Learning Reward Machines for Partially Observable Reinforcement Learning (Abridged Report)

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Abstract

Reward Machines (RMs), originally proposed for specifying problems in Reinforcement Learning (RL), provide an automata-based representation of a reward function that allows an agent to decompose problems into subproblems that can be efficiently learned using off-policy learning. Here we show that RMs can be learned from experience, instead of being specified by the user, and that the resulting problem decomposition can be used to effectively solve partially observable RL problems. We pose the task of learning RMs as a discrete optimization problem and show its effectiveness on three partially observable domains.

1 Introduction

The use of neural networks for function approximation has led to many advances in *Reinforcement Learning (RL)*. Such *deep RL* methods have allowed agents to learn effective policies in many complex environment [22, 18, 2]. However, RL methods (including deep RL ones) often struggle when the environment is *partially observable*. This is because agents in such environments usually require some form of memory to learn optimal behaviour [23]. Recent approaches give memory to RL agents via recurrent neural networks [19, 10, 28, 21] or memory-augmented neural networks [20, 13].

In this work, we show that *Reward Machines (RMs)* are another useful tool for providing memory in a partially observable environment. An RM is an automata-based encoding of a reward function that was proposed as a way to expose the reward function structure [25]. This structure can be exploited by the *Q-Learning for Reward Machines (QRM)* algorithm [25]. QRM has been shown to outperform standard and hierarchical deep RL over a variety of domains. However, QRM was only defined for fully observable environments and required a handcrafted RM.

This paper proposes a method for learning an RM directly from experience in a partially observable environment, in a manner that allows the RM to serve as memory for an RL algorithm. We characterize an objective for RM learning that allows us to formulate the task as a discrete optimization problem and propose an efficient local search approach to solve it. By simultaneously learning an RM and a policy for the environment, we are able to outperform several deep RL baselines that use recurrent neural networks as memory in three domains. We also extend QRM to the case of partial observability.

2 Preliminaries

RL agents learn policies from experience. When the problem is fully-observable, the underlying environment model is typically assumed to be a *Markov Decision Process (MDP)*. An MDP is a tuple

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$\mathcal{M} = \langle S, A, r, p, \gamma \rangle$, where S is a finite set of *states*, A is a finite set of *actions*, $r : S \times A \to \mathbb{R}$ is the *reward function*, $p(s, a, s')$ is the *transition probability distribution*, and γ is the *discount factor*. The agent starts not knowing what r or p are. On every time step t, the agent observes the current state $s_t \in S$ and executes an action $a_t \in A$ following a policy $\pi(a_t|s_t)$. As a result, the state s_t changes to $s_{t+1} \sim p(s_{t+1}|s_t, a_t)$ and the agent receives a reward signal $r(s_t, a_t)$. The goal is to learn the *optimal* policy π^*, which maximizes the future expected discounted reward for every state in S [24].

In partially observable problems, the underlying environment model is typically assumed to be a *Partially Observable Markov Decision Process (POMDP)*. A POMDP is a tuple $\mathcal{P}_\mathcal{O} = \langle S, O, A, r, p, \omega, \gamma \rangle$, where S, A, r, p, and γ are defined as in an MDP, O is a finite set of *observations*, and $\omega(s, o)$ is the *observation probability distribution*. At every time step t, the agent is in exactly one state $s_t \in S$, executes an action $a_t \in A$, receives reward $r_{t+1} = r(s_t, a_t)$, and moves to state s_{t+1} according to $p(s_t, a_t, s_{t+1})$. However, the agent does not observe s_{t+1}, but only receives an observation $o_{t+1} \in O$. This observation provides the agent a clue about s_{t+1} is via ω [4].

RL methods cannot be immediately applied to POMDPs because the transition probabilities and reward function are not necessarily Markovian w.r.t. O. As such, optimal policies may need to consider the complete history $o_0, a_0, \ldots, a_{t-1}, o_t$ when selecting actions. Several partially observable RL methods use a recurrent neural network to compactly represent the history.

3 Reward Machines for Partially Observable Environments

RMs are finite state machines that are used to encode a reward function [25]. They are defined over a set of propositional symbols $\mathcal{P}$ that correspond to high-level features that the agent can detect using a *labelling function* $L : O_\emptyset \times A_\emptyset \times O \to 2^\mathcal{P}$ where (for any set X) $X_\emptyset \triangleq X \cup \{\emptyset\}$. L assigns truth values to symbols in $\mathcal{P}$ given an environment experience $e = (o, a, o')$ where o' is the observation seen after executing action a when observing o. We use $L(\emptyset, \emptyset, o)$ to assign truth values to the initial observation. We call the truth value assignment of $\mathcal{P}$ an *abstract observation* because it provides a high-level view of the low-level environment observations. A formal definition of an RM follows:

Definition 3.1 (reward machine)**.** Given a set of propositional symbols $\mathcal{P}$, a Reward Machine is a tuple $\mathcal{R}_\mathcal{P} = \langle U, u_0, \delta_u, \delta_r \rangle$ where U is a finite set of states, $u_0 \in U$ is an initial state, δ_u is the state-transition function, $\delta_u : U \times 2^\mathcal{P} \to U$, and δ_r is the reward-transition function, $\delta_r : U \times 2^\mathcal{P} \to \mathbb{R}$.

Example 3.1. *The* cookie domain*, shown in Figure 1, has three rooms connected by a hallway. The agent (purple triangle) can move in the four cardinal directions and can only see what it is in the room that it is currently in. There is a button in the yellow room that, when pressed, causes a cookie to randomly appear in the red or blue room (if the environment already contains a cookie, it gets randomly moved to the red or blue room). There is no cookie at the beginning of the episode. The agent receives a reward of $+1$ for each time it reaches a cookie (which removes the cookie).*

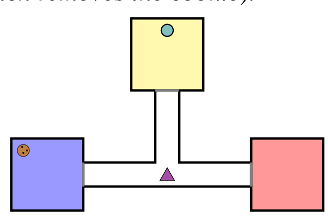
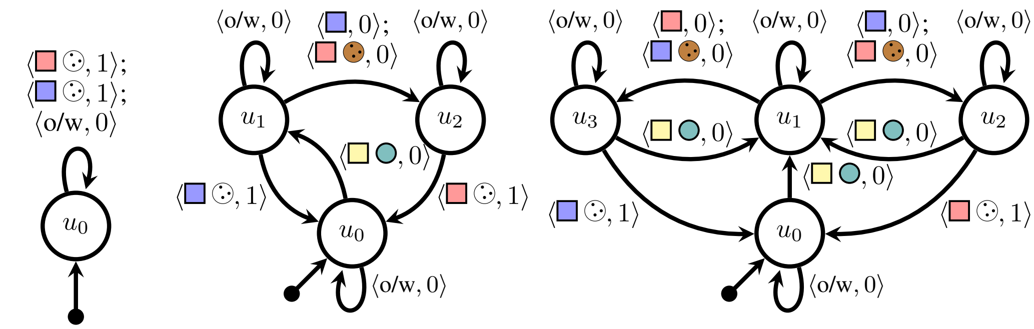


Figure 1: The cookie domain.

RMs decompose problems into a set of high-level states U and define transitions using if-like conditions defined by δ_u. These conditions are over a set of binary properties $\mathcal{P}$ that the agent can detect using L. For example, in the cookie domain, $\mathcal{P} = \{, , , , , , \}$. These properties are true (i.e., part of an experience label according to L) in the following situations: , , , or is true if the agent ends the experience in a room of that color; is true if the agent ends the experience in the same room as a cookie; is true if the agent pushed the button with its last action; and is true if the agent ate a cookie with its last action (by moving onto the space where the cookie was).

Figure 2 shows three RMs for the cookie domain. Each RM starts in the initial state u_0. Edge labels in the figures provide a visual representation of the functions δ_u and δ_r. For example, label $\langle\;, 1\rangle$ between state u_2 and u_0 in Figure 2b represents $\delta_u(u_2, \{,\}) = u_0$ and $\delta_r(u_2, \{,\}) = 1$. Intuitively, this means that if the RM is in state u_2 and the agent's experience ended in room immediately after eating the cookie , then the agent will receive a reward of 1 and the RM will transition to u_0. Any properties not listed in the label are false (e.g. must be false to take the transition labelled $\langle\;, 1\rangle$). We use multiple labels separated by a semicolon (e.g., "$\langle\;, 0\rangle$; $\langle\;, 0\rangle$") to describe different conditions for transitioning between the RM states, each with their own associated reward. The label $\langle$o/w$, r\rangle$ ("o/w" for "otherwise") on an edge from u_i to u_j means that that transition will be made (and reward r received) if none of the other transitions from u_i can be taken.



(a) Naive RM. (b) "Optimal" RM. (c) Perfect RM.

Figure 2: Three possible Reward Machines for the Cookie domain.

Let us illustrate the behaviour of an RM using the one shown in Figure 2c. The RM will stay in u_0 until the agent presses the button (causing a cookie to appear), whereupon the RM moves to u_1. From u_1 the RM may move to u_2 or u_3 depending on whether the agent finds a cookie when it enters another room. It is also possible to associate meanings with being in a RM states: u_0 means that there is no cookie available, u_1 means that there is a cookie in some room (either blue or red), etc.

When learning a policy for a given RM, one simple technique is to learn a policy $\pi(o, u)$ that considers the current observation $o \in O$ and the current RM state $u \in U$. Interestingly, a partially observable problem might be non-Markovian over O, but Markovian over $O \times U$ for some RM $\mathcal{R}_{\mathcal{P}}$.

4 Learning Reward Machines from Traces

Our overall idea is to search for an RM that can be used as external memory by an agent for a given task. As input, our method will only take a set of high-level propositional symbols $\mathcal{P}$, and a labelling function L that can detect them. Then, the key question is what properties should such an RM have.

Three proposals naturally emerge from the literature. The first comes from the work on learning Finite State Machines (FSMs) [3, 30, 7], which suggests learning the smallest RM that correctly mimics the external reward signal given by the environment, as in Giantamidis and Tripakis' method for learning Moore Machines [7]. Unfortunately, such an approach would learn RMs of limited utility, as shown in Figure 2a. This naive RM correctly predicts the reward from the cookie domain (i.e., $+1$ for eating a cookie, zero otherwise) but provides no memory in support of solving the task.

The second proposal comes from the literature on learning Finite State Controllers (FSC) [17] and on model-free RL methods [24]. This work suggests looking for the RM whose optimal policy receives the most reward. For instance, the RM from Figure 2b is "optimal" in this sense. It decomposes the problem into three states. The optimal policy for u_0 goes directly to press the button, the optimal policy for u_1 goes to the blue room and eats the cookie if present, and the optimal policy for u_2 goes to the red room and eats the cookie. Together, these three policies give rise to an optimal policy for the complete problem. This is a desirable property for RMs, but requires computing optimal policies in order to compare the relative quality of RMs, which seems prohibitively expensive. However, we believe that finding ways to efficiently learn "optimal" RMs is a promising future work direction.

Finally, the third proposal comes from the literature on Predictive State Representations (PSR) [15], Deterministic Markov Models (DMMs) [16], and model-based RL [11]. These works suggest learning the RM that remembers sufficient information about the history to make accurate Markovian predictions about the next observation. For instance, the cookie domain RM shown in Figure 2c is *perfect* w.r.t. this criterion. Intuitively, every transition in the cookie environment is already Markovian except for transitioning from one room to another. Depending on different factors, when entering to the red room there could be a cookie there (or not). The perfect RM is able to encode such information using 4 states, where u_0 represents the state where the agent knows that there is no cookie, at u_1 the agent knows that there is a cookie in the blue or the red room, at u_2 the agent knows that there is a cookie in the red room, and at u_3 the agent knows that there is a cookie in the blue room. Since keeping track of more information will not result in better predictions, this RM is *perfect*. Below, we develop a theory about perfect RMs and describe an approach to learn them.

4.1 Perfect Reward Machines: Formal Definition and Properties

The key insight behind perfect RMs is to use their states U and transitions δ_u to keep track of relevant past information such that the partially observable environment $\mathcal{P}_\mathcal{O}$ becomes Markovian w.r.t. $O \times U$.

Definition 4.1 (perfect reward machine)**.** An RM $\mathcal{R}_\mathcal{P} = \langle U, u_0, \delta_u, \delta_r \rangle$ is considered perfect for a POMDP $\mathcal{P}_\mathcal{O} = \langle S, O, A, r, p, \omega, \gamma \rangle$ with respect to a labelling function L if and only if for every trace $o_0, a_0, \ldots, o_t, a_t$ generated by any policy over $\mathcal{P}_\mathcal{O}$, the following holds:

$$\Pr(o_{t+1}, r_{t+1} | o_0, a_0, \ldots, o_t, a_t) = \Pr(o_{t+1}, r_{t+1} | o_t, x_t, a_t) \tag{1}$$

where $x_0 = u_0$ and $x_t = \delta_u(x_{t-1}, L(o_{t-1}, a_{t-1}, o_t))$.

Two interesting properties follow from Definition 4.1. First, if the set of belief states B for the POMDP $\mathcal{P}_\mathcal{O}$ is finite [4], then there exists a perfect RM for $\mathcal{P}_\mathcal{O}$ with respect to some L. Second, the optimal policies for perfect RMs are also optimal for the POMDP (see Appendix A).

Theorem 4.1. *Given any POMDP $\mathcal{P}_\mathcal{O}$ with a finite reachable belief space, there will always exists at least one perfect RM for $\mathcal{P}_\mathcal{O}$ with respect to some labelling function L.*

Theorem 4.2. *Let $\mathcal{R}_\mathcal{P}$ be a perfect RM for a POMDP $\mathcal{P}_\mathcal{O}$ w.r.t. a labelling function L, then any optimal policy for $\mathcal{R}_\mathcal{P}$ w.r.t. the environmental reward is also optimal for $\mathcal{P}_\mathcal{O}$.*

4.2 Perfect Reward Machines: How to Learn Them

We now consider the problem of learning a perfect RM from traces, assuming one exists w.r.t. the given labelling function L. Recall that a perfect RM transforms the original problem into a Markovian problem over $O \times U$. Hence, we should prefer RMs that accurately predict the next observation o' and immediate reward r from the current observation o, RM state u, and action a. This might be achieved by collecting a training set of traces from the environment, fitting a predictive model for $\Pr(o', r | o, u, a)$, and picking the RM that makes better predictions. However, this can be very expensive, especially considering that the observations might be images.

Instead, we propose an alternative that focuses on a necessary condition for a perfect RM: the RM must predict what is *possible* and *impossible* in the environment at the abstract level. For example, it is impossible to be at u_3 in the RM from Figure 2c and make the abstract observation { , },
because the RM reaches u_3 only if the cookie was seen in the blue room or not in the red room.

$$\min_{\langle U, u_0, \delta_u, \delta_r \rangle} \sum_{i \in I} \sum_{t \in T_i} \log(|N_{x_{i,t}, L(e_{i,t})}|) \tag{LRM}$$

$$\text{s.t. } \langle U, u_0, \delta_u, \delta_r \rangle \in \mathcal{R}_\mathcal{P} \tag{2}$$

$$|U| \leq u_{\max} \tag{3}$$

$$x_{i,t} \in U \quad \forall i \in I, t \in T_i \tag{4}$$

$$x_{i,0} = u_0 \quad \forall i \in I \tag{5}$$

$$x_{i,t+1} = \delta_u(x_{i,t}, L(e_{i,t+1})) \quad \forall i \in I, t \in T_i \tag{6}$$

$$N_{u,l} \subseteq 2^{2^\mathcal{P}} \quad \forall u \in U, l \in 2^\mathcal{P} \tag{7}$$

$$L(e_{i,t+1}) \in N_{x_{i,t}, L(e_{i,t})} \quad \forall i \in I, t \in T_i \tag{8}$$

This idea is formalized in the optimization model LRM. Let $\mathcal{T} = \{\mathcal{T}_0, \ldots, \mathcal{T}_n\}$ be a set of traces, such that each trace $\mathcal{T}_i$ is a sequence of observations, actions, and rewards: $\mathcal{T}_i = \{o_{i,0}, a_{i,0}, r_{i,0}, \ldots, o_{i,t_i}, a_{i,t_i}, r_{i,t_i}\}$. We now look for an RM $\langle U, u_0, \delta_u, \delta_r \rangle$ that can be used to predict $L(e_{i,t+1})$ from $L(e_{i,t})$ and the current RM state $x_{i,t}$, where $e_{i,t+1}$ is the experience $(o_{i,t}, a_{i,t}, o_{i,t+1})$ and $e_{i,0}$ is $(\emptyset, \emptyset, o_{i,0})$ by definition. The model parameters are the set of traces $\mathcal{T}$, the set of propositional symbols $\mathcal{P}$, the labelling function L, and a maximum number of states in the RM $u_{\max}$. The model also uses the sets $I = \{0 \ldots n\}$ and $T_i = \{0 \ldots t_i - 1\}$, where I contains the index of the traces and T_i their time steps. The model has two auxiliary variables $x_{i,t}$ and $N_{u,l}$. Variable $x_{i,t} \in U$ represents the state of the RM after observing trace $\mathcal{T}_i$ up to time t. Variable $N_{u,l} \subseteq 2^{2^\mathcal{P}}$ is the set of all the next abstract observations seen from the RM state u and the abstract observations l at some point in $\mathcal{T}$. In other words, $l' \in N_{u,l}$ iff $u = x_{i,t}$, $l = L(e_{i,t})$, and $l' = L(e_{i,t+1})$ for some trace $\mathcal{T}_i$ and time t.

Constraints (2) and (3) ensure that we find a well-formed RM over $\mathcal{P}$ with at most $u_{\max}$ states. Constraint (4), (5), and (6) ensure that $x_{i,t}$ is equal to the current state of the RM, starting from u_0 and following δ_u. Constraint (7) and (8) ensure that the sets $N_{u,l}$ contain every $L(e_{i,t+1})$ that have been seen right after l and u in $\mathcal{T}$. The objective function comes from maximizing the log-likelihood for predicting $L(e_{i,t+1})$ using a uniform distribution over all the possible options given by $N_{u,l}$.

A key property of this formulation is that any perfect RM is optimal with respect to the objective function in LRM when the number of traces tends to infinity (see Appendix A):

Theorem 4.3. *When the set of training traces (and their lengths) tends to infinity and is collected by a policy such that $\pi(a|o) > \epsilon$ for all $o \in O$ and $a \in A$, any perfect RM with respect to L and at most u_{max} states will be an optimal solution to the formulation* LRM*.*

Finally, note that the definition of a perfect RM does not impose conditions over the rewards associated with the RM (i.e., δ_r). This is why δ_r is a free variable in the model LRM. However, we still expect δ_r to model the external reward signals given by the environment. To do so, we estimate $\delta_r(u, l)$ using its empirical expectation over $\mathcal{T}$ (as commonly done when constructing belief MDPs [4]).

4.3 Searching for a Perfect Reward Machine Using Tabu Search

We now describe the specific optimization technique used to solve LRM. We experimented with many discrete optimization approaches—including mixed integer programming [5] (included in Appendix B), Benders decomposition [6], evolutionary algorithms [12], and others—and found local search algorithms [1] to be the most effective at finding high quality RMs given short time limits. In particular, we use Tabu search [8], a simple and versatile local search procedure with convergence guarantees and many successful applications in the literature [27].

In the context of our work, Tabu search starts from a random RM and, on each iterations it evaluates all "neighbouring" RMs. We define the neighbourhood of an RM as the set of RMs that differ by exactly one transition (i.e., removing/adding a transition, or changing its value) and evaluate RMs using the objective function of LRM. When all neighbouring RMs are evaluated, the algorithm chooses the one with lowest values and sets it as the current RM. To avoid local minimum, Tabu search maintains a *Tabu list* of all the RMs that were previously used as the current RM. Then, RMs in the Tabu list are pruned when examining the neighbourhood of the current RM.

5 Simultaneously Learning a Reward Machine and a Policy

We now describe our overall approach for simultaneously finding an RM and learn a policy for it (the pseudo-code is in Appendix C). It starts by collecting a training set of traces $\mathcal{T}$ generated by a random policy during t_{w} "warmup" steps. This set of traces is used to find an initial RM $\mathcal{R}$ using Tabu search. The algorithm then initializes policy π, sets the RM state to the initial state u_0, and sets the current label l to the initial abstract observation $L(\emptyset, \emptyset, o)$. The standard RL learning loop is then followed: an action a is selected following $\pi(o, u)$ where u is the current RM state, and the agent receives the next observation o' and the immediate reward r. The RM state is then updated to $u' = \delta_u(u, L(o, a, o'))$ and the last experience $(\langle o, u\rangle, a, r, \langle o', u'\rangle)$ is used by an RL method to update π. When a terminal state is reached, then the environment and RM are reset.

If on any step, there is evidence that the current RM might not be the best one, our approach will attempt to find a new one. Recall that the RM $\mathcal{R}$ was selected using the cardinality of its prediction sets N (LRM). Hence, if the current abstract observation l' is not in $N_{u,l}$, adding the current trace to $\mathcal{T}$ will increase the size of $N_{u,l}$ for $\mathcal{R}$. As such, the cost of $\mathcal{R}$ will increase and it may no longer be the best RM. Thus, if $l' \notin N_{u,l}$, we add the current trace to $\mathcal{T}$ and search for a new RM. Recall that we use Tabu search, though any discrete optimization method could be applied. Our method only uses the new RM if its cost is lower than $\mathcal{R}$'s. If the RM is updated, a new policy is learned from scratch.

Given the current RM, we can use any RL algorithm to learn a policy $\pi(o, u)$, by treating the combination of o and u as the current state. If the RM is perfect, then the optimal policy $\pi^*(o, u)$ will also be optimal for the original POMDP (Theorem 4.2). However, to exploit the RM structure, we extended the QRM algorithm to work under partial observability (as described in Appendix E).

6 Experimental Evaluation

We tested our approach on three partially observable grid domains. The agent can move in the four cardinal directions and can only see what is in the current room. The first environment is the *cookie domain* described in §3. Each episode is $5,000$ steps long, during which the agent should attempt to get as many cookies as possible. The rest of the environments are described on Appendix D.1.

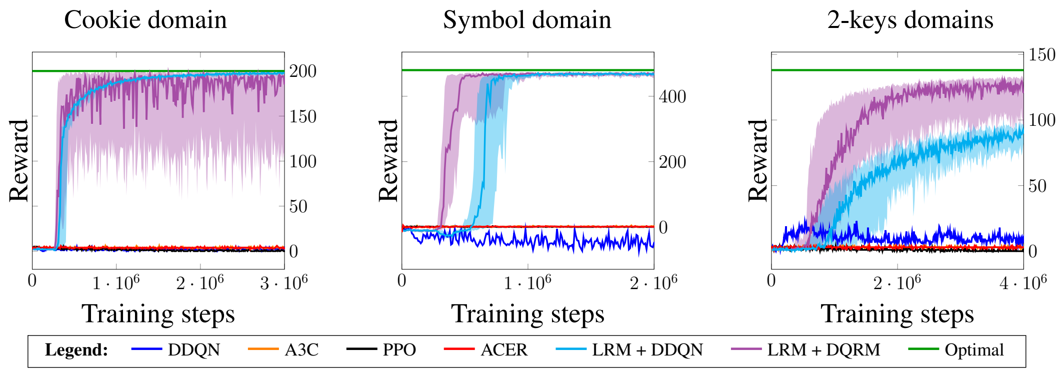


Figure 3: Total reward collected every $10,000$ training steps.

We tested two versions of our Learned Reward Machine (LRM) approach: LRM+DDQN and LRM+DQRM. Both learn an RM from experience as described in §4.2, but LRM+DDQN learns a policy using DDQN [26] while LRM+DQRM uses QRM (Appendix E). We compared against 4 baselines: DDQN [26], A3C [19], ACER [28], and PPO [21]. DDQN uses the concatenation of the last 10 observations as input whereas A3C, ACER, and PPO use an LSTM to summarize the history. The output of the labelling function was also given to the baselines. More details on Appendix D.

Figure 3 shows the total reward that each approach gets every $10,000$ training steps and compares it to the optimal policy. For the LRM algorithms, the figure shows the median performance over 30 runs per domain, and percentile 25 to 75 in the shadowed area. Note that LRM approaches largely outperform all the baselines. A key factor in the strong performance of the LRM approaches is that Tabu search finds high-quality RMs in less than 2.5 minutes using 62 workers (see Appendix D.3).

7 Related Work

State-of-the-art approaches for partially observable RL use Recurrent Neural Networks (RNNs) as memory in combination with policy gradient [19, 28, 21, 10], or use external neural-based memories [20, 13, 9]. While our experiments highlight the merits of our approach w.r.t. RNN-based approaches, we rely on ideas that are largely orthogonal. As such, we believe there is significant potential in mixing these approaches to get the benefit of memory at both the high and low-level.

The effectiveness of automata-based memory has long been recognized in the POMDP literature [4], where the objective is to find policies given a complete specification of the environment. The idea is to encode policies using Finite State Controllers (FSCs) which are FSMs where the transitions are defined in terms of low-level observations from the environment and each state in the FSM is associated with one primitive action. When interacting with the environment, the agent always selects the action associated with the current state in the controller. Meuleau et al. [17] adapted this idea to work in the RL setting by exploiting policy gradient to learn policies encoded as FSCs. RMs can be considered as a generalization of FSC as they allow for transitions using conditions over high-level events and associate complete policies (instead of just one primitive action) to each state.

8 Concluding Remarks

We have presented a discrete optimization-based approach for learning Reward Machines that can be used to solved partially observable RL problems. We believe this work represents an important building block for creating RL agents that can solve cognitively challenging partially observable tasks. Not only did our approach solve problems that were unsolvable by A3C, ACER and PPO, but it did so in a relatively small number of training steps. RM learning provided the agent with memory, but more importantly the combination of RM learning and policy learning provided it with discrete reasoning capabilities that operated at a higher level of abstraction while leveraging deep RL's ability to learn policies from low-level inputs. This work leaves open many interesting questions relating to abstraction, observability, and properties of the language over which RMs are constructed. We believe that addressing these questions will push the boundary of RL problems that can be solved.

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A Theorems and Proof Sketches

When we do have access to a full POMDP model $\mathcal{P}_{\mathcal{O}}$, then the history can be summarized into a *belief state*. A belief state is a probability distribution $b_t : S \to [0,1]$ over S, such that $b_t(s)$ is the probability that the agent is in state $s \in S$ given the history up to time t. The initial belief state is computed using the initial observation o_0: $b_0(s) = \omega(s, o_0)$ for all $s \in S$. The belief state b_{t+1} is then determined from the previous belief state b_t, the executed action a_t, and the resulting observation o_{t+1} as $b_{t+1}(s') \propto \omega(s', o_{t+1}) \sum_{s \in S} p(s, a_t, s') b_t(s)$ for all $s' \in S$. Since the state transitions and reward function are Markovian w.r.t. b_t, the set of all belief states B can be used to construct the belief MDP $\mathcal{M}_B$. Optimal policies for $\mathcal{M}_B$ are also optimal for the POMDP [4]. Below, we use this theory to prove Theorems 4.1 and 4.2.

Theorem A.1. *Given any POMDP $\mathcal{P}_{\mathcal{O}}$ with a finite reachable belief space, there will always exist at least one perfect RM for $\mathcal{P}_{\mathcal{O}}$ with respect to some labelling function L.*

Proof sketch. If the reachable belief space B is finite, we can construct an RM that keeps track of the current belief state using one RM state per belief state and emulating their progression using δ_u and one propositional symbol for every action-observation pair. Thus, the current belief state b_t can be inferred from the last observation, last action, and the current RM state. As such, the equality from Definition 4.1 holds. □

Two interesting properties follow from the definition of a perfect RM. First, if the set of belief states B for the POMDP $\mathcal{P}_{\mathcal{O}}$ is finite, then there exists a perfect RM for $\mathcal{P}_{\mathcal{O}}$ with respect to some L. Second, the optimal policies for perfect RMs are also optimal for the POMDP.

Theorem A.2. *Let $\mathcal{R}_{\mathcal{P}}$ be a perfect RM for a POMDP $\mathcal{P}_{\mathcal{O}}$ w.r.t. a labelling function L, then any optimal policy for $\mathcal{R}_{\mathcal{P}}$ w.r.t. the environmental reward is also optimal for $\mathcal{P}_{\mathcal{O}}$.*

Proof sketch. As the next observation and immediate reward probabilities can be predicted from $O \times U \times A$, an optimal policy over $O \times U$ must also be optimal over $\mathcal{P}_{\mathcal{O}}$. □

A key property of this formulation is that any perfect RM is optimal with respect to objective function in `LRM` when the number of traces tends to infinity:

Theorem A.3. *When the set of training traces (and their lengths) tends to infinity and is collected by a policy such that $\pi(a|o) > \epsilon$ for all $o \in O$ and $a \in A$, any perfect RM with respect to L and at most u_{max} states will be an optimal solution to the formulation `LRM`.*

Proof sketch. In the limit, $l' \in N_{u,l}$ if and only if the probability of observing l' after executing an action from the RM state u while observing l is non-zero. In particular, for all $i \in I$ and $t \in T$, the cardinality of $N_{x_{i,t}, L(e_{i,t})}$ will be minimal for a perfect RM. This follows from the fact that perfect RMs make perfect predictions for the next observation o' given o, u, and a. Therefore, as we minimize the sum over $\log(|N_{x_{i,t}, L(e_{i,t})}|)$, the objective value for a perfect RM must be minimal. □

B Mixed Integer Linear Programming Model for `LRM`

We now present a Mixed Integer Linear Programming Model `MILP` for `LRM`. For this model we assume $|U| = u_{\max}$ and we use $K = 2^{2^{|\mathcal{P}|}}$. Variables $d_{u,u',l} \in \{0,1\}$ represent the possible transitions in the RM for each pair of states $u, u' \in U$ and abstract observation $l \in 2^{\mathcal{P}}$, i.e., $d_{u,u',l} = 1$ iff $\delta_u(u,l) = u'$. Variable $w_{i,t,u} \in \{0,1\}$ indicates if the agent is at state $u \in U$ of the RM on trace $i \in I$ and time step $t \in T_i$, i.e., $w_{i,t,u} = 1$ iff $x_{i,t} = u$. Variable $p_{l,u,l'} \in \{0,1\}$ indicates if $l' \in 2^{\mathcal{P}}$ is a possible next abstract observation at RM state u when observing $l \in 2^{\mathcal{P}}$, i.e., $p_{l,u,l'} = 1$ iff $l' \in N_{u,l}$. Variable $y_{u,l,n} \in \{0,1\}$ represents the cardinality of $N_{u,l}$, i.e., $y_{u,l,n} = 1$ iff $|N_{u,l}| = n$. Lastly, variables $z_{i,t}$ represents the log-likelihood cost for trace $i \in I$ and time step $t \in T_i$, i.e., $z_{i,t} = \log(|N_{x_{i,t}, L(e_{i,t})}|)$. Then, the model is as follows:

$$\min \sum_{i \in I} \sum_{t \in T_i} z_{i,t} \tag{MILP}$$

$$s.t.\ z_{i,t} \geq \sum_{n=1}^{K} y_{u,l,n} \cdot \log(n) - (1 - w_{i,t,u}) \cdot \log(K) \qquad \forall i \in I, t \in T_i, u \in U, l = L(e_{i,t}) \tag{9}$$

$$\sum_{n=1}^{K} y_{u,l,n} = 1 \qquad \forall u \in U, l \in 2^{\mathcal{P}} \tag{10}$$

$$\sum_{l' \in 2^{\mathcal{P}}} p_{l,u,l'} = \sum_{n=1}^{K} y_{u,l,n} \cdot n \qquad \forall u \in U, l \in 2^{\mathcal{P}}, n \in \{1..K\} \tag{11}$$

$$p_{l,u,l'} \geq w_{i,t,u} \qquad \forall i \in I, t \in T_i, l = L(e_{i,t}), l' = L(e_{i,t+1}) \tag{12}$$

$$\sum_{u' \in U} d_{u,u',l} = 1 \qquad \forall u \in U, l \in 2^{\mathcal{P}} \tag{13}$$

$$\sum_{u \in U} w_{i,t,u} = 1 \qquad \forall i \in I, t \in T_i, u \in U \tag{14}$$

$$w_{i,0,u_0} = 1 \qquad \forall i \in I \tag{15}$$

$$w_{i,t+1,u'} \geq w_{i,t,u} + d_{u,u',l} - 1 \qquad \forall i \in I, t \in T_i, u, u' \in U, l = L(e_{i,t+1}) \tag{16}$$

$$d_{u,u',l} \in \{0,1\} \qquad \forall u, u' \in U, l \in 2^{\mathcal{P}} \tag{17}$$

$$w_{i,t,u} \in \{0,1\} \qquad \forall i \in I, t \in T_i, u \in U \tag{18}$$

$$p_{l,u,l'} \in \{0,1\} \qquad \forall u \in U, l, l' \in 2^{\mathcal{P}} \tag{19}$$

$$y_{u,l,n} \in \{0,1\} \qquad \forall u \in U, l \in 2^{\mathcal{P}}, n \in \{1..K\} \tag{20}$$

$$z_{i,t} \geq 0 \qquad \forall i \in I, t \in T_i \tag{21}$$

Constraint (9) models the log-likelihood cost for each time step of a trace. Constraints (10) and (11) compute the cardinality of $N_{u,l}$. Constraint (12) defines the possible predictions given a trace. Constraint (13) enforces that for each RM state an abstract observation can lead to exactly one other RM state. Constraint (14) enforces that at any time step of a trace the agent can be at exactly one RM state. Constraint (15) imposes the initial RM state of a trace and constraint (16) encodes the RM state transitions for a trace. Lastly, constraints (17)-(21) correspond to the variables domains.

C Algorithm for Simultaneously Learning Reward Machines and a Policy

Algorithm 1 shows our overall approach for simultaneously learning an RM and exploiting that RM to learn a policy. The algorithm inputs are the set of propositional symbols $\mathcal{P}$, the labelling function L, a maximum on the number of RM states u_{max}, and the number of "warmup" steps t_{w}. Our approach starts by collecting a training set of traces $\mathcal{T}$ generated by a random policy during t_{w} steps (Line 2). This set of traces is used to find an initial RM $\mathcal{R}$ using Tabu search (Line 3). If later traces show that $\mathcal{R}$ is incorrect, our method will then find a new RM learned using the additional traces.

Lines 4 and 5 initialize the environment and the policy π, and set variables x and l to the initial RM state u_0 and initial abstract observation $L(\emptyset, \emptyset, o)$, respectively. Lines 7–19 are the main loop of our approach. Lines 7–10 are part of the standard RL loop: the agent executes an action a selected following $\pi(o, x)$ and receives the next observation o', the immediate reward r, and a boolean variable *done* indicating if the episode has terminated. Then, the state in the RM x' is updated and the policy π is improved using the last experience $(\langle o, x\rangle, a, r, \langle o', x'\rangle, \textit{done})$. Note that when *done* is true, the environment and RM are reset (Lines 17–18).

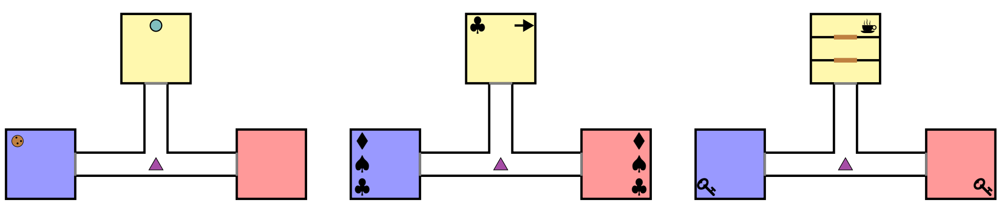
Lines 11–16 involve relearning the RM when there is evidence that the current RM might not be the best one. Recall that the RM $\mathcal{R}$ was selected using the cardinality of its prediction sets N, `LRM`. Hence, if the current abstract observation l' is not in $N_{x,l}$, then adding the current trace to $\mathcal{T}$ will increase the size of $N_{x,l}$ for $\mathcal{R}$. As such, the cost of $\mathcal{R}$ will increase and it may no longer be the best RM. Thus, if $l' \notin N_{x,l}$, we add the current trace to $\mathcal{T}$ and use Tabu search to find a new RM. Note, our method only uses the new RM if its cost is lower than that of $\mathcal{R}$ (Lines 14–16). However, when the RM is updated, a new policy is learned from scratch (Line 16).

Algorithm 1 Learning an RM and a Policy

Input: $\mathcal{P}$, L, A, $u_{\max}$, t_{w}
$\mathcal{T} \leftarrow$ collect_traces(t_{w})
$\mathcal{R}, N \leftarrow$ learn_rm($\mathcal{P}$, L, $\mathcal{T}$, $u_{\max}$)
$o, x, l \leftarrow$ env_get_initial_state(), u_0, $L(\emptyset, \emptyset, o)$
$\pi \leftarrow$ initialize_policy()
for $t = 1$ **to** t_{train} **do**
  $a \leftarrow$ select_action(π, o, x)
  $o', r,$ done $\leftarrow$ env_execute_action(a)
  $x', l' \leftarrow \delta_u(x, L(o, a, o')), L(o, a, o')$
  $\pi \leftarrow$ improve(π, o, x, l, a, r, o', x', l', done, N)
  if $l' \notin N_{x,l}$ **then**
    $\mathcal{T} \leftarrow \mathcal{T} \cup$ get_current_trace()
    $\mathcal{R}', N \leftarrow$ relearn_rm($\mathcal{R}$, $\mathcal{P}$, L, $\mathcal{T}$, $u_{\max}$)
    if $\mathcal{R} \neq \mathcal{R}'$ **then**
      $\mathcal{R}$, done $\leftarrow \mathcal{R}'$, **true**
      $\pi \leftarrow$ initialize_policy()
    end if
  end if
  if done **then**
    $o', x', l' \leftarrow$ env_get_initial_state(), u_0, $L(\emptyset, \emptyset, o)$
  end if
  $o, x, l \leftarrow o', x', l'$
end for
return π

D Experimental Evaluation

D.1 Domains



(a) Cookie domain. (b) Symbol domain. (c) 2-keys domain.

Figure 4: Partially observable environments where the agent can only see what is in the current room.

We tested our approach on three partially observable grid domains (Figure 4). The agent can move in the four cardinal directions and can only see what is in the current room. These are stochastic domains where the outcome of an action randomly changes with a 5% probability.

The first environment is the *cookie domain* (Figure 4a) described in §3. Each episode is $5,000$ steps long, during which the agent should attempt to get as many cookies as possible.

The second environment is the *symbol domain* (Figure 4b). It has three symbols ♣, ♠, and ♦ in the red and blue rooms. One symbol from {♣, ♠, ♦} and possibly a right or left arrow are randomly placed at the yellow room. Intuitively, that symbol and arrow tell the agent where to go, e.g., ♣ and $\rightarrow$ tell the agent to go to ♣ in the east room. If there is no arrow, the agent can go to the target symbol in either room. An episode ends when the agent reaches any symbol in the red or blue room, at which point it receives a reward of $+1$ if it reached the correct symbol and -1 otherwise.

The third environment is the *2-keys domain* (Figure 4c). The agent receives a reward of $+1$ when it reaches the coffee (in the yellow room). To do so, it must open the two doors (shown in brown). Each door requires a different key to open it, and the agent can only carry one key at a time. Initially, the two keys are randomly located in either the blue room, the red room, or split between them.

D.2 Experimental Details

In all domains, we used $u_{\text{max}} = 10$, $t_{\text{w}} = 200,000$, an epsilon greedy policy with $\epsilon = 0.1$, and a discount factor $\gamma = 0.9$. The size of the Tabu list and the number of steps that the Tabu search performs before returning the best RM found is 100.

For LRM+DDQN and LRM+DQRM, the neural network used has 5 fully connected layers with 64 neurons per layer. On every step, we trained the network using 32 sampled experiences from a replay buffer of size 100,000 using the Adam optimizer [14] and a learning rate of 5e-5. The target networks were updated every 100 steps.

DDQN [26] uses the same parameters and network architecture than LRM+DDQN, but its input is the concatenation of the last 10 observations, as commonly done by Atari playing agents. This gives DDQN a limited memory to better handle partially observable domains. A3C, ACER, and PPO use an LSTM to summarize the history. We followed the same testing methodology that was used in their original publications. We ran each approach at least 30 times per domain, and on every run, we randomly selected the number of hidden neurons for the LSTM from $\{64, 128, 256, 512\}$ and a learning rate from (1e-3, 1e-5). We also sampled δ from $\{0, 1, 2\}$ for ACER and the clip range from $(0.1, 0.3)$ for PPO. Other parameters were fixed to their default values.

While interacting with the environment, the agents were given a “top-down" view of the world represented as a set of binary matrices. One matrix had a 1 in the current location of the agent, one had a 1 in only those locations that are currently observable, and the remaining matrices each corresponded to an object in the environment and had a 1 at only those locations that were both currently observable and contained that object (i.e., locations in other rooms are “blacked out"). The agent also had access to features indicating if they were carrying a key, which colour room they were in, and the current status (i.e., occurring or not occurring) of the events detected by the labelling function.

D.3 Tabu Search

Figure 5 evaluates the quality of the RMs found by Tabu search by comparing them to the perfect RM. In each plot, a dot compares the cost of a handcrafted perfect RM with that of an RM $\mathcal{R}$ that was found by Tabu search while running our LRM approaches, where the costs are evaluated relative to the training set used to find $\mathcal{R}$. Being on or under the diagonal line (as in most of the points in the figure) means that Tabu search is finding RMs whose values are at least as good as the handcrafted RM. Hence, Tabu search is either finding perfect RMs or discovering that our training set is incomplete and our agent will eventually fill those gaps.

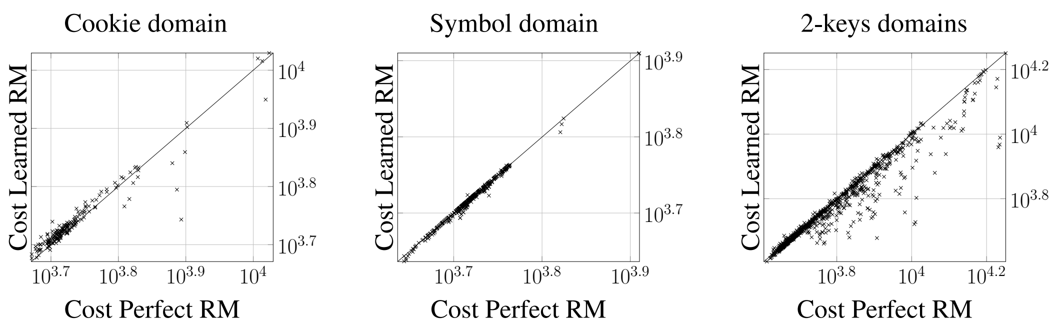


Figure 5: Cost comparison between perfect RM and RM found by Tabu search.

E Q-Learning for Reward Machines under Partial Observability

When learning a policy for a given RM, one simple technique is to learn a policy $\pi(o, u)$ that considers the current observation $o \in O$ and the current RM state $u \in U$ using, for instance, *Q-learning* [29]. Q-learning is a well-known RL algorithm that uses samples of experience of the form (s_t, a_t, r_t, s_{t+1}) to estimate the optimal q-function $q^*(s, a)$. Here, $q^*(s, a)$ is the expected return of selecting action a in state s and following an optimal policy π^*. Deep RL methods like DQN [18] and DDQN [26] represent the q-function as $\tilde{q}_\theta(s, a)$, where $\tilde{q}_\theta$ is a neural network whose inputs are features of the state and action, and whose weights θ are updated using stochastic gradient descent.

However, to exploit the problem structure exposed by the RM, we want to use the QRM algorithm. *Q-Learning for RMs (QRM)* is another way to learn a policy by exploiting a given RM [25]. QRM learns one q-function $\tilde{q}_u$ (i.e., policy) per RM state $u \in U$. Then, given any sample experience, the RM can be used to emulate how much reward would have been received had the RM been in any one of its states. Formally, experience $e = (o, a, o')$ can be transformed into a valid experience $(\langle o, u\rangle, a, \langle o', u'\rangle, r)$ used for updating $\tilde{q}_u$ for each $u \in U$, where $u' = \delta_u(u, L(e))$ and $r = \delta_r(u, L(e))$. Hence, any off-policy learning method can take advantage of these "synthetically" generated experiences to update all subpolicies simultaneously. When tabular q-learning is used, QRM is guaranteed to converge to an optimal policy on fully-observable problems [25]. However, in a partially observable environment, an experience e might be more or less likely depending on the RM state that the agent was in when the experience was collected. For example, experience e might be possible in one RM state u_i but not in RM state u_j. Thus, updating the policy for u_j using e as QRM does, would introduce an unwanted bias to $\tilde{q}_{u_j}$.

We partially address this issue by only updating $\tilde{q}_u$ using (o, a, o') if and only if $L(o, a, o') \in N_{u,l}$, where l was the current abstract observation that generated the experience (o, a, o'). Hence, we do not transfer experiences from u_i to u_j if the current RM does not believe that (o, a, o') is possible in u_j. For example, consider the cookie domain and the perfect RM from Figure 2c. If some experience consists of entering to the red room and seeing a cookie, then this experience will not be used by states u_0 and u_3 as it is impossible to observe a cookie at the red room from those states. Note that adding this rule may work in many cases, but it will not address the problem in all environments. We consider addressing this problem as an interesting area for future work.