Learning Task Automata for Reinforcement Learning Using Hidden Markov Models

Alessandro Abate\textsuperscript{a}, Yousif Almulla\textsuperscript{a,b}, James Fox\textsuperscript{a}, David Hyland\textsuperscript{a} and Michael Wooldridge\textsuperscript{a}

\textsuperscript{a}University of Oxford
\textsuperscript{b}Microsoft Azure Quantum
\{aabate, james.fox, david.hyland, mjw\}@cs.ox.ac.uk, yalmulla@microsoft.com

Abstract. Training reinforcement learning (RL) agents using scalar reward signals is often infeasible when an environment has sparse and non-Markovian rewards. Moreover, handwriting these reward functions before training is prone to misspecification. We learn non-Markovian finite task specifications as finite-state ‘task automata’ from episodes of agent experience within environments with unknown dynamics. First, we learn a product MDP, a model composed of the specification’s automaton and the environment’s MDP (both initially unknown), by treating it as a partially observable MDP and employing a hidden Markov model learning algorithm. Second, we efficiently distil the task automaton (assumed to be a deterministic finite automaton) from the learnt product MDP. Our automaton enables a task to be decomposed into sub-tasks, so an RL agent can later synthesise an optimal policy more efficiently. It is also an interpretable encoding of high-level task features, so a human can verify that the agent’s learnt tasks have no misspecifications. Finally, we also take steps towards ensuring that the automaton is environment-agnostic, making it well-suited for use in transfer learning.

1 Introduction

Reinforcement Learning (RL) can be prohibitively slow (sample inefficient) at learning an optimal policy when the reward signal is sparse and non-Markovian because of the credit assignment problem. However, this setting is common: any task where no reward is given until a sequence of sequential sub-tasks is completed. Consider a medical procedure where the ordering of sub-task completion matters or where one can only enter a room if one already has the key.

Three existing approaches for improving learning in this setting are hierarchical RL \cite{23}, which allows agents to plan at various levels of abstraction; transfer learning, which utilises knowledge learnt from similar tasks \cite{29}; and temporal logic planning approaches, which guide the agent’s exploration by focusing it on the MDP fragment that satisfies a linear temporal logic (LTL) property \cite{14,19,30}. The latter is similar to Icarte et al \cite{19}’s reward machines (finite-state machines that represent non-Markovian reward functions) because an LTL property is often represented as an automaton.

Task specifications are often separable, so an automaton (or reward machine) allows an optimal policy to be found more efficiently by breaking the task into Markovian sub-tasks. Recent work (see Section \cite{5}) has recognised that this automaton is usually a priori unknown, so they learn it concurrently with finding an optimal policy. We focus on how to best learn the task automaton (TA) representing a task specification in sparse, non-Markovian reward environments. To our knowledge, ours is the first model-based approach; our pipeline learns a model of the underlying MDP along with the TA. The aforementioned work on temporal logic planning, sample-efficient model-based RL approaches \cite{35}, or other methods \cite{3} can then synthesise an optimal policy.

Contributions: Our algorithmic pipeline learns both a task specification as a TA (encoded as a deterministic finite automaton (DFA)) and a model of the MDP, from episodes of agent experience within an environment with unknown dynamics and sparse, non-Markovian reward. This improves sample efficiency in three ways: a TA exposes a task specification’s separability, so it allows for solving sub-tasks independently; our model-based approach helps the agent learn an optimal policy more efficiently; and we remove environmental bias from the learned TA for better transfer learning \cite{29}.

We learn the TA via an intermediate product MDP structure, composed of the environment’s ‘spatial’ MDP and the task specification’s TA. The product MDP is partially observable – the agent only observes its state in the spatial MDP and its reward, not the TA-state (its progress through the unknown task). The product MDP is learnt using the Baum-Welch algorithm \cite{36} by first learning an estimate of the spatial MDP using a uniform prior. Then, this learnt spatial MDP is used as an inductive bias for learning the full product MDP. In Section \cite{4} we show that our approach is more efficient than existing SAT-based approaches to learning TAs \cite{1,8,15,34,36} by comparing with Biermann and Feldman’s \cite{12} SAT-based algorithm.

Once the product MDP is learnt, distilling the TA via our ‘Cone Lumping’ method is computationally cheap. This makes the product MDP useful for transfer learning. If the environment changes, the agent only needs to update the affected part of the product MDP before efficiently re-distilling the TA.

This paper also addresses the reward misspecification problem \cite{2} by using a direct task specification to encode a complex, non-Markovian task rather than a scalar reward function. This is because scalar reward functions are brittle with respect to small environmental changes \cite{33}, do not signal a task’s separability, and can be difficult for a human to interpret and verify whether they result in the desired behaviour. In contrast, our learnt TA reveals the full task specification. Since our pipeline works in unknown environments where
many high-level tasks may exist, agents using our pipeline can learn multiple tasks in one TA. Although we focus on deterministic TAs in this paper (i.e., DFAs), our approach can be straightforwardly extended to learning probabilistic automata [10] [24]. Although the paper is self-contained, for brevity, we relegate many proposition proofs to our supplementary material, Appendix A.

2 Setup

An agent’s interaction with its environment can be viewed at many levels of abstraction, amongst which a low and fine-grained description is often modelled by a Markov Decision Process (MDP). However, agents can also recognise higher-level features of the environment (e.g., chairs or tables). These are included in a labelled MDP (in Section 2.1) using a set of (atomic) propositional variables from an alphabet of labels $\cal{AP}$, which are assigned truth values at every MDP state via a labelling function $\ell$. Task specifications refer to sequential compositions of these high-level features and can be encoded as TAs (in Section 2.2), which graphically represent the structure of tasks that an agent can get reward from completing. A TA and the MDP can be combined into a single structure, a product MDP (in Section 2.3) to provide a holistic representation of the agent’s exploration.

2.1 MDP Environment

Definition 1. A Markov Decision Process (MDP) is a tuple $\cal{M} = (S, A, s_0, P, R, \gamma)$, where $S$ and $A$ are finite sets of states and actions, $s_0$ is the initial state (or distribution over states), $P: S \times A \times S \rightarrow [0, 1]$ is the transition probability distribution, $R : (S \times A)^+ \rightarrow S \rightarrow \mathbb{R}$ is a (non-Markovian) reward function, and $\gamma \in [0, 1]$ is the discount factor. A labelled MDP is a tuple $\cal{M} = (S, A, s_0, P, R, \gamma, \cal{AP}, L)$; an MDP enriched with $\cal{AP}$, a finite alphabet of atomic propositions (labels), and $L: S \rightarrow 2^{\cal{AP}}$, a labelling function.

A sequence of states and actions $s_0, a_0, s_1, \ldots, a_{n-1}, s_n$ is called a trajectory. A state or action trajectory is the restriction to just the sequence of states $(s_i)_{i=0}^n \in S^+$ or actions $(a_i)_{i=0}^n \in A^+$. A state trajectory is attainable if $\prod_{i=0}^n P(s_{i+1} | s_i, a_i) > 0$ for some action trajectory $(a_i)_{i=0}^n$, and impossible otherwise. A trajectory is accompanied by a reward sequence $(r_i)_{i=0}^n$ and a sequence of labels, called a trace, $(\ell_i)_{i=0}^n \in (2^{\cal{AP}})^*$, where $L(s_i) = \ell_i$ for all $0 \leq i \leq n$. A (history-based) policy $\pi: (S \times A)^+ \times A \rightarrow [0, 1]$ is a function mapping trajectories to probability distributions over actions, where $\pi(a_t | s_0, a_0, \ldots, a_t, s_t)$ gives the probability of the agent choosing action $a_t$ at state $s_t$ given the (historical) trajectory $s_0, a_0, \ldots, s_t$.

Memoryless policies are a special case where the distribution over actions only depends on the last state (standard in RL because storing entire histories is intractable). The agent starts at $s_0$ in each exploration episode and, at each time step $t$, in state $s_t$, it selects action $a_t$ with probability $\pi(a_t | s_t)$, before transitioning to a new state $s_{t+1}$ with probability $P(s_{t+1} | s_t, a_t)$ whilst receiving a reward $r_t = R(s_0, a_0, \ldots, s_t, a_t, s_{t+1})$. The agent’s task is to find a policy $\pi$ that maximises the expected sum of discounted reward $\mathbb{E}_s [\sum_{t=0}^\gamma r_t]$. A policy $\pi$ is fully mixed if every action at every state is chosen with zero-probability (i.e., $\pi(a | s) > 0$ for all $s \in S$ and $a \in A$). We assume the agent observes state trajectories, traces, and reward sequences, as it explores the labelled MDP.\[1\]

1. This must encompass the initial transition, as evidenced by the use of the non-empty repetition operator $\ast$. 

Figure 1: (a) The labelled MDP environment and (b) 5 state TA representing a task specification for Example 1.

Given the initial state $s_0$, fixing the agent’s policy $\pi$ in an MDP $\cal{M}$ induces a Markov chain (MC) $\cal{M}_\pi$ if all state transitions, the reward function’s output is independent of the last action (i.e., $R(\zeta, a_i, s_{t+1}) = R(\zeta, a_j, s_{t+1})$ for all $a_i, a_j \in A$, where $\zeta \in (S \times A)^+$). Definition 1’s reward function is non-Markovian because it depends upon the full trajectory up until that point. A Markovian reward function $R : S \times A \times S \rightarrow \mathbb{R}$ only depends on the last transition. State-based rewards could also be handled straightforwardly.

Example 1. An RL agent is in Figure 1a’s environment. The task is to collect coffee $\text{coffee}$ for the guest on a couch $\text{couch}$ before turning on the TV $\text{tv}$ and then ascending the stairs (Figure 1b). The carpet $\text{carpet}$ and book $\text{book}$ do not affect whether the agent can achieve its goal. The arrow next to the silhouette indicates the initial state.

Example 1’s MDP environment is shown in Figure 1a. The agent’s possible actions $A$ are to move in the adjacent up, down, left, and right directions; the MDP’s state space cardinality $|S|$ is 25; and the transition dynamics are initially unknown (as discussed later, stochasticity in the dynamics derives from randomised action execution). The set of (atomic) propositional variables $\cal{AP} \equiv \{\text{coffee}, \text{couch}, \text{tv}\}$ represent the high-level features of the environment. Empty cells are implicitly labelled $L(s) = \emptyset$ (i.e., the MDP state $s \in S$ has no high-level environmental feature of interest).

If the agent only gets a positive reward upon completing the full task specification, this cannot be expressed with a Markovian reward function with respect to the MDP’s state space $S$ because the agent cannot go between states labelled $\text{coffee}$ and $\text{couch}$ in one timestep, let alone complete all four subtasks. So, the agent must learn an optimal policy in an environment with a non-Markovian reward function that provides sparse feedback. This challenge of planning using full trajectories can be surmounted by recognising that the agent also observes traces of high-level features in $\cal{AP}$. By maintaining a memory of complete subtasks (e.g., coffee collected) at this higher-level of abstraction (with smaller dimension), the agent can overcome the ‘curse of dimensionality’ and synthesise an optimal policy more efficiently by exploiting the compositionality of many tasks.

2.2 Task Specification

Linear temporal logic (LTL) or Linear Dynamic Logic (LDL), evaluated with respect to finite automata (LTLF/LDLF), is often used to express a task specification as temporally extended goals, or constraints on plans because this mitigates the sample inefficiency of RL in non-Markovian environments [14]. In fact, Littman et al. [22] argue that task specifications are superior to reward functions for specifying behaviour, as they are environment independent. We exploit the fact that the expressive power of both LTLF and LTLF is subsumed by the class of regular expressions, so they can be represented by deterministic or non-deterministic finite automata (DFAs/NFAs) [3].
Definition 2. A Non-Deterministic Finite Automaton (NFA) is a tuple $\mathcal{N} = (\Sigma, Q_0, \Sigma, \delta, F)$, where $Q$ is a finite set of states, $q_0 \in Q$ is the initial state, $\Sigma$ is a finite alphabet, $\delta : Q \times \Sigma \rightarrow 2^Q$ is a non-deterministic transition function, and $F \subseteq Q$ is the set of accepting states. If $\delta(q, \alpha) = 1$ for all $q \in Q$ and $\alpha \in \Sigma$, then $\mathcal{N}$ is deterministic and is called a Deterministic Finite Automaton (DFA).

Let $\Sigma^*$ be the set of all finite words over $\Sigma$. A finite word $w = \alpha_1 \alpha_2 \ldots \alpha_n \in \Sigma^*$ is accepted by an NFA $\mathcal{N}$ if there exists a finite run $u_0, u_1, \ldots, u_n \in \Sigma^*$ where $u_0 = q_0, u_{i+1} = \delta(u_i, \alpha_{i+1})$ for $0 \leq i < n$, and $u_n \in F$. In a DFA, only one path follows $w$, as each transition is deterministic, so the final state must be accepting, otherwise the word is rejected. The set of all accepted words is the language recognised by $\mathcal{N}$, denoted by $L(\mathcal{N})$. A DFA is trivially an NFA and any NFA can be converted into an equivalent DFA using Rabin and Scott’s subset construction method, so NFAs and DFAs both classify the recognition of regular languages.

Definition 3. A Task Automaton (TA) $\mathcal{A}$ is a DFA $(Q, q_0, \Sigma, \delta, F)$ with $\Sigma = 2^{AP}$, where $AP$ is a set of propositional variables inherited from the labelled MDP $M$.

We define a TA as a DFA to make our presentation as clear as possible. However, other types of automaton may also be used, such as lecarte et al’s [18]’s reward machines which, rather than having a set of accepting states (as in DFAs), outputs a reward function at each state. We define a TA as a DFA to make our presentation as clear as possible. We now give our three-step algorithmic pipeline for learning an MDP $M \otimes T$ with $T$ a TA.

Step 1: Learn the Product MDP

Input: put agent into an (unknown) labelled MDP $M$
Output: $T \otimes T^*$ that represents a task specification

1: $\text{Observe} \leftarrow$ collect episodes of corresponding trajectories, traces, and reward sequences.
2: function $\text{LearnProductMDP}(\text{Observe})$ \hspace{1cm} \textbf{Step 1}
3: Use an HMM/POMDP learning algorithm to learn estimates of (i) the spatial MDP, $M^*$’s transition probability distribution $P^*$, (ii) the product MDP $M \otimes T^*$’s transition probability distribution $P^\otimes$.
4: function $\text{DILUX}(M \otimes T^*, \text{Observe})$ \hspace{1cm} \textbf{Step 2}
5: Determinise $M \otimes T^*$ using Cone Lumpining to return the MDP-restricted $T^*$.
6: function $\text{PostProcess}(\hat{T}^*, \text{Observe})$ \hspace{1cm} \textbf{Step 3}
7: Remove environmental bias and minimise $\hat{T}^*$.

3.1 Step 1: Learn the Product MDP

Although the agent’s interactions with its environment are fully modelled by the product MDP, the product MDP is only partially observable. The agent observes MDP states as well as the associated labels and rewards but does not observe the TA states it visits. So, Step 1 involves learning the product MDP’s transition function $P^\otimes$ by viewing the agent’s interaction with the (product MDP) environment as a partially-observable Markov Decision Process (POMDP).

Definition 5. A Partially-Observable Markov Decision Process (POMDP) is a tuple $\mathcal{P} = (S, A, S_0, P, R, \gamma, O, Z)$ where
\( (S,A,s_0,P,R,\gamma) \) is an MDP, \( O \) is an observation set, and \( Z : O \times S \rightarrow [0,1] \) is an observation probability function, where \( Z(o | s) \) is a probability that observation \( o \in O \) is seen when the agent is at the hidden state \( s \in S \).

**Remark 1.** \( \mathcal{P}^\circ := (S^\circ, A, s_0^\circ, \mathcal{P}^\circ, R, \gamma, O, Z) \) is a POMDP that models an agent interacting with a product MDP\( M \otimes A' = (S^M, A^M, s_0^M, \mathcal{P}^M, R^M, \gamma) \), where the agent makes observations from the set \( O = S \times \{0,1\} \) according to the deterministic observation function \( Z : O \times S^\circ \rightarrow \{0,1\} \).

Remark 1 follows from Definitions 4 and 5. The agent’s observations in the POMDP \( \mathcal{P}^\circ \) are from \( S \times \{0,1\} \), where the latter component is a binary value corresponding to the co-domain of the reward function \( R^\circ \). At each time step, the agent transitions from a hidden state \( s_t \in S^\circ \) to \( s_{t+1} = (s_{t+1}, q_{t+1}) \) in the product MDP, but observes just \( \{s_{t+1}, \chi_F(q_{t+1})\} \) with probability 1. The product MDP state \( s_{t+1}^\circ \) is partially obscured from the agent. Recall \( \chi_F \) is the indicator function on the set of accepting states \( F \) in the TA \( A' \). If a policy \( \pi \) is chosen by the agent interacting with the POMDP \( \mathcal{P}^\circ \), then the POMDP becomes a partially observable Markov chain \( \mathcal{P}^\circ_{\pi} \), known as a Hidden Markov Model (HMM) \([26]\).

To learn the product MDP \( M \otimes A' \), we can employ any algorithm for learning HMMs or POMDPs and apply it to \( \mathcal{P}^\circ \) or \( \mathcal{P}^\circ_{\pi} \). We use the Baum-Welch algorithm (BW) \([8]\), due to its popularity and the ability to steer optimisation towards a desired local optimum (see Section 4) and, for further details, Appendices C and D. We learn \( \mathcal{P}^\circ_{\pi} \) in two stages. (i) Learn an estimate \( \mathcal{P} \) of the true spatial MDP \( M' \)’s transition probability distribution \( P \) using a fully mixed exploration policy \( \pi \). This can be any fully mixed policy, but we chose a uniform policy, \( \pi \) is a valid transition probability matrix. \( \mathcal{P} \) is isomorphic to the product MDP, \( M \otimes A' \). So, every hidden state of the learned model must correspond to a state \( s \in S \) in the true product MDP.

BW requires an initial guess on the number of hidden states \( |S^\circ| = |S| \times |Q| \). Since the agent can observe the MDP states, we only need guess the number of TA states \( K \). Furthermore, this guess only needs to be as large as the true \( k \) (i.e., \( k \geq Q \)). If \( k \) is too high, it generates duplication in the learnt matrix, which is easily identified. For a sufficient upper bound for \( k \) one can: use the label set cardinality, use a TA simplicity assumption, or identify the minimum number of distinct labels needed for task completion using successful exploration episodes. We did the latter. Further details about the convergence criterion and other hyper-parameters (such as the episode length and the number of episodes) are in Section 4.

To encode the learnt spatial MDP’s transition probability distribution \( \mathcal{P} \) as an inductive bias for learning \( \mathcal{P}^\circ \), we take the Kronecker product between a \( k \times k \) identity matrix and \( P^\circ \) (the matrix induced from \( P \) and \( \pi \)) to form the basis of the initial estimate of the product MDP’s transition matrix. For example, with a three-state TA:

\[
I_{3 \times 3} \otimes_K \mathcal{P} = \begin{pmatrix}
\mathcal{P} & 0 & 0 \\
0 & \mathcal{P} & 0 \\
0 & 0 & \mathcal{P}
\end{pmatrix}.
\]

Then, a small positive probability \( \varepsilon > 0 \) is added to each zero entry in the above construction to ensure that all expressions in the HMM learning procedure are well-defined. The probability \( \varepsilon \) can take any positive value, but we chose a value inversely proportional to \( |S^\circ| \) for consistency across experiments. Finally, each row is normalised so that the resulting initial estimate of the product MDP’s transition matrix \( \mathcal{P}^\circ \) is a valid transition probability matrix.

Concentrating on learning \( \mathcal{P}^\circ \) (the process is the same for learning \( \mathcal{P} \)), BW begins with initial estimates for the hidden transition distribution \( P^\circ_\tau \) (an \( |S|^\circ \times |S|^\circ \) matrix constructed from the inductive bias, as explained), the observation probability function \( Z \) (an \( |S|^\circ \times |O| \) matrix), and the initial state distribution (a vector \( \rho \in [0,1]^{\mid S^\circ} \) defined as \( \rho_\tau \equiv \Pr(s_0^\circ = s_0^\circ) \)). Then it finds the \( \mathcal{P}^\circ_\tau \) and \( Z \) that maximises the likelihood of obtaining the set of observation sequences \( O = \{o_1, \ldots, o_T\} \in (O^+)^T \).

**Definition 6.** Two product MDPs \( M_1 \otimes A_1 \) and \( M_2 \otimes A_2 \) with the same action spaces \( A_1 = A_2 \) are observationally equivalent, denoted \( M_1 \otimes A_1 \cong M_2 \otimes A_2 \), if for any observation sequence, any action trajectory, and all \( \tau \in N \), it holds that \( \Pr^\circ_\tau ([o_1]_{t=0}^\tau) \equiv \Pr^\circ_\tau ([o_2]_{t=0}^\tau) \), where \( \mathcal{P}^\circ_\tau = (M_1 \otimes \omega_0 \otimes A, Z) \). The observation spaces need not be identical for this to hold.

**Proposition 1.** The observational equivalence relation \( \cong \) is an equivalence relation since it is reflexive, symmetric, and transitive.

**Proposition 2.** Let \( M \) be a labelled MDP. For any two TAs \( A, A' \), if \( \mathcal{L}(A') = \mathcal{L}(A) \), then \( M \otimes A \cong M \otimes A' \).

**Proposition 1** says we can find the quotient set of all product MDPs identical for this to hold.

**Step 1:** Given state trajectories and reward sequences from interacting with the initially unknown product MDP \( M \otimes A' \), learn an estimate \( \mathcal{M} \otimes A' \in [M \otimes A'] \).

**Definition 7.** The digraph \( G = (E, V) \) underlying an MDP \( M \) with state space \( S \) and transition probability function \( \mathcal{P} \) has \( V = S \) and \( E = \{s_i \rightarrow s_j : \exists_k \in A \text{ s.t. } P(s_j | s_i, a_k) > 0\} \). \( M \) is structurally correct with respect to another MDP \( M' \) if the digraph underlying \( M \) is isomorphic to \( M' \).

Any algorithm which learns a maximum likelihood estimate (MLE) for the HMM parameters is asymptotically structurally correct, provided it converges to the true MLE and belongs in \([M \otimes A']\). So, every hidden state of the learned model must correspond to a state \( s^\circ \in S^\circ \) in the true product MDP \( M \otimes A' \).
Proposition 3. Suppose an agent is given a structurally correct product MDP \( M \otimes A \) belonging to \([M \otimes A] \), where \( M \) is the true MDP underlying the product MDP, and the agent can observe \( s \) and \( q \) for all \( (s, q) \in S^\pi \). Then, the agent can learn the MDP-restricted TA \( A_{M \otimes A} \), but may not be able to learn the full TA \( A \).

From Step 1, the agent knows the digraph of \( M \otimes A \) and an estimate \( \hat{P} \) for the transition probability function of the true MDP \( M \). Therefore, we first compute a product MC \( \hat{M} \) by assigning to the agent a fully mixed policy \( \pi \). We now recognise that when the edges of the digraph underlying \( M \otimes A \) are labelled according to each edge’s target state (recall that the agent observes traces), it results in an NFA whose accepting states are those in which reward 1 is obtained (see Appendix B for a worked example).

Proposition 4. Given a labelled product MC \( M \otimes A \) with binary reward, labelling every edge \( (s, q) \rightarrow (s', q') \) according to the label of its target state’s MDP component (i.e., in this case, \( L(s_j) = \ell \)) results in an NFA.

This NFA can be converted into a DFA with language equal to the MDP-restricted TA \( A_{M \otimes A} \) using the subset construction method [25].

Proposition 5. Let \( N \) be the NFA underlying the learnt product MC \( M \otimes A \). Then, \( L(N) = L(A_{M \otimes A}) \), where \( A_{M \otimes A} \) is the MDP-restricted true TA.

However, the subset-construction algorithm has worst-case exponential time complexity in the size of the NFA (i.e., \( O(2^{|S|}) \)). We therefore introduce our more efficient Cone Lumping method for determining NFAs that underlie MDPs, which explicitly leverages their product structure. ‘Lumping’ aligns with related literature (e.g., [9]). Our key insight is that out-going edges from a product state \( (s, q) \in S^\pi \) of a product MDP \( M \otimes A \) that have the same label must transition to the same next TA state. Every time this occurs, the product states are merged. When representing state transitions sequentially from left to right, this merging criterion looks for a cone structure to merge all states on the right-hand side (Figure 2).

Lemma 1 (Cone Lumping). Given a labelled product MC \( M \otimes A \), let \( E^\pi_{\ell}(s, q) = \{(s, q) \overset{\ell}{\rightarrow} (s', q') : L(s_j) = \ell \} \) be the set of all out-going edges from state \( (s, q) \) in the digraph underlying \( M \otimes A \) with label \( \ell \). Since any TA transition \( q \overset{\ell}{\rightarrow} q' \) is deterministic, then \( q_1 = q_2 \) for any pair \( q_1, q_2 \in \{q' : (s, q) \overset{\ell}{\rightarrow} (s', q') \} \). Thus, for a product state \( (s, q) \), \( \{(q' : (s, q) \overset{L(s_j)}{\rightarrow} (s', q')) : L(s_j) = \ell \} = 1 \).

Performing Cone Lumping for all \( (s, q) \in S^\pi \) until a fixed point is reached (i.e., no more states can be merged), obtains a TA accepting (at minimum) \( L(A_{M \otimes A}) \), and at most \( L(A) \) (by construction of the product MDP). This is because all non-determinism in the NFA underlying \( M \otimes A \) comes from the possible existence of multiple out-going edges with the same label from a product state.

![Figure 2: Schematics of “Cone Lumping”.](image-url)

Proposition 6. Cone Lumping determinises any product MDP in \( O(|S|^3) \), exponentially faster than Rabin and Scott [25]’s subset-construction \( O(2^{|S|}) \) algorithm.

Cone Lumping therefore efficiently converts an NFA underlying a labelled MC into a DFA (our TA in this work, Section 3) and it assists in transfer learning because the hardness is confined to learning the product MDP. If the MDP or TA changes slightly, the agent only has to relearn the affected part of the product MDP, before using Cone Lumping to efficiently distil the new TA. In practice, this uses the transition probability distribution \( P^\pi_{\ell} \) of the old MDP and TA’s product MDP as an initial estimate for the new product MDP. The parts of the MDP and TA that remain the same will not need updating, so Baum-Welch only needs to update the parts that have changed. This speeds up convergence significantly [38]. Finally, this process can also be useful outside of our work, e.g., for simulation or model reduction studies [20].

3.3 Step 3: Remove environmental bias and minimise the learnt TA

The TA distilled from the product MDP in Step 2 is in general not unique (cf. Section 3.1). If the TA is a DFA, as has been this paper’s focus, it can be minimised using, for instance, Hopcroft [16]’s algorithm in \( O(n \log n) \). However, the TA might also not be minimal due to environmental bias. If a certain label must be traversed by the agent to reach a necessary label for achieving the underlying task specification, automaton-learning algorithms cannot differentiate the importance of the two labels and will therefore assume that both are necessary TA transitions, even when the former is unnecessary.

Theorem 1. Given an arbitrary product MDP \( M \otimes A \), the TA distilled from \( M \otimes A \) may not be unique because there can exist \( A \neq A' \), with or without \( L(A \neq A') \), such that \( M \otimes A \equiv M \otimes A' \).

Proof sketch by (counter)example. Let \( M \) be the labelled MDP defined by the environment in Figure 1a and \( A \) and \( A' \) be the TAs in Figures 3a and 3b respectively, where \( A \) is the true TA. Then, \( A' \) satisfies \( M \otimes A' \equiv M \otimes A \). In Figure 1a a \( \equiv \)-label must be traversed immediately prior to reaching the \( \equiv \)-label, no matter which MDP path to \( \equiv \) is taken. Because reward is only obtained upon reaching \( \equiv \), there is no way to identify from the reward signal if the sequence \( (\equiv, \equiv) \) is necessary for reward, or just reaching \( \equiv \) suffices. The agent does not know which of the two task specifications, expressed by the TAs \( A \) and \( A' \), is sufficient.

Corollary 1. In general, it is impossible to verify that a TA \( A \) is the TA that underpins the product MDP \( M \otimes A \) (i.e., that \( A' = A \)), even given knowledge of \( M \) and \( M \otimes A \).

![Figure 3: Two TAs for Example 1’s environment in Figure 1a to show the learned TA can be environmentally biased.](image-url)
Thus, to minimize environmental bias, we must use counterfactual reasoning in our post-processing step to select among the set of TAs \( \mathcal{A} \) such that \( \mathcal{A} : \mathcal{M} \otimes \mathcal{A} = \mathcal{M} \otimes \mathcal{A} \) the TA that requires the smallest alphabet to explain its behaviour.

**Step 3:** For every label in \( L(S) \), guess that it has no effect in the supposed true TA \( \mathcal{A} \) (i.e., the agent self-loops on every TA state). To check this guess, first merge any states of the learned-automaton \( \mathcal{A} \) that have a non-loop edge between them with this label, then check if the resulting TA outputs the correct acceptance/rejection on every word in the set of observed sequences.

This post-processing only removes labels that are never meaningful to \( \mathcal{A} \); it does not remove labels that are necessary somewhere, but may still exist ‘wrongfully’ in \( \mathcal{A} \) due to environmental bias. Further post-processing can address this by looking for neighbourhoods of (possibly same-labelled) states that entirely surround another label, then checking, as above, whether these are necessary in \( \mathcal{A} \).

### 4 Experimental Results

Although the main contributions of this paper are theoretical, our experiments (available at [https://github.com/dkhyland/TALearner](https://github.com/dkhyland/TALearner)) evaluate the efficacy of Algorithm 1’s pipeline. To our knowledge, we are the first to focus on the task of learning both the TA and spatial MDP starting from no a-priori knowledge. Our experiments assess our pipeline’s ability to scale up to 5x5 MDP grid-worlds and 5-state TAs and benchmark, where possible, to related work. These sizes are comparable to or beyond those handled in all related work (see Section 5).

Figure 4 illustrates the three grid worlds and the three-, four-, and five-state TAs used for our experiments. The grid worlds all share a common set of high-level environmental features \( \mathcal{A}P \equiv \{ \text{start}, \text{couch}, \text{coffee} \} \), which have been distributed randomly across the grid. The agent can visit every action and state within the grid world.

For all experiments, the convergence criterion was taken to be the point when the difference between the transition matrix estimates over one pass through the training data achieves a maximum absolute row sum less than \( 10^{-6} \). In practice, this is sufficient to ensure that a structurally correct product MDP is learned.

The episode length and number of episodes used in the training data are hyperparameters that can affect both the convergence time and the structural correctness of the learnt transition matrix. In practice, choosing the episode length so that the agent achieves (on average) the goal in between 20 – 50% of the episodes, ensures that the agent sufficiently explores all states in the product MDP. Additionally, a general trend was observed that for larger product MDPs, more training episodes were required to obtain a structurally correct estimate of the transition matrix. The number of episodes that were sufficient for convergence in our experiments was less in our model-based approach than in model-free approaches in related work (Section 5).

Exact hyperparameters used and full results are presented in Table 1 in Appendix E.

Step 1 of our algorithm (learning the product MDP) is implemented in C++ (see Appendices D and E for more details), and the remaining steps are implemented in Python. All experiments are the average of 3 runs (with negligible standard errors) and were conducted on an Intel Xeon Gold 6248 (2.50GHz) CPU. Cone Lumping (Step 2) determines the NFA underlying the product MDP for the 5x5 grid and 5-state TA in Figure 1 in 0.43s, and removing environmental bias (Step 3) takes 0.8ms. This also confirms the usefulness of these steps for other purposes (argued in Sections 3.2 and 5.3).

Figure 4a demonstrates our approach’s superiority over the uniform baseline. We plot the convergence times of Step 1 for our approach (in red) against the two baselines for the 3 state TA and 3 different grid sizes. As the size of the grid increases, the time taken to learn an accurate estimate of the product MDP trends towards the idealised baseline. This is because the time taken to learn \( \hat{P} \) in the first stage becomes negligible compared with learning the TA. Thus, learning the TA via a larger (and therefore ostensibly more complex) structure first, the product MDP, does not noticeably increase the time complexity of the process. This also demonstrates why our process is useful for transfer learning (Section 3.2).

Figure 5a demonstrates our approach’s superiority over the uniform baseline. We plot the convergence times of Step 1 for our approach (in red) against the two baselines for the 3 state TA and 3 different grid sizes. As the size of the grid increases, the time taken to learn an accurate estimate of the product MDP trends towards the idealised baseline. This is because the time taken to learn \( \hat{P} \) in the first stage becomes negligible compared with learning the TA. Thus, learning the TA via a larger (and therefore ostensibly more complex) structure first, the product MDP, does not noticeably increase the time complexity of the process. This also demonstrates why our process is useful for transfer learning (Section 3.2).

Figure 5b shows the dependence of the convergence time on the sizes of the MDP environment and TA. Increasing the TA size increases the number of sub-tasks the agent must complete before receiving reward. This Figure also shows how our algorithm’s efficiency compares with related work. We presented the codebases of
five related works (see Appendix F for details) the same sequences used in our smallest experiment (3x3 grid with a 3-state TA), but none of these could successfully learn the TA (or threw a recursion error). We were, however, able to perform some benchmarks against an implementation of Biermann and Feldman’s SAT-based algorithm in the libalf library to infer a hypothesis reward machine consistent with the data for the 3- and 4-state TAs. We used the same set of sequences that were used in our algorithm for comparison, which were labelled as positive or negative sequences depending on whether the agent received a reward. With a 4-state TA, ours had a lower convergence time in a 4x4 gridworld than BF managed in even a 3x3 gridworld, and BF timed out at 150,000s when trying to learn the 5-state TA in the 3x3 gridworld.

Learning an automaton from data is NP-hard \[\text{(13)}\], so under standard complexity assumptions, the time taken to solve this problem will necessarily grow exponentially as a function of the size of the TA. The most appropriate method will depend on the use-case as different approaches choose to relax different assumptions. For example, Corazza et al \[\text{(8)}\] and Dohmen et al \[\text{(10)}\] extend the SAT-based approach to noisy rewards and the \(L^*\) approach to learning probabilistic automata, respectively.

Our method is most appropriate in the following situations. First, when one does not assume the presence of an oracle (required for \(L^*\)). Second, if the reward environment is sparse, i.e. where the agent must follow a sequence of non-rewarding steps before getting a reward if and only if it completes the full task. Third, when sample-efficiency is critical (as in many real-world scenarios) since our model-based approach requires fewer episodes to learn the TA. Fourth, for transfer learning: our approach can readily handle the underlying MDP or TA changing slightly. For example, suppose the initial task specification is to get coffee for the guest on the couch. Then, the furniture is rearranged and the task changes from collecting coffee to collecting tea. Only the affected part of the product MDP needs to be re-learnt before performing the subsequent computationally cheap steps (2 and 3) in our algorithmic pipeline. Other methods would need to start learning the new TA from scratch each time. Finally, the stochastic nature of our approach has advantages over the discrete approaches of related work; e.g., we can easily incorporate active-learning to more intelligently guide the agent’s exploration \[\text{(3)}\]. Furthermore, our stochastic approach allows for entropy-based uncertainty quantification and it will always generate an estimate of the solution even with few exploration episodes.

5 Related Research

SAT-based approaches \[\text{(1}\text{,} \text{8}\text{,} \text{15}\text{,} \text{34}\text{,} \text{36)}\] generate a hypothesis automaton (equivalent to a temporal specification) and then verify whether this agrees with the agent’s observations during exploration. We showed that these are less efficient than our approach by benchmarking against the only available codebase that learnt an automaton from our traces. Meanwhile, Icarte et al \[\text{(12)}\] use Tabu search, which relies on already knowing a partial model, and Furelos-Blanco et al \[\text{(11)}\] use an Answer Set Programming algorithm, which assumes a known upper bound for the maximum finite distance between TA states. Our assumptions are weaker than these as we are only required to guess an upper bound on the number of TA states (in Section \text{4} we explained why this is easy to do) and we do not require any a priori knowledge about the spatial MDP. Also, all of these approaches are local, whereas ours is complete in the sense that our TA captures all sequential behaviour seen in the traces (high-level features).

\[\text{21}\text{,} \text{28}\text{,} \text{33)}\] all consider probabilistic approaches to learning specifications. Their maximum entropy approaches (inspired by Ziebart et al \[\text{(29)}\]’s variant of inverse reinforcement learning) start from an initial pool of candidate specifications. In contrast, our maximum-likelihood approach does not a priori require any structure of the specification or the spatial MDP environment. Meanwhile, \[\text{11}\text{,} \text{12}\text{,} \text{27)}\] use Angluin’s \(L^*\) algorithm to learn a TA, relying on an oracle for equivalence and membership queries. We assume that the agent cannot access an oracle and must learn the TA fully autonomously, which aligns with the standard setup of model-free RL (note that \(L^*\) was not originally developed for RL applications). Because this means our training data cannot be provided as input to \(L^*\), we cannot benchmark fairly against these approaches.

6 Conclusions and Future work

We have introduced an unsupervised pipeline for an RL agent to learn task specifications, encoded as deterministic, finite automata known as ‘task automata’, in unknown environments with sparse and non-Markovian rewards. The agent first learns a product MDP – a composition of the task automaton with the environment’s MDP before distilling out a task automaton using our efficient ‘Cone Lumping’ method. Finally, our post-processing routine, which is useful for any method that learns automata in RL, minimises environmental bias and simplifies the learnt task automaton.

As future work, we are extending to environments with multiple tasks (i.e., cases where an agent can achieve reward by satisfying multiple different task specifications); introducing active learning to further improve the efficiency of the rate-limiting Step 1; and trying different techniques for learning HMMs/POMDPs (e.g., spectral learning \[\text{17)}\]. We are also interested in multi-agent settings, where agents get rewarded according to different tasks or have to optimally share information to learn a common task. Finally, we intend to extend to cases where the task automata encode \(\omega\)-regular LTL properties, which require evaluation over infinite trajectories.

Acknowledgements

Fox was supported by the EPSRC Centre for Doctoral Training in Autonomous Intelligent Machines and Systems (Reference: EP/S024050/1) and Wooldridge was supported by a UKRI Turing AI World Leading Researcher Fellowship (Reference: EP/W002949/1).
References

[1] Eden Abadi and Ronen I Brafman, ‘Learning and solving regu-
lar decision processes’, in 29th International Joint Conference on Artificial Intelligence, IJCAI 2020, pp. 1948–1954. Interna-
tional Joint Conferences on Artificial Intelligence, (2020).

[2] Dario Amodei, Chris Olah, Jacob Steinhardt, Paul Christi-
ano, John Schulman, and Dan Mané, ‘Concrete problems in ai
safety’, arXiv preprint arXiv:1606.06565, (2016).

[3] Brigham Anderson and Andrew Moore, ‘Active learning for
hidden markov models: Objective functions and algorithms’, in Proceedings of the 22nd international conference on Machine
learning, pp. 9–16, (2005).

[4] Dana Angluin, ‘Learning regular sets from queries and counterexamples’, Information and computation, 75(2), 87–
106, (1987).

[5] Christel Baier and Joost-Pieter Katoen, Principles of model
checking, MIT press, 2008.

[6] Leonard E Baum and Ted Petrie, ‘Statistical inference for prob-
abilistic functions of finite state markov chains’, The annals of mathematical statistics, 37(6), 1543–1563, (1966).

[7] Alan W Bjerrum and Jerome A Feldman, ‘On the synthesis of finite-state machines from samples of their behavior’, IEEE
transactions on Computers, 100(6), 592–597, (1972).

[8] Jan Corazza, Ivan Gavran, and Daniel Neider, ‘Reinforcement
learning with stochastic reward machines’, in Proceedings of the AAAI Conference on Artificial Intelligence, volume 36, pp. 6429–6436, (2022).

[9] Salem Derisavi, Holger Hermanns, and William H Sanders, ‘Optimal state-space lumping in markov chains’, Information Processing Letters, 87(6), 309–315, (2003).

[10] Taylor Dohmen, Noah Topper, George Atia, Andre Beckus, Ashutosh Trivedi, and Alvaro Velasquez, ‘Inferring probabil-
istic reward machines from non-markovian reward signals for reinforcement learning’, in Proceedings of the Interna-
tional Conference on Automated Planning and Scheduling, volume 32, pp. 574–582, (2022).

[11] Daniel Furelos-Blanco, Mark Law, Anders Jonsson, Krysia
Broda, and Alessandra Russo, ‘Induction and exploitation of subgoal automata for reinforcement learning’, Journal of Arti-
ficial Intelligence Research, 70, 1031–1116, (2021).

[12] Maor Gaon and Ronen Brafman, ‘Reinforcement learning with non-markovian rewards’, in Proceedings of the AAAI Conference on Artificial Intelligence, volume 34, pp. 3980–3987, (2020).

[13] E Mark Gold, ‘Complexity of automaton identification from
given data’, Information and control, 37(3), 302–320, (1978).

[14] Mohammadhossein Hasanbeig, Alessandro Abate, and Daniel
Kroening, ‘Logically-constrained reinforcement learning’, arXiv preprint arXiv:1801.08099, (2018).

[15] Mohammadhossein Hasanbeig, Natasha Yogananda Jeppu, Alessandro Abate, Tom Melham, and Daniel Kroening, ‘Deep-
synth: Automata synthesis for automatic task segmentation in
deep reinforcement learning’, in Proceedings of the AAAI Con-
ference on Artificial Intelligence, volume 35, pp. 7647–7656, (2021).

[16] John Hopcroft, ‘An n log n algorithm for minimizing states in a
finite automaton’, in Theory of machines and computations,
189–196, Elsevier, (1971).

[17] Daniel Hsu, Sham M Kakade, and Tong Zhang, ‘A spectral al-
gorithm for learning hidden markov models’, Journal of Com-
puter and System Sciences, 78(5), 1460–1480, (2012).

[18] Rodrigo Toro Icarte, Toryn Q Klassen, Richard Valenzano,
and Sheila A McIlraith, ‘Reward machines: Exploiting reward
function structure in reinforcement learning’, Journal of Artifi-
cial Intelligence Research, 73, 173–208, (2022).

[19] Kishor Jothimurugan, Suguman Bansal, Osbert Bastani, and Raje
vur, ‘Compositional reinforcement learning from logical
specifications’, Advances in Neural Information Processing
Systems, 54, 10026–10039, (2021).

[20] K. G. Larsen and A. Skou, ‘Bisimulation through probabilistic
testing’, Information and computation, 94(1), 1–28, (1991).

[21] Niklas Lauffer, Beyazit Yalcinkaya, Marcell Vazquez-
Chanlatte, Ameesh Shah, and Sanjit A Seshia, ‘Learning
deterministic finite automata decompositions from examples
and demonstrations’, in Conference on Formal MEthods in
Computer-Aided Design–FMCAD 2022, p. 325.

[22] Michael L Littman, Ufak Topcu, Jie Fu, Charles Isbell, Min
Wen, and James MacGlashan, ‘Environment-independent task
specifications via GLTL’, arXiv preprint arXiv:1704.04341, (2017).

[23] Shubham Pateria, Budhimagga Subagdja, Ah-hwee Tan, and
Chai Quek, ‘Hierarchical reinforcement learning: A compre-
hensive survey’, ACM Computing Surveys (CSUR), 54(5), 1–35, (2021).

[24] Michael O Rabin, ‘Probabilistic automata’, Information and
control, 6(3), 230–245, (1963).

[25] Michael O Rabin and Dana Scott, ‘Finite automata and their
decision problems’, IBM journal of research and development,
3(2), 114–125, (1959).

[26] Lawrence R Rabiner, ‘A tutorial on hidden markov models and
selected applications in speech recognition’, Proceedings of the IEEE, 77(2), 257–286, (1989).

[27] Gavin Rens, Jean-François Raskin, Raphaël Reynaud, and Gi-
useppe Marra, ‘Online learning of non-markovian reward mod-
els’, in Proceedings of the Thirteenth International Conference on Agents and Artificial Intelligence, volume 2, pp. 74–66.
Scitepress, (2020).

[28] Raed Saqr, ‘Reward learning using structural mo-
tifs in inverse reinforcement learning’, arXiv preprint
arXiv:2209.13489, (2022).

[29] Matthew E Taylor and Peter Stone, ‘Cross-domain transfer for
reinforcement learning’, in Proceedings of the 24th interna-
tional conference on Machine learning, pp. 879–886, (2007).

[30] Sylvie Thiébaux, Charles Grettton, John Slaney, David Price,
and Produljd Kabanza, ‘Decision-theoretic planning with non-
markovian rewards’, Journal of Artificial Intelligence Re-
search, 25, 17–74, (2006).

[31] Noah Topper, George Atia, Ashutosh Trivedi, and Alvaro
Velasquez, ‘Active grammatical inference for non-markovian
planning’, in Proceedings of the International Conference on
Automated Planning and Scheduling, volume 32, pp. 647–651, (2022).

[32] Rodrigo Toro Icarte, Ethan Walddie, Toryn Klassen, Rick Valen-
zano, Margarita Castro, and Sheila McIlraith, ‘Learning reward
machines for partially observable reinforcement learning’, Adv-
ces in Neural Information Processing Systems, 32, 15523–
15534, (2019).

[33] Marcell Vazquez-Chanlatte, Susmit Jha, Ashish Tiwari,
Mark K Ho, and Sanjit Seshia, ‘Learning task specifi-
cations from demonstrations’, Advances in Neural Information Processing Systems, 31, 5367–5377, (2018).
[34] Christos Verginis, Cevahir Koprulu, Sandeep Chinchali, and Ufuk Topcu, ‘Joint learning of reward machines and policies in environments with partially known semantics’, arXiv preprint arXiv:2204.11833, (2022).

[35] Tingwu Wang, Xuchan Bao, Ignasi Clavera, Jerrick Hoang, Yeming Wen, Eric Langlois, Shunshi Zhang, Guodong Zhang, Pieter Abbeel, and Jimmy Ba, ‘Benchmarking model-based reinforcement learning’, arXiv preprint arXiv:1907.02057, (2019).

[36] Zhe Xu, Ivan Gavran, Yousef Ahmad, Rupak Majumdar, Daniel Neider, Ufuk Topcu, and Bo Wu, ‘Joint inference of reward machines and policies for reinforcement learning’, in Proceedings of the International Conference on Automated Planning and Scheduling, volume 30, pp. 590–598, (2020).

[37] Zhe Xu, Bo Wu, Aditya Ojha, Daniel Neider, and Ufuk Topcu, ‘Active finite reward automaton inference and reinforcement learning using queries and counterexamples’, in International Cross-Domain Conference for Machine Learning and Knowledge Extraction, pp. 115–135. Springer, (2021).

[38] Fanny Yang, Sivaraman Balakrishnan, and Martin J Wainwright, ‘Statistical and computational guarantees for the baum-welch algorithm’, in 2015 53rd Annual Allerton Conference on Communication, Control, and Computing (Allerton), pp. 658–665. IEEE, (2015).

[39] Brian D Ziebart, Andrew L Maas, J Andrew Bagnell, Anind K Dey, et al., ‘Maximum entropy inverse reinforcement learning’, in AAAI, volume 8, pp. 1433–1438. Chicago, IL, USA, (2008).
Learning Task Automata for Reinforcement Learning Using Hidden Markov Models (Supplementary Material)

A Proofs of Technical Results

Proposition 2. Let $\mathcal{M}$ be a labelled MDP. For any two TAs $\mathcal{A}$, $\mathcal{A}'$, if $L(\mathcal{A}) = L(\mathcal{A}')$, then $\mathcal{M} \otimes \mathcal{A} \cong \mathcal{M} \otimes \mathcal{A}'$.

Proof. Consider the two product Markov processes $\mathcal{M} \otimes \mathcal{A}$ and $\mathcal{M} \otimes \mathcal{A}'$ constructed by composing the MDP $\mathcal{M}$ with each TA $\mathcal{A}$ and $\mathcal{A}'$. At each time step $t$, the agent’s observation $o_t$ is a pair in $S \times \{0, 1\}$. Therefore, observation sequences restricted to the first component of the observation pair are state trajectories, and restricted to the second component are reward sequences $(\chi x(q_i))_{i=0}^\infty \in \{0, 1\}^\ast$. The probabilities of state trajectories must be equal for $\mathcal{M} \otimes \mathcal{A}$ and $\mathcal{M} \otimes \mathcal{A}'$, since they are constructed from identical environments $\mathcal{M}$, and the probabilities of reward sequences must be equal because the languages of $\mathcal{A}$ and $\mathcal{A}'$ are identical by assumption.

Proposition 3. Suppose an agent is given a structurally correct product MDP $\mathcal{M} \otimes \mathcal{A}$ belonging to $[\mathcal{M} \otimes \mathcal{A}]$, where $\mathcal{M}$ is the true MDP underlying the product MDP, and the agent can observe $s$ and $q$ for all $(s, q) \in S^\ast$. Then, the agent can learn the MDP-restricted TA $\mathcal{A}^\ast_{\mathcal{M}}$ but may not be able to learn the full TA $\mathcal{A}$.

Proof. Start with the product MDP $\mathcal{M} \otimes \mathcal{A}$, where the agent can observe the MDP and TA state components ($s$ and $q$) of each product MDP state $s^\circ = (s, q)$. Induce a product MC $\mathcal{M}_s \otimes \mathcal{A}$ by employing a random exploration policy $\pi$. Note that any exploration policy can be used here, provided that every action is chosen at every state with non-zero probability. For each transition $P^\circ((s_j, q_j) \mid (s_i, q_i)) > 0$ in $\mathcal{M}_s \otimes \mathcal{A}$, add the edge $q_i \xrightarrow{L(s_i)} q_j$ to the candidate TA (unless it already exists). After going through all such transitions in the product MDP, all TA transitions accessible by an MDP-attainable trace must have been exhausted. We have therefore created the MDP-restricted TA $\mathcal{A}^\ast_{\mathcal{M}}$, which may not be equal to the true underlying TA $\mathcal{A}$ because there might exist a path in $\mathcal{A}$ that corresponds with a trace that cannot be generated by an agent exploring in $\mathcal{M}$.

Proposition 4. Given a labelled product MC $\mathcal{M}_s \otimes \mathcal{A}$ with binary reward, labelling every edge $(s_i, q) \rightarrow (s_j, q_j)$ according to the label of its target state’s MDP component (i.e., in this case, $L(s_i) = t_j$), results in an NFA.

Proof. An NFA is a tuple $(Q, q_0, \Sigma, \delta, F)$ (Definition 2). The set of states $Q$ is the set of states of the product MDP. The state $q_0$ is the same as the initial state of the product MDP (since the initial states of the MDP $\mathcal{M}$ and TA $\mathcal{A}$ are known). $\Sigma = 2^{AP}$ since these are the possible labels of the edges. $\delta$ is indeed a non-deterministic transition function since from any state $s \in S$, there may be multiple $s_i \in S$ such that a transition from $s$ to $s_i$ is possible, and $L(s_i) = \ell$. That is, multiple possible next states may exist, which all have the same label. Finally, the accepting states $F$ are the accepting states of the product MC $\mathcal{M}_s \otimes \mathcal{A}$ – i.e., the states where the reward observed is non-zero.

Proposition 5. Let $\mathcal{N}$ be the NFA underlying the learnt product MC $\mathcal{M}_s \otimes \mathcal{A}$, then, $L(\mathcal{N}) = L(\mathcal{A}_{\mathcal{M}})$, where $\mathcal{A}_{\mathcal{M}}$ is the MDP-restricted true TA.

Proof. $\mathcal{N}$ accepts precisely those words that terminate at an accept state of the product MC $\mathcal{M}_s \otimes \mathcal{A}$, and because a product state is an accept state if and only if its TA-component is accepting, the language recognised by $\mathcal{N}$ must be contained in the language of the true underlying TA. Moreover, because the set of paths in $\mathcal{N}$ underlying $\mathcal{M}_s \otimes \mathcal{A}$ is precisely the set of MDP-attainable paths of the true TA, the language of $\mathcal{N}$ is precisely the language of the MDP-restricted TA $\mathcal{A}_{\mathcal{M}}$.

Proposition 6. Cone Lumping determinises any product MDP in $O(|S^\circ|^3)$, exponentially faster than Rabin and Scott’s subset-construction $O(2^{|S^\circ|})$ algorithm.

Proof. Our implementation of Cone Lumping (Lemma 1) uses iterations that involve looping over all states in $S^\circ$ and all out-going transitions at each state and then merging any successor-state with the same label from $2^{|S^\circ|}$ into one equivalence class that is used as the new state. The iterations end when no states can be ‘lumped’ into the same equivalence class (corresponding to the same TA state). In the worst case, only one state is subtracted from the NFA upon each iteration, implying that there are at most $|S^\circ| - 1$ iterations. This also implies that, in the worst case, the number of successor-states that need to be checked on iteration $i$ is $|S^\circ| - i^2$: there are $|S^\circ| - i$ states left in the model, and from any of these there are at most $|S^\circ| - i$ out-going edges (in the worst case, the underlying graph is fully-connected). Thus, the worst-case number of check-operations before this algorithm terminates is $\sum_{i=2}^{|S^\circ|} i^2 = \frac{1}{6}|S^\circ|(|S^\circ| + 1)(|S^\circ| + 2) - 1 = O(|S^\circ|^3)$. In the common case where there are precisely $k$ permitted out-going transitions from any state in the model (e.g., gridworld environments), this complexity reduces to $\sum_{i=2}^{|S^\circ|} i \cdot k = \frac{k}{2}|S^\circ|(|S^\circ| + 1) - k = O(|S^\circ|^2)$.

2 A state $(s', q')$ such that $(s, q) \rightarrow (s', q')$ is called a successor-state of $(s, q)$.
A product MDP is of size $|S \times Q|$, so we use a simple $3 \times 3$ grid-world with a three state TA (Figure 6a) to use as an easy demonstration of cone lumping. The task specification here again can still not be expressed by a Markovian reward function because the agent cannot go from either ☕ to the stairs 🕊 in one step. A product MDP in this environment can be learnt using Step 1 of our pipeline. We then induce a product MC by assigning to the agent a fully mixed policy $\pi$. Figure 6b then shows the NFA underlying this product MC, where the edges have been labelled as instructed in Proposition 5 and $(s_{21}, q_2)$ is the only accepting state.

For the Cone Lumping step, any two outgoing edges from a product state of this NFA underlying a labelled product MC that have the same label must transition to the same next TA state (cf. Section 3.2). Observe that this is the case in Figure 6b; for example, every edge labelled with $\emptyset$ outgoing from $(s_{00}, q_0) \in S^\otimes$ ends up in a TA state with $q_0$ as its TA component. Cone Lumping efficiently converts the NFA in Figure 6b into the DFA in Figure 6a.

In the main text, we also mentioned that Cone Lumping helps transfer learning because the hardness has been confined to learning the product MDP. If the spatial MDP or the TA changes slightly, the agent only has to relearn the affected part of the product MDP, then can use Cone Lumping to efficiently find the new TA. For instance, if after learning the TA from exploring the spatial MDP in Figure 6a, the agent was then put in a new $3 \times 3$ grid-world with no carpets present. The agent only has to re-learn the parts of the product MDP associated with MDP states $s_{20}$ and $s_{22}$ before applying our efficient Cone Lumping method again. It would then find that the old TA still applies.

Figure 6: A simple MDP (a) and TA (b). (c) The NFA underlying the product MDP constructed from this MDP and TA under a fully mixed policy $\pi$. MDP states $S$ are labelled $s_{xy}$ (for $x, y \in \{0, 1, 2\}$) corresponding to the horizontal ($x$) and vertical ($y$) cell position in the grid.
C Baum-Welch Algorithm

This section more completely introduces the Baum-Welch algorithm [3] that we use to implement Step 1 of our TA learning pipeline. Recall there are two stages of Baum-Welch: i) learning the transition probability distribution \( \bar{P} \) of the MDP \( \mathcal{M} \) and ii) learning the transition probability distribution \( \bar{P} \) of the product MDP \( \mathcal{M} \otimes \mathcal{S} \). Both follow the same procedure, where the result of the former is used for the initial parameters (an inductive bias) of the latter (see Section 3.1). Since it is the ultimate goal of this procedure, we spell out the procedure for the latter where the hidden Markov model is \( \bar{P} = (\mathcal{S}, s_0^\mathcal{S}, P_{ij}^\mathcal{S}, R, \gamma, O, Z) \) (constructed from the product MDP and a fully mixed policy \( \pi \)).

Baum-Welch uses an ‘expectation-maximisation’ method to find the hidden transition matrix and the observation (or emissions) distribution \( Z \) that maximises the likelihood of obtaining the given set of observation sequences,

\[
O = (o_1, ..., o_T) \in (O^*)^T.
\]

Formally, we represent this optimisation problem as:

\[
\langle \bar{P}, Z \rangle = \arg \max_{\langle \bar{P}, Z \rangle} \Pr \{ O \mid \langle \bar{P}, Z \rangle \}.
\]

**Defining HMM Parameters.** The hidden Markov chain’s state space is the set \( \mathcal{S} \) and, as is commonly done, we will view the transition probability function \( P_{ij}^\mathcal{S} : \mathcal{S} \times \mathcal{S} \rightarrow [0, 1] \) as a matrix, with elements

\[
P_{ij}^\mathcal{S} = P_{ij}^\mathcal{S} = P_{ij}^\mathcal{S} \mid s_{i-1} = s_i^\mathcal{S}.
\]

This representation is induced by a bijective mapping, so no information is lost.

Formally, we represent this optimisation problem as:

\[
\langle \hat{P}^\mathcal{S}, \hat{Z} \rangle = \arg \max_{\langle \bar{P}, Z \rangle} \Pr \{ O \mid \langle \bar{P}, Z \rangle \}.
\]

We do the same for the distribution \( Z \), but call the matrix \( E^Z \) (for ‘emissions from \( Z \’):

\[
E_{ij}^Z \equiv Z(o_t = o_i \mid s_i = s_j^\mathcal{S}).
\]

Here, \( o_i \) represents the \( i \)-th element of the finite observation set \( O \) under any fixed ordering. Thus, \( E^Z_{ij} \) is the probability that observation \( O_i \) is emitted when the hidden state is \( s_j^\mathcal{S} \).

Under these definitions, \( P_{ij}^\mathcal{S} \) is an \( | \mathcal{S}^\mathcal{S} | \times | \mathcal{S}^\mathcal{S} | \) matrix and \( E^Z \) is an \( | \mathcal{S}^\mathcal{S} | \times | O | \) matrix.

Lastly, we define the initial state distribution \( \rho \in [0, 1]|\mathcal{S}^\mathcal{S}| \) by

\[
\rho_j \equiv \Pr[s_0^\mathcal{S} = s_j^\mathcal{S}].
\]

In our application, the starting state is always known to be the same, so this distribution will always have support 1.

**Initialisation.** We initialise \( P_{ij}^\mathcal{S} \) using the fact that we have an estimate of the transition matrix for the MDP \( \bar{P} \) as an inductive bias and we initialise \( E^Z \) according to the deterministic observation mapping \( (s, q) \mapsto (s, \chi_X(q)) \) (see Appendix D).

\[
\sum_{\langle s_j^\mathcal{S}, s_k^\mathcal{S} \in \mathcal{S} \rangle} P_{ij}^\mathcal{S} = 1
\]

\[
\sum_{\langle o_j, o_i \in \mathcal{O} \rangle} E^Z_{ij} = 1.
\]

**Forward Procedure.** This first variable is the probability that the input model is in hidden state \( s_i^\mathcal{S} \) at time \( t \) in the given observation sequence \( o_{t+1}, ..., o_T \):

\[
\alpha_i(t) \equiv \Pr \{ o_1, ..., o_t, s_t^\mathcal{S} = s_i^\mathcal{S} \mid \langle \bar{P}, Z \rangle \}
\]

Then, the following recursive relations are used to compute these variables for later use in the update step:

1. \( \alpha_i(1) = \pi_i E^Z_{i,o_1} \)
2. \( \alpha_i(t + 1) = E^Z_{i,o_{t+1}} \sum_{j=1}^{\mathcal{S}} \alpha_j(t) P_{ij}^\mathcal{S} \)

**Backward Procedure.** These variables are calculated backwards temporally for ‘smoothing’ of the calculated probabilities:

\[
\beta_i(t) \equiv \Pr \{ o_{t+1}, ..., o_T \mid s_t^\mathcal{S} = i, \langle \bar{P}, Z \rangle \}
\]

Then, the following recursive relations are used to compute these variables for use in the update step:

1. \( \beta_i(T) = 1 \)
2. \( \beta_i(t) = \sum_{j=1}^{\mathcal{S}} \beta_j(t + 1) P_{ij} E^Z_{i,o_{t+1},j} \).
Calculate Update Parameters. The first update parameter is
\[
\gamma_i(t) = \Pr[s_t^o = i \mid (o_t)_{t=1}^T, (P^o_n, Z)] = \frac{\Pr[s_t^o = s_t^o, (o_t)_{t=1}^T \mid (P^o_n, Z)]}{\Pr[(o_t)_{t=1}^T \mid (P^o_n, Z)]} = \frac{\alpha_i(t)\beta_j(t)}{\sum_{k=1}^{\alpha_i(t)} \alpha_j(t)\beta_j(t)}.
\]
Note that by the definitions of \(\alpha_i(t)\) and \(\beta_i(t)\), \(\sum_{j=1}^{\alpha_i(t)} \alpha_j(t)\beta_j(t)\) is a sum over all possible hidden state transitions from time \(t\) that manifest the same observation sequence \((o_t)_{t=1}^T\).

The other update parameter is
\[
\xi_{ij}(t) = \Pr[s_t^o = i, s_{t+1}^o = j \mid (o_t)_{t=1}^T, (P^o_n, Z)] = \frac{\Pr[(o_t)_{t=1}^T \mid (P^o_n, Z)]}{\alpha_i(t)\beta_j(t)}.
\]
(by Bayes’ Theorem)

where the final denominator here is a sum over all possible hidden state transitions from time \(t\) to \(t+1\) which can give rise to the specific observation sequence \((o_t)_{t=1}^T\).

Update Step. We calculate the actual model updates with the following equations:
\[
\tilde{P}^o_{ij} = \frac{\sum_{t=0}^{T-1} \xi_{ij}(t)}{\sum_{t=0}^{T-1} \gamma_i(t)} = \sum_{t=0}^{T-1} \Pr[s_t^o = i, s_{t+1}^o = j \mid (o_t)_{t=1}^T, (P^o_n, Z)] = \sum_{t=0}^{T-1} \Pr[s_{t+1}^o = j \mid (o_t)_{t=1}^T, (P^o_n, Z)] \sum_{t=0}^{T-1} \gamma_i(t),
\]
where \(\chi_{o_t=j}\) is the indicator function for \(o_t = j \in O\).

After this step, we re-define \(P^o_n := \tilde{P}^o\) and \(E^\pi_{ij} := \tilde{E}^\pi\), and repeat all the steps with the same observation data \((o_t)_{t=1}^T\). Baum-Welch implementations usually keep track of the magnitude of changes from iteration to iteration, terminating when changes become negligible, or when a user-defined maximum number of iterations is reached.

D Mathematical Implementation of HMM Learning

Here we discuss any non-trivial linear algebra used by us to encode the models and data structures for the Baum-Welch algorithm.

As usual for MDPs, given the choice of some action \(a \in A\) at any time \(t\), the transition matrix \(T^a_{P^o_n} \in [0, 1]^{|S| \times |S|}\) corresponding to \(P^o_n\) in \(\mathcal{M} \otimes A\) is
\[
(T^a_{P^o_n})_{(s, q), (s', q')} \equiv P^o_n((s, q), a).
\]

The primary non-trivial linear algebra tool used is the Kronecker product. Usually, this is denoted with the symbol \(\otimes\), but we use \(\otimes_K\) to avoid confusion with our notation for the product MDP.

Definition 9. The Kronecker product of two matrices \(A, B\) is the block-matrix
\[
A \otimes_K B \equiv \begin{pmatrix} A_{11}B & A_{12}B & \cdots & A_{1m}B \\ A_{21}B & A_{22}B & \cdots & A_{2m}B \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1}B & A_{n2}B & \cdots & A_{nm}B \end{pmatrix},
\]
where each \(A_{ij}B\) is the \(B\)-sized matrix of the scalar \(A_{ij}\) multiplied by \(B\).

The mathematical setup for converting a product MDP into an HMM is as follows (applies to any matrix-based implementation, this is not unique to our programmatic implementation).

We construct the product MDP according to Definition 4 and store it as a rank-3 tensor with each layer corresponding to the dynamics induced by a specific action. This implies that the dimensions of the tensor \((T\) above) correspond to \(|S| \times |Q| \times |S| \times |Q| \times |A|\). Each “action layer” is equal to the matrix given by Equation 1 above.

We convert this product MDP to a Markov chain by summing and normalising to the fully mixed policy \(\pi\). This results in an \(|S| \times |Q| \times |S| \times |Q|\) transition matrix, representing the true transition dynamics of the Hidden Markov model we will be looking to solve.

The HMM learning algorithm takes as input a set of observation sequences and initial guesses for the transition and emission dynamics of the system. Note that this requires assuming a fixed number of hidden states in the system. Since we know the number of MDP states, estimating the right number of hidden states corresponds to guessing the number of TA states \(k\), which is unknown a priori. However, all that is actually required is that our guess \(k\) is greater than or equal to the true number of TA states \(|Q|\) because guessing too many states will just generate duplication in the learnt matrix - which can easily be identified. It is easy to come up with an upper bound on the size of the underlying TA.
that is sufficient for there to be enough hidden states in the learned product MDP to capture the dynamics over $S \times Q$; for instance, we could base it on the cardinality of the set of labels or on some type of simplicity assumption that the task specification is unlikely to have more than 10 states perhaps. We then initialise $p_{\text{initial estimate}}$ as a $k|S| \times k|S|$ stochastic matrix by taking the Kronecker product between a $k \times k$ identity matrix and $P_\pi$ (the estimate for the MDP’s transition matrix after being induced by the fully mixed policy $\pi$).

The observations seen consist of the MDP state component $s$, label $L(s)$, and reward. This corresponds to setting the true emissions matrix (also known as the observation probability matrix) $E^Z_k$ to the block matrix

$$
E^Z_k := \begin{pmatrix}
S \times \{q_0\} & S \times \{r = 0\} & S \times \{r = 1\} \\
S \times \{q_1\} & I & 0 \\
\vdots & \vdots & \vdots \\
S \times \{q_{k-1}\} & I & 0 \\
S \times \{q_k\} & 0 & I
\end{pmatrix} = \otimes K I_{|S| \times |S|},
$$

where $I_{|S| \times |S|}$ is the $|S| \times |S|$ identity matrix, and the adjacent binary matrix is $k \times 2$. Thus, for all product states with TA state $q \neq q_k$, the observation is just the physical state and reward 0, i.e. $\langle s, 0 \rangle$, and in the case $q = q_k$, the TA is an accepting state (by the assumption that there is one accepting TA state and that we number it with $k$) so the observation for $\langle s, q_k \rangle$ is $\langle s, 1 \rangle$. Note that the mission output from each specific product state is deterministic in our setting.

### E Further experimental details

Table 1 contains the key hyperparameters used in our experiments and presents the precise mean times to convergence across 3 runs of each experiment.

| Algorithm | Grid size | TA size | Episode Length | No. Episodes | Convergence Time (s) |
|-----------|-----------|---------|----------------|--------------|---------------------|
| Ours      | $3 \times 3$ | 3       | 34             | 275          | 26.3                |
| Ours      | $3 \times 3$ | 4       | 34             | 275          | 382.3               |
| Ours      | $3 \times 3$ | 5       | 70             | 500          | 5,232.7             |
| BF        | $3 \times 3$ | 3       | 34             | 275          | 63.7                |
| BF        | $3 \times 3$ | 4       | 34             | 275          | 18,188.3            |
| BF        | $3 \times 3$ | 5       | 70             | 500          | Timeout (>150,000)  |
| Ours      | $4 \times 4$ | 3       | 80             | 500          | 600.7               |
| Ours      | $4 \times 4$ | 4       | 90             | 1000         | 3,824.7             |
| Ours      | $4 \times 4$ | 5       | 80             | 1000         | 38,025.0            |
| Ours      | $5 \times 5$ | 3       | 85             | 2000         | 2,625.7             |
| Ours      | $5 \times 5$ | 4       | 100            | 2000         | 16,819.7            |
| Ours      | $5 \times 5$ | 5       | 140            | 2000         | 68,977.7            |

### F Comparisons with Related work

We attempted to benchmark our algorithm against several existing passive DFA learning libraries. Two well-established and commonly-used approaches to this are the RPNI algorithm (used in, e.g. [55, 57]) and SAT-based algorithms (used in e.g. [1, 2, 15, 34, 56]). The results of our comparisons are summarised in Table 2. Of the six implementations we tried, only the SAT-based approach from the libalf library was able to successfully learn the 3-state TA in our 3x3 gridworld. As Table 2 and Figure 4b demonstrate, our algorithm runs significantly faster than the RPNI algorithm indicating its better efficiency compared to existing approaches. Additionally, most of the libraries we attempted to run using the same dataset that we used for our experiments were not able to learn the correct TA, as evidenced by the results in Table 2. This highlights the general applicability of our approach in passively learning DFAs.

| Library   | Algorithm | Result | URL |
|-----------|-----------|--------|-----|
| AALpy     | dfa-identify | SAT-based | Wrong DFA (Fig. 3) | [AALpy](https://github.com/DES-Lab/AALpy) |
| Inferrer  | RPNI      | Recursion error | [Inferrer](https://github.com/steynvl/inferrer) |
| FlexFringe | SAT-based | Throws error | [FlexFringe](https://github.com/tudelft-cda-lab/FlexFringe) |
| Libalf    | RPNI      | Wrong DFA | [Libalf](https://github.com/libalf/libalf) |
| Libalf    | SAT-based | Works | [Libalf](https://github.com/libalf/libalf) |

3 In our application, accepting states cannot be left after achieving the goal, so it suffices in every case to have just one accepting state.
Learning an automaton from data is an NP-complete problem [13], so under standard complexity assumptions, the convergence time will, in the worst case, always grow exponentially with instance size. Nevertheless, as remarked in our experimental section, a 5×5 MDP grid world with a 5-state TA is comparable to that of related research. For example, in [1] their largest problem is the “Maze domain” with a five-state TA, MDP size 4×4 and in [12] their largest is a five-state TA and a 5×5 MDP. Other works such as [11, 21, 36] do go to slightly larger MDP worlds, but they employ SAT-based approaches, which assume knowledge of the underlying environment, unlike ours.

Figure 7: TA learnt using the AALpy library with the same data set used to learn the 3-state TA in the 3×3 gridworld.