : \Sigma^O \rightarrow \mathbb{N}_0$ for $s \in TS$ returns output frequencies observed after $s$:

$$\forall o \in \Sigma^O : \text{fq}(s)(o) = S(s \cdot o)$$

**Complete Query.** Trace frequencies retrieved via $\text{fq}$ are generally used to compute empirical output distributions $\mu$ following a sequence $s$ in $TS$, i.e. the learner computes $\mu(o) = \frac{\text{fq}(s)(o)}{\sum_{o' \in \Sigma^O} \text{fq}(s)(o')}$ to approximate $M(s)(o)$. The complete query $\text{cq}$ takes a sequence $s$ as input and signals whether $s$ should be used to approximate $M(s)$, e.g. to perform statistical tests. We base $\text{cq}$ on a threshold $n_c > 0$ by defining:

$$\text{cq}(s) = \begin{cases} 
\text{true} & \text{if } \sum_{o \in \Sigma^O} S(s \cdot o) \geq n_c \\
\text{true} & \text{if } \exists s', o, i : \text{s.t. } s' \cdot o \cdot i \ll s \land \text{cq}(s') \land S(s \cdot o) = 0 \\
\text{false} & \text{otherwise}
\end{cases}$$

---

4 This query serves a similar role as in [13].
Algorithm 5 Refine query

1: rare ← \{s | s ∈ (S ∪ Lt(S)) ∗ E : ¬cq(s)\} \Comment{select incomplete sequences}
2: trie ← BUILD_TREE(rare) \Comment{build trie}
3: for i ← 1 to n_sample do \Comment{collect n_sample new samples}
4: new_trace ← SAMPLE_SUL(trie) \Comment{new trace}
5: S ← S ∪ \{new_trace\} \Comment{add new trace}
6: function SAMPLE_SUL(trie)
7: node ← root(trie) \Comment{initialise SUL and observe initial output}
8: loop \Comment{loop}
9: input ← randSel({i ∈ ΣI | ∃o ∈ ΣO, n : node \overset{i}{\to} n}) \Comment{random input}
10: output ← step(i) \Comment{execute SUL and observe output}
11: trace ← trace · i · o \Comment{did we leave the trie?}
12: if trace ∉ trie or trace labels leaf then
13: return trace \Comment{move in trie}
14: node' ← n with node \overset{i}{\to} n \Comment{did we leave the trie?}
15: node ← node'
16: end loop

Note that for a complete s, all prefixes of s are also complete. Additionally, if cq(s), we assume that we have seen all extensions of s; therefore, we set for each o with S(s · o) = 0 all extensions of s · o to be complete (second clause). The threshold n_c is user-specifiable in our implementation.

Refine Query. Refine queries serve the purpose of refining our knowledge about output distributions along previously observed traces. Therefore, we select rarely observed traces and resample them. We implemented this through the procedure outlined in Algorithm 5.

First, we build a trie from rarely observed traces (Lines 1 and 2), where edges are labelled by input-output pairs and nodes are labelled by traces reaching the nodes. This trie is then used for directed online-testing of the SUL via SAMPLE_SUL (Lines 6 to 16) with the goal of reaching a leaf of the trie. In this way, we create n_sample new samples and add them to the multiset of samples S.

Equivalence Query. Equivalence queries are often implemented via (conformance) testing in active automata [23], e.g., via the W-method [16] method for deterministic models. Such testing techniques generally execute some test suite to find counterexamples to conformance between a model and the SUL. In our setup, a counterexample is a test sequence inducing a different output distribution in the hypothesis H than in the SUL. Since we cannot directly observe those distributions, we apply two strategies to find counterexamples during equivalence queries. First, we search for counterexamples with respect to the structure of H via testing. Second, we check for statistical conformance between all traces S collected so far and H, which allows us to detect incorrect output distributions.

Note that all traces to the state q_{chaos} are guaranteed to be counterexamples, as chaos is not part of the original output alphabet Σ_O. For this reason, we do not search for other counterexamples if q_{chaos} is reachable in H. In slight abuse of terminology, we implement this by returning none from eq(H). \text{L^*_mdp} in Algorithm 4 will then issue further \text{rfq} queries, lowering uncertainty about state transitions, which in turn causes q_{chaos} to be unreachable eventually.
Testing of Structure. Our goal in testing is to sample a trace of the SUL that is not observable on the hypothesis. For that, we adapted a randomised testing strategy from Mealy machines to MDPs, which proved effective in previous work [2]. In this work, we generated test cases for active automata learning by interleaving random walks in hypotheses with paths leading to randomly chosen transitions. By generating many of these tests, we aim at covering hypotheses adequately, while exploring new parts of SUL’s state space through random testing. Here, we aim at covering randomly chosen states and apply an online testing procedure, as the SUL is stochastic. This procedure is outlined in Algorithm 6.

The algorithm takes a hypothesis and qSched as input, where qSched is a mapping from states to schedulers. Given q ∈ Q, qSched(q) is a scheduler maximising the probability of reaching q, i.e. it selects inputs optimally with respect to reachability of q. For optimal reachability, there exist schedulers that are memoryless and deterministic [19], which means that they take only the last state in the current execution path into account and that input choices are not probabilistic. Therefore, a scheduler qSched(q) is a function s : Q → ΣI. In Algorithm 6, we start by randomly choosing a target state qtarget from the states reachable from the initial state (Line 3), which are given by reachable(Q, qcurr). Then, we execute the SUL, either with random inputs (Line 6) or with inputs leading to the target (Line 8), which are computed using schedulers. If we observe an output which is not possible in the hypothesis, we return a counterexample (Line 12), alternatively we may stop with probability pstop (Line 15). If we reach the target or it becomes unreachable, we simply choose a new target state (Line 17).

For each equivalence query, we repeat Algorithm 6 up to ntest times and report the first counterexample we find. In case we find a counterexample c, we resample it up to nretest times or until cq(c), to get more accurate information about it.

Algorithm 6 State-coverage-based testing for counterexample detection

| Input: | H = (Q, ΣI, ΣO, q0, δ, L), schedulers qSched |
|--------|------------------------------------------------|
| Output: | counterexample test sequence s ∈ TS or none |
| 1: | qcurr ← q0 >> current state |
| 2: | trace ← reset |
| 3: | qtarget ← randSel(reachable(Q, qcurr)) >> choose a target state |
| 4: | loop |
| 5: | if coinFlip(prand) then |
| 6: | in ← randSel(ΣI) >> next input leads towards target |
| 7: | else |
| 8: | in ← qSched(qtarget) >> random next input |
| 9: | out ← step(in) >> perform input |
| 10: | qcurr ← ∆(qcurr, in · out) >> output not possible in hypothesis |
| 11: | return trace · in >> return counterexample |
| 12: | qcurr ← qtarget >> if qcurr = ⊥ then |
| 13: | trace ← trace · in · out |
| 14: | if coinFlip(pstop) then |
| 15: | return none >> stop with probability pstop |
| 16: | if qcurr = qtarget or qtarget ∉ reachable(Q, qcurr) then |
| 17: | qtarget ← randSel(reachable(Q, qcurr)) >> choose new target |

Testing of Structure. Our goal in testing is to sample a trace of the SUL that is not observable on the hypothesis. For that, we adapted a randomised testing strategy from Mealy machines to MDPs, which proved effective in previous work [2]. In this work, we generated test cases for active automata learning by interleaving random walks in hypotheses with paths leading to randomly chosen transitions. By generating many of these tests, we aim at covering hypotheses adequately, while exploring new parts of SUL’s state space through random testing. Here, we aim at covering randomly chosen states and apply an online testing procedure, as the SUL is stochastic. This procedure is outlined in Algorithm 6.

The algorithm takes a hypothesis and qSched as input, where qSched is a mapping from states to schedulers. Given q ∈ Q, qSched(q) is a scheduler maximising the probability of reaching q, i.e. it selects inputs optimally with respect to reachability of q. For optimal reachability, there exist schedulers that are memoryless and deterministic [19], which means that they take only the last state in the current execution path into account and that input choices are not probabilistic. Therefore, a scheduler qSched(q) is a function s : Q → ΣI. In Algorithm 6, we start by randomly choosing a target state qtarget from the states reachable from the initial state (Line 3), which are given by reachable(Q, qcurr). Then, we execute the SUL, either with random inputs (Line 6) or with inputs leading to the target (Line 8), which are computed using schedulers. If we observe an output which is not possible in the hypothesis, we return a counterexample (Line 12), alternatively we may stop with probability pstop (Line 15). If we reach the target or it becomes unreachable, we simply choose a new target state (Line 17).

For each equivalence query, we repeat Algorithm 6 up to ntest times and report the first counterexample we find. In case we find a counterexample c, we resample it up to nretest times or until cq(c), to get more accurate information about it.
Checking Conformance to $S$. For each sequence $t \cdot i \in TS$ with $i \in \Sigma^I$ such that $\text{cq}(t \cdot i)$, we check for consistency between the information stored in $S$ and the hypothesis $\mathcal{H}$ by evaluating two conditions:

1. Is $t$ observable in $\mathcal{H}$? If it is not, then we determine the longest observable prefix $t'$ of $t$ such that $t' \cdot i' \cdot v = t$, where $i'$ is a single input, and return $t' \cdot i'$ as counterexample from $\text{eq}(\mathcal{H})$.
2. Otherwise we determine $q = \langle o, \text{row}(r) \rangle$ reached by $t$ in $\mathcal{H}$, where $r \in R$, and return $t \cdot i$ as counterexample if $\text{diff}_f(t \cdot i, r \cdot i)$ is true. This statistical check approximates the comparison $M(t \cdot i) \neq M(r \cdot i)$, to check if $t \equiv_M r$. Therefore, it checks implicitly $M(t \cdot i) \neq H(t \cdot i)$, as $t \equiv_H r$.

4.3 Convergence of $L^\ast_{mdp}$

In the following, we will show that the sampling-based $L^\ast_{mdp}$ learns the correct MDP. Based on the notion of language identification in grammar inference [21], we describe our goal as producing an MDP isomorphic to the canonical MDP modelling the SUL with probability one in the limit. To show identification in the limit, we introduce slight simplifications. Firstly, we disable trimming of the observation table (see Sect. 4.1), i.e. we do not remove rows. Second, we set $p_{\text{rand}} = 1$ for equivalence testing and we do not stop at the first detected difference between SUL and hypothesis, but solely based on a $p_{\text{stop}} < 1$; i.e. all input choices are uniformly randomly and the length of each test is geometrically distributed with $p_{\text{stop}}$. This is motivated by the common assumption that sampling distributions do not change during learning [21]. Third, we change the function $\text{rank}$ in Algorithm 3 to assign ranks based on a lexicographic ordering of traces instead of a rank based on observed frequencies, such that the trace consisting only of the initial SUL output has the largest rank. We actually implemented both types of rank functions and found that the frequency-based function led to better accuracy, but would require more complex proofs. We let the number of samples for learning approach infinity, therefore we do not use a stopping criterion. Finally, we concretely instantiate $\text{cq}$ by setting $n_c = 1$, since $n_c$ is only relevant for applications in practice.

Proof Structure. We show convergence in two major steps: (1) we show that the hypothesis structure derived from a sampling-based observation table converges to the hypothesis structure derived from the corresponding observation table with exact information. (2) Then, we show that if counterexamples exist, we will eventually find them. Through that, we eventually arrive at a hypothesis with the same structure as the canonical MDP $\text{can}(M)$, where $M$ is the SUL semantics. Given a hypothesis with correct structure, it follows by the law of large numbers that the estimated transition probabilities converge to true probabilities, thus the hypotheses converge to an MDP isomorphic to $\text{can}(M)$.

A key point of the proofs concerns the convergence of statistical test applied by $\text{diff}_f$, which is based on Hoeffding bounds [22]. With regard to that, we apply similar arguments as Carrasco and Oncina [12, p.11-13 & Appendix]. Given
convergence of \textit{diff}, we also rely on the convergence of the exact learning algorithm \( L_{\text{new}}^* \) discussed in Sect. 3. Another important point is that the shortest traces in each equivalence class of \( S/\equiv_M \) do not form loops in \( \text{can}(M) \). Hence, there are finitely many such traces. Furthermore, for a given \( \text{can}(M) \) and some hypothesis MDP, the shortest counterexample has bounded length, therefore it suffices to check finitely many test sequences to check for overall equivalence.

**Auxiliary Definitions & Notation.** We show convergence in the limit of the number of sampled system traces \( n \). We take \( n \) into account through a data-dependent \( \alpha_n \) for the Hoeffding bounds used by \textit{diff} defined in Def.\[30\]. More concretely, let \( \alpha_n = \frac{1}{n^r} \) for \( r > 2 \) as used by Mao et al.\[30\], which implies \( \sum_n \alpha_n n < \infty \). For the remainder of this section, let \( \langle S_n, E_n, \hat{T}_n \rangle \) be the closed and consistent observation table containing the first \( n \) samples stored by the teacher in the multiset \( S_n \). Furthermore, let \( H_n \) be the hypothesis \( \text{hyp}(S_n, E_n, \hat{T}_n) \), let the semantics of the SUL be \( M \) and let \( M \) be the canonical MDP \( \text{can}(M) \). We say that two MDPs have the same structure, if their underlying graphs are isomorphic, i.e. exact transition probabilities may be different.

**Theorem 4 (Convergence).** Given a data-dependent \( \alpha_n = \frac{1}{n^r} \) for \( r > 2 \), such that \( \sum_n \alpha_n n < \infty \), then with probability one, the hypothesis \( H_n \) is isomorphic to \( M \), except for finitely many \( n \).

Hence, we learn an MDP that is minimal with respect to the number of states and output-distribution equivalent to the SUL.

**Hoeffding-Bound-Based Difference Check.** First, we briefly discuss the Hoeffding-bound-based test applied by \textit{diff}. Recall, that for two test sequences \( s \) and \( s' \), we test for each \( o \in \Sigma^O \) if the probability \( p \) for observing \( o \) after \( s \) is different than the probability \( p' \) for observing \( o \) after \( s' \). This is implemented through:

\[
\exists o \in \Sigma^O : \left| \frac{f(s)(o)}{n_1} - \frac{f(s')(o)}{n_2} \right| > \left( \sqrt{\frac{1}{n_1}} + \sqrt{\frac{1}{n_2}} \right) \cdot \sqrt{\frac{1}{2} \ln \frac{2}{\alpha(n_1, n_2)}} = \epsilon_\alpha(n_1, n_2)
\]

As pointed out by Carrasco and Oncina \[12\] p.11-13 \& Appendix], this test works with confidence level above \((1 - \alpha)^2\) and for large enough \( n_1 \) and \( n_2 \) it tests for difference and equivalence of \( p \) and \( p' \). More concretely, for convergence, \( n_1 \) and \( n_2 \) must be such that \( 2\epsilon_\alpha(n_1, n_2) \) is smaller than the smallest absolute difference between any two different \( p \) and \( p' \). As our data-dependent \( \alpha_n \) decreases only polynomially, \( \epsilon_\alpha(n_1, n_2) \) tends to zero for increasing \( n_1 \) and \( n_2 \). Hence, the test implemented by \textit{diff} converges to an exact comparison between \( p \) and \( p' \).

In the remainder of the paper, we ignore Condition 2.a for \textit{diff}, which checks if the sampled distributions have the same support. By applying a data-dependent \( \alpha_n \), as defined above, Condition 2.b converges to an exact comparison between output distributions, thus 2.a is a consequence of 2.b in the limit. Therefore, we only consider the Hoeffding-based tests of Condition 2.b.
**Access Sequences.** The exact learning algorithm $L^*_\text{mdp}$ presented in Sect. 8 iteratively updates an observation table. Upon termination it arrives at an observation table $(S, E, T)$ producing a hypothesis $H = (Q_h, \Sigma^I, \Sigma^O, q_0h, \delta_h, L_h) = \text{hyp}(S, E, T)$. Let $S_{\text{acc}} \subseteq S$ be the set of shortest access sequences leading to states in $Q$ given by $S_{\text{acc}} = \{ s | s \in S, \exists s' \in S : s' \ll s \land s \neq s' \land \delta_h^*(q_0h, s) = \delta_h^*(q_0h, s') \}$ (the shortest traces in each equivalence class of $S/\equiv_M$). By this definition, $S_{\text{acc}}$ forms a directed spanning tree in the structure of $H$. There are finitely many different spanning trees for a given hypothesis, therefore there are finitely many different $S_{\text{acc}}$. Hypothesis models learned by $L^*_\text{mdp}$ are isomorphic to $M$, thus there are finitely many possible final hypotheses. Let $S$ be the finite union of all access sequence sets $S_{\text{acc}}$ forming spanning trees in all valid final hypotheses. Let $L = \{ s \cdot i \cdot o | s \in S, i \in \Sigma^I, o \in \Sigma^O, M(s \cdot i)(o) > 0 \}$ be one-step extensions of $S$ with non-zero probability. Observe that for the correct construction of correct hypotheses in $L^*_\text{mdp}$, it is sufficient for $\text{eqRow}_E$ to approximate $M$-equivalence (see Def. 4) for traces in $L$. Consequently, the approximation of $\text{eqRow}_E$ via $\text{compatible}_E$ needs to hold only for traces in $L$.

**Hypothesis Construction.**

**Theorem 5 (Compatibility Convergence).** Given $\alpha_n$ such that $\sum_n \alpha_n n < \infty$, then with probability one: $\text{compatible}_E(s, s') \Leftrightarrow \text{eqRow}_E(s, s')$ for all traces $s, s'$ in $L$, except for finitely many $n$.

**Proof.** Let $A_n$ be the event that $\text{compatible}_E(s, s') \not\Leftrightarrow \text{eqRow}_E(s, s')$ and $p(A_n)$ be the probability of this event. In the following, we derive a bound for $p(A_n)$ based on the confidence level of applied tests in Def. 9 which is above $(1 - \alpha_n)^2$ [12]. An observation table stores $|S \cup Lt(S)| \cdot |E|$ cells, which gives us an upper bound on the number of tests performed for computing $\text{compatible}_E(s, s')$ for two traces $s$ and $s'$. However, note that cells do not store unique information; multiple cells may correspond to the same test sequence in $TS$, therefore it is simpler to reason about the number of tests in calls to $\text{diff}_f(c, c') = \text{diff}_\text{fq}(c, c')$ with respect to $S_n$. A single call to $\text{diff}_\text{fq}$ involves either 0 or $|\Sigma^O|$ tests. We apply tests only if we have observed both $c$ and $c'$ at least once, therefore we perform at most $2 \cdot |\Sigma^O| \cdot n$ different tests for all pairs of observed test sequences. The event $A_n$ may occur if any test produces an incorrect result, i.e., it yields a Boolean result different from the comparison between the true output distributions induced by $c$ and $c'$. This leads to $p(A_n) \leq 2 \cdot |\Sigma^O| \cdot n \cdot (1 - (1 - \alpha_n)^2)$, which implies $p(A_n) \leq 4 \cdot |\Sigma^O| \cdot n \cdot \alpha_n$. By choosing $\alpha_n$ such that $\sum_n \alpha_n n < \infty$, we have $\sum_n p(A_n) < \infty$ and we can apply the Borel-Cantelli lemma like Carrasco and Oncina [12], which states $A_n$ happens only finitely often. Hence, there is an $N_{\text{comp}}$ such that for $n > N_{\text{comp}}$, we have $\text{compatible}_E(s, s') \Leftrightarrow \text{eqRow}_E(s, s')$ with respect to $S_n$.

**Lemma 8.** Under the assumed uniformly randomised equivalence testing strategy, for every $s \cdot i \cdot o \in L : S_n(s \cdot i \cdot o) > 0$ after finitely many $n$. 
Proof. Informally, we will eventually sample all traces \( t \in \overline{T} \). The probability \( p_L \) of sampling \( t = o_0 \cdot i_1 \cdot o_1 \cdots o_n \cdot i \cdot o \) during a test, where \( t[\ll k] \) is the prefix of \( t \) of length \( k \), is given by (note that we may sample \( t \) as a prefix of another sequence):

\[
p_L = \frac{1}{\sum_{n=0}^{\infty} M(t[\ll 1])(o_1) \cdots M(t[\ll n])(o_n) \cdot M(t[\ll n+1])(o)(1-p_{\text{stop}})^n}
\]

Since every \( t \in \overline{T} \) is observable, we have \( M(t[\ll 1])(o_1) \cdots M(t[\ll n])(o_n) \cdot M(t[\ll n+1])(o) > 0 \), thus \( p_L > 0 \). Hence, there is a finite \( N_L \) such that for all \( s \cdot i \cdot o \in \overline{T} : S_n(s \cdot i \cdot o) > 0 \) for \( n > N_L \).

Lemma 9. If \( \text{compatible}_E(s, s') \iff \text{eqRow}_E(s, s') \), then the set of representatives \( R \) computed by Algorithm 3 for the closed and consistent observation table \( \langle S_n, E_n, T_n \rangle \) is prefix-closed.

Proof. Recall that we assume the function rank to impose a lexicographic ordering on traces. This simplifies showing prefix-closedness of \( R \), which we do by contradiction. Assume that \( R \) is not prefix-closed. In that case, there is a trace \( r \) of length \( n \) in \( R \) with a prefix \( r_p \) of length \( n - 1 \) that is not in \( R \). As \( r_p \notin R \), we have \( r_p \neq \text{rep}(r_p) \) and \( \text{rank}(r_p) < \text{rank}(\text{rep}(r_p)) \), because the representative \( \text{rep}(r_p) \) has the largest rank in its class \( eq(r_p) \). Since \( S_n \) is prefix-closed and \( R \subseteq S_n, r_p \in S_n \). Let \( i \in \Sigma^t \) and \( o \in \Sigma^O \) such that \( r_p \cdot i \cdot o = r \). Algorithm 3 enforces \( \text{compatible}_E(r_p, \text{rep}(r_p)) \) and due to consistency, we have that \( \text{compatible}_E(r_p \cdot i \cdot o, \text{rep}(r_p) \cdot i \cdot o) = \text{compatible}_E(r, \text{rep}(r_p) \cdot i \cdot o) \). Since \( r \) is a representative in \( R \), \( \text{rep}(r_p) \cdot i \cdot o \in eq(r) \). Representatives \( r \) have the largest rank in their compatibility class \( eq(r) \) and \( r \neq \text{rep}(r_p) \cdot i \cdot o \), thus \( \text{rank}(r) > \text{rank}(\text{rep}(r_p) \cdot i \cdot o) \).

In combination we have \( \text{rank}(r_p) < \text{rank}(\text{rep}(r_p)) \) and \( \text{rank}(r_p \cdot i \cdot o) > \text{rank}(\text{rep}(r_p) \cdot i \cdot o) \) which is a contradiction given the lexicographic ordering on traces imposed by rank. Consequently, \( R \) must be prefix-closed under the premises of Lemma 9.

Lemma 10. Let \( \langle S_n, E_n, T_n \rangle \) be the exact observation table corresponding to the sampling-based observation table \( \langle S_n, E_n, \overline{T}_n \rangle \), i.e. with \( \overline{T}_n(s) = \text{odq}(s) \) for \( s \in (S_n \cup Ltr(S_n)) \cdot E \). Then, \( \overline{T}_n(r \cdot i)(o) > 0 \iff T_n(r \cdot i)(o) > 0 \) for \( r \in R, i \in \Sigma^t, o \in \Sigma^O \) after finitely many \( n \).

Proof. First, we will show for prefix-closed \( R \) (Lemma 9) that \( R \subseteq \overline{S} \), if \( \text{compatible}_E(s, s') \iff \text{eqRow}_E(s, s') \). \( \overline{S} \) contains all traces corresponding to simple paths of \( \text{can}(M) \), therefore we show by contradiction that no \( r \in R \) forms a cycle in \( \text{can}(M) \).

Assume that \( r \) forms a cycle in \( \text{can}(M) \), i.e. it visits states multiple times. We can split \( r \) into three parts \( r = r_p \cdot r_c \cdot r_s \), where \( r_p \in TR \) such that \( r_p \) and \( r_p \cdot r_c \) reach the same state, and \( r_s \in (\Sigma^t \times \Sigma^O)^* \) is the longest suffix such that \( r_s \) visits every state of \( \text{can}(M) \) at most once. As \( R \) is prefix-closed, \( R \) includes \( r_p \) and \( r_p \cdot r_c \) as well. The traces \( r_p \) and \( r_p \cdot r_c \) reach the same state.
in \( \text{can}(M) \), thus we have \( \rho \equiv_M \rho \cdot r \) which implies \( \text{eqRow}_E(\rho, \rho \cdot r) \) and \( \text{compatible}_E(\rho, \rho \cdot r) \). By Algorithm 3 all \( r \in R \) are pairwise not compatible with respect to \( \text{compatible}_E \) leading to a contradiction, thus no \( r \) visits a state of \( \text{can}(M) \) more than once and we have \( R \subseteq \overline{S} \).

Hence, every observable \( r_i = r \cdot i \cdot o \) for \( r \in R, i \in \Sigma^I \) and \( o \in \Sigma^O \) is in \( \overline{L} \), as \( \overline{L} \) includes all observable extensions of \( \overline{S} \). By Lemma 8 we will sample \( r_i \) eventually, i.e. \( \hat{T}_n(r \cdot i)(o) > 0 \) and therefore \( T_n(r \cdot i)(o) > 0 \Leftrightarrow \hat{T}_n(r \cdot i)(o) > 0 \) after finitely many \( n \).

**Lemma 11.** The chaos state \( q_{\text{chaos}} \) is not reachable in \( \mathcal{H}_n \), except for finitely many \( n \).

**Proof.** We add a transition from state \( q = \langle \text{last}(r), \text{row}(r) \rangle \) with input \( i \) to \( q_{\text{chaos}} \) if \( cq(r \cdot i) = \text{false} \). As we consider \( n_c = 1 \), \( cq(r \cdot i) = \text{true} \) if there is an \( o \) such that \( \hat{T}_n(r \cdot i)(o) > 0 \). Lemma 10 states that \( T_n(r \cdot i)(o) > 0 \) for any observable \( r \cdot i \cdot o \) after finitely many \( n \). Thus, Lemma 11 implies \( cq(r \cdot i) = \text{true} \) for all \( r \in R \) and \( i \in \Sigma^I \), therefore the chaos is unreachable in \( \mathcal{H}_n \), except for finitely many \( n \).

Combining Theorem 5, Lemma 10 and Lemma 11 it follows that, after finitely many \( n \), hypotheses created in the sampling-based setting have the same structure as in the exact setting.

**Corollary 1.** Let \( \langle S_n, E_n, T_n \rangle \) be the exact observation table corresponding to the sampling-based observation table \( \langle S_n, E_n, \hat{T}_n \rangle \), i.e. \( T_n(s) = \text{odq}(s) \) for \( s \in (S_n \cup \text{Lt}(S_n)) \cdot E \). Then there exists a finite \( N_{\text{struct}} \) such that the exact hypothesis \( \text{hyp}(S_n, E_n, T_n) \) has the same structure as \( \mathcal{H}_n \) for \( n > N_{\text{struct}} \).

**Equivalence Queries.**

**Theorem 6 (Convergence of Equivalence Queries).** Given \( \alpha_n \) such that \( \sum_n \alpha_n < \infty \), an observation table \( \langle S_n, E_n, \hat{T}_n \rangle \) and a hypothesis \( \mathcal{H}_n \), then with probability one, \( \mathcal{H}_n \) has the same structure as \( M \) or we find a counterexample to equivalence, except for finitely many \( n \).

According to Corollary 1 there is an \( N_{\text{struct}} \) such that \( \mathcal{H}_n \) has the same structure as in the exact setting and \( \text{compatible}_E(s, s') \Leftrightarrow \text{eqRow}_E(s, s') \) for \( n > N_{\text{struct}} \). Therefore, we assume \( n > N_{\text{struct}} \) for the following discussion of counterexample search through the implemented equivalence queries \( \text{eq} \). Let \( H_n \) be the semantics of \( \mathcal{H}_n \). Recall that we apply two strategies for checking equivalence:

1. Random testing with a uniformly randomised scheduler (\( p_{\text{rand}} = 1 \)): this form of testing of testing can find traces \( s \cdot o \), with \( s \in TS \) and \( o \in \Sigma^O \), such that \( H(s)(o) = 0 \) and \( M(s)(o) > 0 \). While this form of search is coarse, we store all sampled traces in \( S_n \) that is used by our second counterexample search strategy performing a fine-grained analysis.
2. Checking conformance with $S_n$: for all observed test sequences, we statistically check for differences between output distributions in $H_n$ and distributions estimated from $S_n$ through applying $\text{diff}_{\text{eq}}$. Applying that strategy finds counterexample sequences $s \in T\mathcal{S}$ such that $M(s) \neq \perp$ (as $s$ must have been observed) and approximately $M(s) \neq H(s)$.

Case 1. If $H_n$ and $\mathcal{M}$ have the same structure and $n > N_{\text{struct}}$, such that $\text{eqRow}_E(s, s') \iff \text{compatible}_E(s, s')$, we may still find counterexamples that are spurious due to inaccuracies. Therefore, we will show that adding a prefix-closed set of traces to the set of short traces $S_n$ does not change the hypothesis structure, as this is performed by Algorithm 4 in response to counterexamples returned by $\text{eq}$.

**Lemma 12.** If $H_n$ has the same structure as $\mathcal{M}$ and $n > N_{\text{struct}}$, then adding a prefix-closed set of observable traces $S_t$ to $S_n$ will neither introduce closedness-violations nor inconsistencies, i.e. $\langle S_n \cup S_t, E_n, T_n \rangle$ is closed and consistent. Consequently, the hypothesis structure does not change, i.e. $H_n$ and $\text{hyp}(S_n \cup S_t, E_n, T_n)$ have the same structure.

**Proof.** Let $t$ be a trace in $S_t$ and $q_t = \delta_n^*(t)$ be the hypothesis state reached by $t$, which exists because $H_n$ has the same structure as $\mathcal{M}$. Let $t_s \in S_n$ be a short trace also reaching $q_t$. Since $\mathcal{M}$ and $H_n$ have the same structure, $t$ and $t_s$ also reach the same state of $\mathcal{M}$, therefore $t \equiv_t t_s$ (by reaching the same state both traces lead to the same future behaviour), implying $\text{eqRow}_E(t, t_s)$. With $n > N_{\text{struct}}$, we have $\text{compatible}_E(t, t_s)$. By the same reasoning, we have $\text{compatible}_E(t \cdot i \cdot o, t_s \cdot i \cdot o)$ for any $i \in \Sigma^1, o \in \Sigma^0$ with $M(t \cdot i)(o) > 0$; which is the condition for consistency of observation tables, i.e. adding $t$ to $S_n$ leaves the observation tables consistent.

Furthermore because $\langle S_n, E_n, T_n \rangle$ is closed, there exists a $t'_s \in S_n$, with $\text{compatible}_E(t_s \cdot i \cdot o, t'_s)$. Since $\text{compatible}_E(t \cdot i \cdot o, t_s \cdot i \cdot o)$ and because $\text{compatible}_E$ is transitive for $n > N_{\text{struct}}$, we have $\text{compatible}_E(t \cdot i \cdot o, t'_s)$. Hence, adding $t$ as to $S_n$ does not violate closedness, because for each observable extensions of $t$, there exists a compatible short trace $t'_s$.

Case 2. If the hypothesis $H_n$ does not have the same structure as $\mathcal{M}$ and $n > N_{\text{struct}}$, then $H_n$ has fewer states than $\mathcal{M}$ (following Lemma 1 given that $H$ is consistent with $\tilde{T}_n$ and $\text{compatible}_E(s, s') \iff \text{eqRow}_E(s, s')$). Since $\mathcal{M}$ is minimal with respect to the number of states, $H_n$ and $\mathcal{M}$ are not equivalent, thus a counterexample to observation equivalence exists and we are guaranteed to find any such counterexample after finitely many samples.

**Lemma 13.** If $\text{compatible}_E(s, s') \iff \text{eqRow}_E(s, s')$ for traces $s$ and $s'$ in $S_n$, then the hypothesis $H_n$ derived from $\langle S_n, E_n, T_n \rangle$ is the smallest MDP consistent with $\tilde{T}_n$.

**Proof.** Recall that for a given observation table $\langle S, E, T \rangle$, the exact learning algorithm $L_{\text{mdp}}^*$ derives the smallest hypothesis consistent with $T$. By Corollary 1...
$\mathcal{H}_n$ is the smallest MDP consistent $T$. As $\text{diff} \, \tilde{T}_n$ does not produce spurious results for $n > N_{\text{struct}}$ (Theorem [10]), $\mathcal{H}_n$ is also the smallest MDP consistent with $\tilde{T}_n$ with respect to $\text{diff} \, \tilde{T}_n$.

**Lemma 14.** Let $n_q$ be the number of states of $\mathcal{M}$, $C = \bigcup_{i=0}^{n_q^2+1} (\Sigma^2 \times \Sigma^1)^i$ and $C^{\text{obs}} = \{c | c \in C : M(c) \neq \bot\}$. For any other MDP $\mathcal{M}'$ with at most $n_q$ states and semantics $\mathcal{M}'$, iff $\forall c \in C^{\text{obs}} : M(c) = M'(c)$, then $\mathcal{M} \equiv_{\text{od}} \mathcal{M}'$.

Hence, there is a finite set $C^{\text{obs}}$ of sequences with lengths bounded by $n_q^2 + 1$ such that if we test all sequence in $C^{\text{obs}}$, we can check equivalence with certainty.

**Proof.** Let $\mathcal{M}$ and $\mathcal{M}'$ with states $Q$ and $Q'$ as defined above, i.e. $|Q| = n_q$ and $|Q'| \leq n_q$, and let $\text{reachQSeq}(t) \in (Q \times Q')^*$ be the sequence of state-pairs visited along a trace $t$ by $\mathcal{M}$ and $\mathcal{M}'$, respectively. $\mathcal{M} \equiv_{\text{od}} \mathcal{M}'$ iff for all $t \in \mathcal{TR}$ and $i \in \Sigma^t$, we have $M(t \cdot i) = M'(t \cdot i)$. If the length of $t \cdot i$ is at most $n_q^2 + 1$, then $t \cdot i \in C$. Otherwise, $\text{reachQSeq}(t)$ contains duplicated state pairs, because $|Q \times Q'| \leq n_q^2$. For $t$ longer than $n_q^2$, we can remove loops on $Q \times Q'$ from $t$ to determine a trace $t'$ of length at most $n_q^2$ such that $\text{reachQSeq}(t)[|t|] = \text{reachQSeq}(t')[|t'|]$, i.e. such that $t$ and $t'$ reach the same state pair. Since $t$ reaches the same state as $t'$ in $\mathcal{M}$ and in $\mathcal{M}'$, we have $M(t \cdot i) = M'(t' \cdot i)$ and $M'(t \cdot i) = M'(t' \cdot i)$, thus $M(t \cdot i) = M'(t \cdot i) \Leftrightarrow M(t' \cdot i) = M'(t' \cdot i)$. Consequently for all $t \cdot i \in \mathcal{TR} \cdot \Sigma^t$, either $t \cdot i \in C$, or there is a $t' \cdot i \in C$ leading to the same check between $\mathcal{M}$ and $\mathcal{M}'$.

We further restrict $C$ to $C^{\text{obs}}$, by considering only observable test sequences in $C$. This restriction is justified by Remark [1]. In summary:

\[
\mathcal{M} \equiv_{\text{od}} \mathcal{M}' \Leftrightarrow \forall c \in \mathcal{TS} : M(c) = M'(c)
\]
\[
\Leftrightarrow \forall c \in C : M(c) = M'(c)
\]
\[
\Leftrightarrow \forall c \in C^{\text{obs}} : M(c) = M'(c)
\]

**Lemma 15.** Under the randomised testing strategy with $p_{\text{rand}} = 1$ and $p_{\text{stop}} < 1$, all $c$ in $C^{\text{obs}}$ have non-zero probability to be observed.

**Proof.** Due to $p_{\text{rand}} = 1$ and $p_{\text{stop}} < 1$ we apply uniformly randomised inputs during testing and each test has a length that is distributed dependent on $p_{\text{stop}}$. Let $c = o_0i_1o_1 \cdots o_{n-1}i_n$ be a sequence in $C^{\text{obs}}$ with $c[\ll k]$ being its prefix of length $k$, then the probability $p_c$ of observing $c$ is (note that we may observe $c$ as a prefix of another sequence):

\[
p_c = \frac{1}{|\Sigma|_n} M(c[\ll 1])(o_1) \cdot M(c[\ll 2])(o_2) \cdots M(c[\ll n-1])(o_{n-1}) \cdot (1 - p_{\text{stop}})^{n-1}
\]

By definition of $C^{\text{obs}}$, we have $M(c[\ll j])(o_j) > 0$ for all indexes $j$ and $c$ in $C^{\text{obs}}$, therefore $p_c > 0$. 

\[L^*-\text{Based Learning of Markov Decision Processes (Extended Version)}\]
In every round of \( L_{\text{mdp}}^c \), we check for conformance between \( S_n \) and the hypothesis \( \mathcal{H}_n \) and return a counterexample if we detect a difference via \( \text{diff}_R \). Since we apply \( \text{diff}_R \), we follow a similar reasoning as for the convergence of hypothesis construction. Here, we approximate \( M(c) \neq H(c) \) for \( c \in T_S \) by \( \text{diff}_R(t \cdot i, r \cdot i) \), where \( c = t \cdot i \) for a trace \( t \), input \( i \) and the hypothesis state \( \langle \text{last}(r), \text{row}(r) \rangle \) reached by \( t \), where \( r \in R \) is the corresponding representative short trace.

**Lemma 16.** Given \( \alpha_n \) such that \( \sum_n \alpha_n n < \infty \), then with probability one \( M(c) \neq H(c) \Leftrightarrow \text{diff}_R(t \cdot i, r \cdot i) \) for \( c = t \cdot i \in C_{\text{obs}} \) and \( r \) as defined above, except for finitely many \( n \).

**Proof.** We use the identity \( H(t \cdot i) = H(r \cdot i) \) for traces \( t \) and \( r \) and inputs \( i \), which holds because \( t \) and \( r \) reach the same state in the hypothesis \( \mathcal{H} \). Applying that, we test for \( M(t \cdot i) \neq H(t \cdot i) \) by testing \( M(t \cdot i) \neq H(r \cdot i) \) via \( \text{diff}_R(t \cdot i, r \cdot i) \).

We perform \(|\Sigma^O|\) tests for each unique observed sequence \( c \), therefore we apply at most \( n \cdot |\Sigma^O| \) tests. Let \( B_n \) be the event that any of these tests is wrong, that is, \( M(t \cdot i) \neq H(r \cdot i) \Leftrightarrow \text{diff}_R(t \cdot i, r \cdot i) \) for at least one observed \( c = t \cdot i \). Due to the confidence level greater than \((1 - \alpha_n)^2\) of the tests, the probability \( p(B_n) \) of \( B_n \) is bounded by \( p(B_n) \leq n \cdot |\Sigma^O| \cdot (1 - (1 - \alpha_n)^2) \leq 2 \cdot n \cdot |\Sigma^O| \cdot \alpha_n \). By choosing \( \alpha_n \) such that \( \sum_n \alpha_n n < \infty \), we can apply the Borel-Cantelli lemma as above. Hence, \( B_n \) only happens finitely often, thus there is a \( N_1 \) such that for all \( n > N_1 \) we have \( M(t \cdot i) \neq H(r \cdot i) \Leftrightarrow \text{diff}_R(t \cdot i, r \cdot i) \) for all observed \( c = t \cdot i \).

Furthermore, the probability of observing any \( c \) of the finite set \( C_{\text{obs}} \) during testing is greater than zero (Lemma [13]), thus there is a finite \( N_2 \) such that \( S_n \) contains all \( c \in C_{\text{obs}} \) for \( n > N_2 \). Consequently, there is an \( N_{\text{cex}} \), such that \( \text{Lemma 16} \) holds for all \( n > N_{\text{cex}} \).

**Putting Everything Together.** We have established that after finitely many \( n \), the sampling-based hypothesis \( \mathcal{H}_n \) has the same structure as in the exact setting (Corollary [1]). Therefore, certain properties of the exact learning algorithm \( L_{\text{mdp}}^e \) hold for the sampling-based \( L_{\text{mdp}}^c \) as well. The derived hypotheses are therefore minimal, i.e., they have at most as many states as \( M \). As with \( L_{\text{mdp}}^e \), adding a non-spurious counterexample to the trace set \( S_n \) introduces at least one state in the derived hypotheses. Furthermore, we have shown that equivalence queries return non-spurious counterexamples, except for finitely many \( n \) (Theorem [1]). Consequently, after finite \( n \) we arrive at a hypothesis \( \mathcal{H}_n \) with the same structure as \( M \). We derive transition probabilities by computing empirical means, thus by the law of large numbers these estimated probabilities converge to the true probabilities. Hence, we learn a hypothesis \( \mathcal{H}_n \) isomorphic to the canonical MDP \( M \) in the limit as stated by Theorem [4].
More efficient parameters. So far, we discussed a particular parametrisation of $L^\ast_{mdp}$. Among others, we used uniformly random input choices for equivalence testing with $p_{rand} = 1$, and instantiated $cq$ to accept samples as complete after only $n_c = 1$ observation. This simplified the proof, but is inefficient in practical experiments. However, the arguments based on $n_c = 1$, such as Lemma 10 and Lemma 11, are easily extended to small constant values of $n_c$. Since the samples are collected independently, any observation that occurs at least once after a finite number of steps also occurs at least $n_c$ times after a finite number of steps.

5 Experiments

In active automata learning, our goal is generally to learn an MDP which is equivalent to the true MDP modelling the SUL. This changes in the stochastic setting, where we want to learn a model close to true model, as equivalence can hardly be achieved. Note that we perform experiments with known models, which we treat as a black boxes during learning. As a reference, we also learn models and perform the same measurements with IOALERGIA. Our experiments aim to measure the similarity between the learned models and the true model:

1. We compute the discounted bisimilarity distance between the true models and the learned MDPs [7,8]. We adapted the distance measure from MDPs with rewards to labelled MDPs by defining a distance of 1 between states with different labels.
2. Additionally, we perform probabilistic model-checking. We compute and compare maximal probabilities of manually defined temporal properties with all models. The computation is done via Prism [28].

Experimental results and the implementation can be found in the evaluation material [38].

Measurement Setup. As in [30], we configure IOALERGIA with a data-dependent significance parameter for the compatibility check, by setting $\epsilon_N = \frac{10000}{N}$, where $N$ is the total combined length of all traces used for learning. This parameter serves a role analogous to the $\alpha$ parameter for the Hoeffding bounds used by $L^\ast_{mdp}$. In contrast to IOALERGIA, we observed that $L^\ast_{mdp}$ shows better performance with non-data-dependent $\alpha$, therefore we set $\alpha = 0.05$ for all experiments. Motivated by convergence guarantees given in [30], we collect traces for IOALERGIA by sampling with a scheduler that selects inputs according to a uniform distribution. The length of these traces is geometrically distributed with a parameter $p_l$ and the number of traces is chosen such that IOALERGIA and $L^\ast_{mdp}$ learn from approximately the same amount of data.

We implemented $L^\ast_{mdp}$ and IOALERGIA in Java. In addition to our Java implementations, we use Prism 4.4 [28] for probabilistic model-checking, and an adaptation of the MDPDist library available at [6] for computing bisimilarity distances. We performed the experiments with a Lenovo Thinkpad T450 with 16 GB RAM, an Intel Core i7-5600U CPU with 2.6 GHz and running Xubuntu Linux 18.04.
Table 2. Results for learning the first gridworld example.

|               | true model | $L^*_\text{mdp}$ | IoAlergia |
|---------------|------------|------------------|-----------|
| # outputs     | -          | 3101959          | 3103607   |
| # traces      | -          | 391530           | 387746    |
| time [s]      | -          | 118.377          | 21.4420   |
| # states      | 35         | 35               | 21        |
| $d_{\alpha, \beta}$ | -          | 0.1442           | 0.5241    |
| $P_{\text{max}}(F^{\leq 11}(\text{goal}))$ | 0.9622 | 0.9651 | 0.2306 |
| $P_{\text{max}}(\neg G U^{\leq 14}(\text{goal}))$ | 0.6499 | 0.6461 | 0.1577 |
| $P_{\text{max}}(\neg S U^{\leq 19}(\text{goal}))$ | 0.6912 | 0.6768 | 0.1800 |

5.1 First Gridworld

Models similar to our gridworlds have, e.g., been considered in the context of learning control strategies [20]. Basically, a robot moves around in a world of tiles of different terrains. It may make errors in movement, e.g. move south west instead of south with an error probability depending on the target terrain. Our aim is to learn an environment model, i.e. a map. Figure 2 shows the first gridworld used for evaluation. Black tiles are walls and other terrains are represented by different shades of grey and letters (Sand, Mud, Grass & Concrete). A circle marks the initial location and a double circle marks a goal location. Four inputs enable movement in four directions. Observable outputs include the different terrains, walls, and a label indicating the goal. The true model of this gridworld has 35 different states.

We set the sampling parameters to $n_{\text{re} \text{s} \text{ample}} = n_{\text{re} \text{t} \text{e} \text{s} \text{t}} = 300$, $n_{\text{te} \text{s} \text{t}} = 50$, $p_{\text{s} \text{top}} = 0.25$ and $p_{\text{ran} \text{d}} = 0.25$. As stopping parameter served $t_{\text{un} \text{a} \text{m} \text{b}} = 0.99$, $r_{\text{m} \text{i} \text{n}} = 500$ and $r_{\text{m} \text{a} \text{x}} = 4000$. Finally, the parameter $p_{l}$ for IoAlergia’s geometric trace length distribution was set to 0.125.

Results. Table 2 shows the measurement results for learning the first gridworld. Our active learning stopped after 1147 rounds, sampling 391530 traces (Row 2) with a combined number of outputs of 3101959 (Row 1). The bisimilarity distance discounted with $\lambda = 0.9$ to the true model is 0.144 for $L^*_\text{mdp}$ and 0.524 for IoAlergia (Row 5); thus it can be assumed that model checking the $L^*_\text{mdp}$ model produces more accurate results. This is indeed true for our three evaluation queries in the last three rows. These model-checking queries ask for the maximum probability (quantified over all schedulers) of reaching the goal within a varying number of steps. The first query does not restrict the terrain visited before the goal, but the second and third require to avoid G and S, respectively. The absolute difference to the true values is at most 0.015 for $L^*_\text{mdp}$, but the results for IoAlergia differ greatly from the true values. One reason is that the
IoAlergia model with 21 states is significantly smaller than the minimal true model, while the $L^*_{\text{MDP}}$ model has as many states as the true model. IoAlergia is faster than $L^*_{\text{MDP}}$, which applies time-consuming computations during equivalence queries. However, the runtime of learning-specific computations is often negligible in practical applications, such as learning of protocol models \cite{39,35}, as the communication with the SUL usually dominates the overall runtime. Given the smaller bisimilarity distance and the lower difference to the true probabilities computed with Prism, we conclude that the $L^*_{\text{MDP}}$ model is more accurate.

### 5.2 Second Gridworld

Fig. 3 shows the second gridworld used in our evaluation. As before, the robot starts in the initial location in the top left corner and can only observe the different terrains. The goal location is in the bottom right corner in this example. The true MDP representing this gridworld has 72 states. We configured learning as for the first gridworld, but collect more samples per round by setting $n_{\text{retest}} = n_{\text{resample}} = 1000$. Table 3 shows the measurement results for learning.

We sampled 515,950 traces with a combined number of outputs of 3,663,415, i.e. the combined length of all traces is in a similar range as before, although we sampled more traces in a single round. This is the case because learning stopped already after 500 rounds. We used similar model-checking queries as

### Table 3. Results for learning the second gridworld example.

|                | true model | $L^*_{\text{MDP}}$ | IoAlergia |
|----------------|------------|--------------------|-----------|
| # outputs      | -          | 3,663,415          | 3,665,746 |
| # traces       | -          | 515,950            | 457,927   |
| time [s]       | -          | 166.8550           | 15.1360   |
| # states       | 72         | 72                 | 31        |
| $\delta_{0.9}$| -          | 0.1121             | 0.5763    |
| $P_{\text{max}}(F^{\leq14}(\text{goal}))$ | 0.9348 | 0.9404 | 0.0208 |
| $P_{\text{max}}(F^{\leq12}(\text{goal}))$ | 0.6712 | 0.6796 | 0.0172 |
| $P_{\text{max}}(-M U^{\leq18}(\text{goal}))$ | 0.9743 | 0.9750 | 0.0196 |
| $P_{\text{max}}(-S U^{\leq20}(\text{goal}))$ | 0.1424 | 0.1644 | 0.0240 |
Table 4. Results for learning the shared coin consensus protocol.

|                | true | $L^*_\text{mdp}$ | IOALERGIA |
|----------------|------|-----------------|-----------|
| # outputs      | -    | 537 665         | 537 885   |
| # traces       | -    | 98 064          | 67 208    |
| time [s]       | -    | 31 885.8510     | 33 548.80 |
| # states       | 272  | 163             | 94        |
| $\delta_{0.9}$| -    | 0.1142          | 0.4482    |
| $P_{\text{max}}(F(\text{finished} \land p_1\text{heads} \land p_2\text{tails}))$ | 0.1069 | 0 | 0 |
| $P_{\text{max}}(\neg F(\text{finished} \land p_1\text{tails} \land p_2\text{tails}))$ | 0.5556 | 0.6765 | 0.6594 |
| $P_{\text{max}}(\text{counter} \neq 5 \land \neg F(\text{finished}))$ | 0.3333 | 0.3899 | 0.5356 |
| $P_{\text{max}}(\text{counter} \neq 4 \land \neg F(\text{finished}))$ | 0.4286 | 0.5191 | 0.6682 |
| $P_{\text{max}}(F^+ (\text{finished} \land p_1\text{heads} \land p_2\text{tails}))$ | 0.0017 | 0 | 0 |
| $P_{\text{max}}(F^{-\omega} (\text{finished} \land p_1\text{tails} \land p_2\text{tails}))$ | 0.2668 | 0.3066 | 0.2694 |
| $P_{\text{max}}(\text{counter} \neq 5 \land F^+ \text{finished})$ | 0.2444 | 0.2928 | 0.4460 |
| $P_{\text{max}}(\text{counter} \neq 4 \land F^{-\omega} \text{finished})$ | 0.2634 | 0.3246 | 0.5050 |

in the previous example and we can again see that the difference between the true model and the $L^*_\text{mdp}$ model is much smaller than for IOALERGIA. However, compared to the previous example, the absolute difference between $L^*_\text{mdp}$ and the true model with respect to model-checking has slightly increased.

5.3 Shared Coin Consensus

This example is a randomised consensus protocol by Aspnes and Herlihy [5]. In particular, we used a model of the protocol distributed with the PRISM model checker [28] as a basis for our experiments. We generally performed only minor adaptations such as adding action labels for inputs, but we also slightly changed the functionality by doing that. For the purpose of this evaluation these changes are immaterial, though.

We consider only the configuration with the smallest state space of size 272 with two processes and constant $K$ set to 2. Basically, the SUL has two inputs $go_1$ and $go_2$, one for each process, where executing input $go_i$ causes process $p_i$ to perform exactly one step. The outputs of the SUL comprise the counter state, the processes’ coin states, as well as additional propositions, e.g., denoting that the protocol finished. Note that we need to make the coin states visible, to be able to model the SUL with deterministic MDPs. In this experiment, we basically learn the state machine underlying the protocol, which we cannot observe directly.

We set the learning parameters to $n_{\text{resample}} = n_{\text{retest}} = n_{\text{test}} = 50$, $p_{\text{stop}} = 0.25$ and $p_{\text{rand}} = 0.25$. We controlled stopping with $t_{\text{unamb}} = 0.99$, $r_{\text{min}} = 500$ and $r_{\text{max}} = 4000$. Finally, we set $p_t = 0.125$ for IOALERGIA.

A thorough discussion of the model and related experiments can be found at [http://www.prismmodelchecker.org/casestudies/consensus_prism.php](http://www.prismmodelchecker.org/casestudies/consensus_prism.php) Accessed: June 28, 2019
Table 4 shows the measurement results for learning a model of the shared coin consensus protocol. Compared to the previous example, we need a significantly lower sample size of 98,064 traces containing 537,665 outputs, although the models are much larger. A reason for this is that there is a relatively large number of outputs in this example, such that states are easier to distinguish from each other. The bisimilarity distance is in a similar range as before for $L^*_{\text{mdp}}$, which is again significantly smaller than IoALERGIA’s bisimilarity distance. The $L^*_{\text{mdp}}$ model is again larger than the IoALERGIA model, but in this example it is smaller than the true model. This happens because many states are never reached during learning, as reaching them within a bounded number of steps has a very low probability – see e.g. the fifth model-checking query determining the maximum probability of finishing the protocol within less than 40 steps, but without consensus, as $p_1$ chooses heads and $p_2$ chooses tails. Here, we also see that the model-checking results computed with the IoALERGIA model are more accurate in some cases, but $L^*_{\text{mdp}}$ produces more accurate results overall. The absolute difference from the true values averaged over all model-checking results is about 0.066 for $L^*_{\text{mdp}}$, approximately half of IoALERGIA’s average absolute difference of 0.138. We see an increase in runtime compared to the gridworld examples, which is caused by the larger state space, since the precomputation time for equivalence testing grows with the state space.

5.4 Slot machine

The slot machine originally served as an example in [29,30], as an adaptation from another model, and we used it subsequently in [3] as well. It has three reels, each of them controlled by a separate input. Initially they are blank, but after a reel is spun, it may either show apple or bar. A play generally spans $m$ rounds (spins) and after that a prize is awarded. It is $Pr_{10}$, if all reels show bar, it is $Pr_{2}$, if two reels show bar, and otherwise it is $Pr_{0}$. The probability of bar decreases with decreasing number of remaining rounds. Finally, there is also a fourth input stop, which with equal probability either stops the game or grants two extra rounds, but the remaining rounds cannot exceed $m$.

For our experiments, we configured the slot machine with $m = 3$. In this configuration, the true minimal model has 109 states. We configured sampling for IoALERGIA with $p_l = 0.125$ and we set the following parameters for $L^*_{\text{mdp}}$: $n_{\text{resample}} = n_{\text{retest}} = n_{\text{test}} = 300$, $p_{\text{stop}} = 0.25$, $p_{\text{rand}} = 0.25$, $r_{\text{min}} = 500$ and $r_{\text{max}} = 20000$. To demonstrate the influence of the parameter $t_{\text{unamb}}$, we performed experiments with $t_{\text{unamb}} = 0.9$ and $t_{\text{unamb}} = 0.99$.

Table 5 and Table 6 show the results for $t_{\text{unamb}} = 0.9$ and $t_{\text{unamb}} = 0.99$, respectively. Configured with $t_{\text{unamb}} = 0.9$, $L^*_{\text{mdp}}$ stopped after 2988 rounds and it stopped after 12,879 rounds, if configured with $t_{\text{unamb}} = 0.99$. We see here that learning an accurate model of the slot machine requires a large amount of samples; in the case of $t_{\text{unamb}} = 0.99$, we sampled 7,542,332 traces containing 24,290,643 outputs. These are almost 10 times as many outputs as for the gridworld examples. However, we also see that sampling more traces clearly pays off. The $L^*_{\text{mdp}}$ results shown in Table 6 are much better than those shown in Table 5.
|               | true | $L^\ast_{\text{mdp}}$ | IoAlergia |
|---------------|------|----------------------|-----------|
| # outputs     | -    | 4,752,687            | 4,752,691 |
| # traces      | -    | 1,567,487            | 594,086   |
| time [s]      | -    | 3380.9610            | 60.3480   |
| # states      |      | 109                  | 109       |

| $\delta_{0.9}$ | 0.1632 | 0.2983 |
| $\mathbb{P}_{\text{max}}(F(\text{Pr}10))$ | 0.3637 | 0.3769 | 0.4169 |
| $\mathbb{P}_{\text{max}}(F(\text{Pr}2))$ | 0.6442 | 0.6697 | 0.6945 |
| $\mathbb{P}_{\text{max}}(F(\text{Pr}0))$ | 1.0000 | 1.0000 | 1.0000 |
| $\mathbb{P}_{\text{max}}(X\langle X(\text{bar-bar-blank})\rangle))$ | 0.1600 | 0.1615 | 0.1639 |
| $\mathbb{P}_{\text{max}}(X\langle X(\text{apple-bar-bar})\rangle))$ | 0.2862 | 0.2865 | 0.2776 |
| $\mathbb{P}_{\text{max}}(\neg(F^{\leq10}(\text{end})))$ | 0.2500 | 0.3013 | 0.3283 |
| $\mathbb{P}_{\text{max}}(X\langle X(\text{apple-apple-apple})\rangle \land (F(\text{Pr}0)))$ | 0.0256 | 0.0262 | 0.0107 |

Notably the state space stayed the same way. Thus, the model learned with fewer traces presumably includes some incorrect transitions. This is exactly what our stopping heuristic aims to avoid; it aims to avoid ambiguous membership of traces in compatibility classes to reduce the uncertainty in creating transitions.

We also see in both settings that $L^\ast_{\text{mdp}}$ models are more accurate than IoAlergia models, with respect to bisimilarity distance and with respect to model-checking results. While the experiment with $t_{\text{unamb}} = 0.99$ required the most samples among all experiments, it also led to the lowest bisimilarity distance. It is also noteworthy that model-checking results for the $L^\ast_{\text{mdp}}$ model are within a low range of approximately 0.01 of the true results. A drawback of $L^\ast_{\text{mdp}}$ compared to IoAlergia is again the learning runtime, as $L^\ast_{\text{mdp}}$ required about 5 hours while learning with IoAlergia took only about 8.7 minutes. However, in a non-simulated environment, the sampling time would be much larger than 5 hours, such that the learning runtime becomes negligible. Consider for instance a scenario where sampling a single trace takes 20 milliseconds. The sampling time of $L^\ast_{\text{mdp}}$ is about 42 hours in that scenario, i.e. about 8.4 times the learning runtime.

5.5 Discussion & Threats to Validity

Our case studies demonstrated that $L^\ast_{\text{mdp}}$ is able to achieve better accuracy than IoAlergia. The bisimilarity distances of $L^\ast_{\text{mdp}}$ models to the true models were generally lower and the model checking results were more accurate. These observations will be investigated in further case studies. It should be noted though that the considered systems have different characteristics. The gridworld has small state-space, but is strongly connected and the different terrains lead to different probabilistic decisions, e.g. if we try to enter mud there is a probability of 0.4 of entering one of the neighbouring tiles, whereas entering concrete is generally successful (the probability of entering other tiles instead is 0). The
Table 6. Results for learning the slot machine with $t_{unamb} = 0.99$.

|                      | true           | $L^*_\text{MDP}$ | IoALERGIA |
|----------------------|----------------|------------------|-----------|
| # outputs            | -              | 24,290,643      | 24,282,985|
| # traces             | -              | 7,542,332       | 3,036,332 |
| time [s]             | -              | 18,047.9610     | 518.8520  |
| # states             | 109            | 109             | 97        |
| $\delta_{0.9}$      | 0.0486         | 0.2518          |
| $P_{\max}(F(Pr10))$ | 0.3637         | 0.3722          | 0.3901    |
| $P_{\max}(F(Pr2))$  | 0.6442         | 0.6552          | 0.6997    |
| $P_{\max}(F(Pr0))$  | 1.0000         | 1.0000          | 1.0000    |
| $P_{\max}(\neg(F<10(\text{end})))$ | 0.2500 | 0.2606 | 0.4000 |
| $P_{\max}(X(X(\text{apple-apple-apple})))$ & $\wedge (F(Pr0)))$ | 0.0256 | 0.0264 | 0.0128 |

consensus protocol has a large state space with many different outputs and finishing the protocol takes at least 14 steps. The slot machines requires states to be distinguished based on subtle differences in probabilities, as the probability of seeing bar decreases in each round.

$L^*_\text{MDP}$ has several parameters that affect performance and accuracy. We plan to investigate the influence of parameters in further experiments. For the present experiments, we fixed most of the parameters except for $n_{retest}$, $n_{test}$ and $n_{resample}$ and we observed that results are robust with respect to these parameters. We, e.g., increased $n_{resample}$ from 300 for the first gridworld to 1000 for the second gridworld. Both settings led to approximately the same results, as learning simply performed fewer rounds with $n_{resample} = 1000$. Hence, further experiments will examine if the fixed parameters are indeed appropriately chosen and if guidelines for choosing other parameters can be provided.

$L^*_\text{MDP}$ and IoALERGIA learn from different traces, thus the trace selection may actually be the main reason for the better accuracy of $L^*_\text{MDP}$. We examined if this is the case, by learning IoALERGIA models from two types of traces: traces with uniform input selection and traces sampled during learning with $L^*_\text{MDP}$. We noticed that models learned from $L^*_\text{MDP}$ traces altogether led to less accurate results, especially in terms of bisimilarity distance, and therefore we reported only results for models learned from traces with uniformly distributed inputs.

6 Related Work

In the following, we discuss techniques for learning both model structure and transition probabilities in case of probabilistic systems. There are many learning approaches for models with a given structure, e.g., for learning control strategies [20]. Covering these approaches is beyond the scope of this paper.

We build upon Angluin’s $L^*$ [4], thus our work shares similarities with other $L^*$-based work like active learning of Mealy machines [36]. Interpreting MDPs
as functions from test sequences to output distributions is similar to the interpretation of Mealy machines as functions from input sequences to outputs [37].

Volpato and Tretmans presented an \( L^* \)-based technique for non-deterministic input-output transition systems [43]. They simultaneously learn an over- and an under-approximation of the SUL with respect to the input output conformance (ioco) relation [40]. Inspired by that, \( L^*_\text{mdp} \) uses completeness queries and we add transitions to a chaos state in case we have low information. Beyond that, we consider systems to behave stochastically rather than non-deterministically. While [43] leaves the concrete implementation of queries unspecified, \( L^*_\text{mdp} \)'s implementation closely follows Sect. 4. Early work on ioco-based learning for non-deterministic systems has been presented by Willemse [44]. Khalili and Tacchella [26] addressed non-determinism by presenting an \( L^* \)-based algorithm for non-deterministic Mealy machines. Like Volpato and Tretmans [43], they assume to be able to observe all possible outputs in response to input sequences applied during learning. Our implementation does not require this assumption by checking for compatibility, i.e. approximate equivalence, between output distributions. Both these approaches assume a testing context, as we do.

Most sampling-based learning algorithms for stochastic systems are passive, i.e. they assume preexisting samples of system traces. Their roots can be found in grammar inference techniques like Alergia [11] and rlips [12], which identify stochastic regular languages. We share with these techniques that we also apply Hoeffing bounds [22] for testing for difference between probability distributions. Alergia has been extended to MDPs by Mao et al. [29,30]. The extension is called IoAlergia and basically creates a tree-based representation of the sampled system traces and repeatedly merges compatible nodes to create an automaton. Finally, transition probabilities are estimated from observed output frequencies. Like \( L^*_\text{mdp} \), IoAlergia converges in the limit, but showed worse accuracy in Sect. 5. It was adapted to an active setting by Chen and Nielsen [15]. They proposed to generate new samples to reduce uncertainty in the data. In contrast to this, we base our sampling not only on the data collected so far (refine queries), but also on the current observation table and the derived hypothesis MDPs (refine & equivalence queries), i.e. we take information about the SUL's structure into account. In previous work, we presented a different approach to apply IoAlergia in an active setting which takes reachability objectives into account with the aim of maximising the probability of reaching desired events [3].

\( L^* \)-based learning for probabilistic systems has also been presented by Feng et al. [17]. They learn assumptions in the form of probabilistic finite automata for compositional verification of probabilistic systems. Their learning algorithm requires queries returning exact probabilities, hence it is not directly applicable in a sampling-based setting. The learning algorithm shares similarities with an \( L^* \)-based algorithm for learning multiplicity automata [10], a generalisation of deterministic automata. Further query-based learning in a probabilistic setting has been described by Tzeng [41]. He presented a query-based algorithm for learning probabilistic automata and described an adaptation of Angluin’s \( L^* \) for learning Markov chains. In contrast to our exact learning algorithm \( L^*_\text{mdp} \),
which relies on output distribution queries, Tzeng’s algorithm for Markov chains queries the generating probabilities of strings. Castro and Gavalda review passive learning techniques for probabilistic automata with a focus on convergence guarantees and present them in a query framework [14]. Unlike MDPs, the learned automata cannot be controlled by inputs.

7 Conclusion

We presented $L^*$-based learning of MDPs. For our exact learning algorithm $L^*_{\text{MDP}}$, we assumed an ideal setting that allows to query information about the SUL with exact precision. Subsequently, we relaxed our assumptions, by approximating exact queries through sampling SUL traces via directed testing. These traces serve to infer the structure of hypothesis MDPs, to estimate transition probabilities and to check for equivalence between SUL and learned hypotheses. The resulting sampling-based $L^*_{\text{MDP}}$ iteratively learns approximate MDPs which converge to the correct MDP in the large sample limit. We implemented $L^*_{\text{MDP}}$ and compared it to IoALERGIA [30], a state-of-the-art passive learning algorithm for MDPs. The evaluation showed that $L^*_{\text{MDP}}$ is able to produce more accurate models. To the best of our knowledge, $L^*_{\text{MDP}}$ is the first $L^*$-based algorithm for MDPs that can be implemented via testing. Experimental results and the implementation can be found in the evaluation material [38].

The evaluation showed promising results, therefore we believe that our technique can greatly aid the black-box analysis of reactive systems such as communication protocols. While deterministic active automata learning has successfully been applied in this area [18,39], networked environments are prone to be affected by uncertain behaviour that can be captured by MDPs. $L^*_{\text{MDP}}$ converges in the limit, therefore a potential direction for future work is an analysis with respect to probably approximately correct (PAC) learnability [42,14]. A challenge towards this goal will be the identification of a distance measure suited to verification [30]. Furthermore, $L^*_{\text{MDP}}$ provides room for experimentation, e.g. different testing techniques could be applied in equivalence queries.

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