Certified Reinforcement Learning with Logic Guidance

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Abstract This paper proposes the first model-free Reinforcement Learning (RL) framework to synthesise policies for unknown, and continuous-state Markov Decision Processes (MDPs), such that a given linear temporal property is satisfied. We convert the given property into a Limit Deterministic Büchi Automaton (LDBA), namely a finite-state machine expressing the property. Exploiting the structure of the LDBA, we shape a synchronous reward function on-the-fly, so that an RL algorithm can synthesise a policy resulting in traces that probabilistically satisfy the linear temporal property. This probability (certificate) is also calculated in parallel with policy learning when the state space of the MDP is finite: as such, the RL algorithm produces a policy that is certified with respect to the property. Under the assumption of finite state space, theoretical guarantees are provided on the convergence of the RL algorithm to an optimal policy, maximising the above probability. We also show that our method produces "best available" control policies when the logical property cannot be satisfied. In the general case of a continuous state space, we propose a neural network architecture for RL and we empirically show that the algorithm finds satisfying policies, if there exist such policies. The performance of the proposed framework is evaluated via a set of numerical examples and benchmarks, where we observe an improvement of one order of magnitude in the number of iterations required for the policy synthesis, compared to existing approaches whenever available.

1 Introduction

Markov Decision Processes (MDPs) are a family of stochastic processes adopted in automatic control, computer science, economics, and biology inter alia, for modelling sequential decision-making problems [86]. By choosing relevant actions over states, a decision maker (or an agent) can move probabilistically

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between states [78] and receives a scalar reward. The outcomes from taking actions are in general probabilistic and not fully under the control of the agent [11]. An MDP is said to be solved when at any given state the agent is able to choose most favourable actions so that the accrued reward is expected to be maximum in the long run: in other words, the goal is to find an optimal action selection policy that returns the maximum expected reward [78] (possibly discounted over time).

When state and action spaces are finite, the stochastic behaviour of the MDP is encompassed by a transition probability matrix, which represents its mathematical model. In problems where this matrix is available, the most immediate method to solve a given MDP is to use Dynamic Programming (DP). DP iteratively applies a Bellman operation on a value function expressing the expected reward of interest, which is defined over the "entire state space" of the MDP [11]. Due to its reliance on the whole state space and its known computational costs, the applicability of DP can be practically quite limited. When the state and action spaces are not finite, approximate DP is often employed. This approximation can be applied over the state or action space [9, 24, 85, 98], or over the value function [73, 93, 99].

In practice, holding full knowledge about the stochastic behaviour of the MDP (namely, its model) is often infeasible. Consider a robotic motion planning problem as an example: at a given state taking a particular action might move the robot to a different state each time due to several factors both in the environment where the robot operates and also in the mechanics of the robot; thus, the robot planning problem can be modelled as an MDP in which the state are observable but transition probabilities are unknown. In these scenarios classical DP is of limited utility, because of its assumption of a perfectly known model [102].

Reinforcement Learning (RL), on the other hand, is an algorithm that is widely used to train an agent to interact with an unknown MDP. RL is inspired by cognitive and behavioural psychology, where a reinforcement is the outcome of an action that will strengthen an agent's future behaviour, whenever that behaviour is anticipated by a specific stimulus. A key feature of RL is its sole dependence on these set of experiences, which, in the form of traces, have a time sequentiality. This makes RL inherently different than DP, in the sense that it can solve an MDP without having access to any prior knowledge about the MDP model.

Learning by collecting experience in RL is accomplished via two different methods: model-based learning and model-free learning. Model-based RL attempts to first model the MDP structure (or its transition probabilities), and then based on the built model it synthesises the optimal policy via DP or other planning algorithms. The second method, model-free RL, learns an optimal policy directly by mapping state-action pairs to their expected reward, without the need for a model. Model-free RL is proved to converge to the same action selection policy as DP (over the original MDP) under mild assumptions [11,112]. Both RL methods are extensively used in a variety of

applications from robotics [43,87,103], resource management [42,69], traffic management [91] and flight control [3], chemistry [119], and gaming [72,97].

Classical RL is focused on problems where the MDP states are finite. Nonetheless, many interesting real-world control tasks require actions to be taken in response to high-dimensional or real-valued sensory inputs [22]. As an example, consider the problem of drone control, in which the drone state is represented as its Euclidean position $(x, y, z) \in \mathbb{R}^3$: the physical space of an MDP modelling the stochastic behaviour of the drone is uncountably infinite, namely continuous.

The simplest way to solve an (uncountably) infinite-state MDP with RL is to discretise the state space and to resort to conventional RL to find an approximate optimal policy [99]. Unfortunately, the resulting discrete model can be often inaccurate and may not capture the full dynamics of the original MDP, leading to a sub-optimal policy synthesis. One might argue that by increasing the number of discrete states this problem can be solved, however the more the discrete states, the more expensive and time-consuming the learning process is. Thus, MDP discretisation has to always deal with the trade off between accuracy and curse of dimensionality.

A more elaborate solution is to gather a set of experience samples and then use an approximation function constructed via regression from the samples set over the entire state space. A number of methods are available to approximate the expected reward function, e.g. sparse coarse coding [101], kernel-based modelling [77], tree-based regression [26], basis functions [16], etc. Among these methods, neural networks offer great promise in approximating the expected reward, due to their ability to generalise [48], and as a result there exist numerous successful applications of neural networks in RL for uncountably infinite or very large MDPs, e.g. TD-Gammon [105], Asynchronous Deep RL [71], Neural Fitted Q-iteration (NFQ) [89], CACLA [109] and Deep Qnetworks (DQN) [72]. DQN are arguably one of the recent breakthroughs in RL, whereby human-level game play has been achieved on a number of Atari 2600 games. DQN attains this only by receiving available high-level information, namely the image visible on the game-screen and the score. This means that it is general enough that the rules of different games do not have to be explicitly encoded for the agents to learn successful control policies at the price of very high sample complexity.

Despite its generality, DQN is not a natural representation of how humans perceive these games, since humans already have prior knowledge and associations regarding many elements that appear on-screen and their corresponding function, e.g. "keys open doors". Given the useful domain knowledge that human experts can offer, and the otherwise huge challenge posed by randomly and exhaustively exploring large state spaces, new approaches have arisen that intend to combine human domain knowledge and insight with the ability of RL to eventually converge to near-optimal policies. These include apprenticeship learning, imitation learning, and expert demonstrations [2,7,12,47,50,68,74,84,110], and have already shown great improvements over the state-of-the-art learning methods. However, these approaches are very much biased towards the human

behaviour and might not be able to find a global optimal control policy when the human teacher believes that a local optimum is actually global. Introducing useful associations to RL in a formal way allows the agent to lift its initial knowledge about the problem and to efficiently find the global optimal policy, while avoiding an exhaustive exploration in the beginning or being biased towards human beliefs.

Contributions of This Work: Linear Temporal Logic (LTL) [83] is a formal language that allows to express formal engineering requirements and specifications, to the extent that there exists a substantial body of research on extraction of LTL properties from natural language sentences, e.g. [36, 76, 116]. LTL can express time-dependent properties, such as safety and liveness, and further allows one to specify complex (e.g., repeating, sequential, conditional) tasks. Given an LTL specification, in this paper we propose the first algorithm for model-free RL, which allows to synthesise a control policy for a continuousstate MDP (and its simpler, finite-state case), such that the generated traces satisfy the LTL property (with maximal probability in finite-state case). In this work, the problem of "policy synthesis" is separated from (and does not depend to) that of "model learning" and can be addressed directly via model-free RL. This is not the case in existing LTL synthesis algorithms, all of which rely on the process of (1) first learning a model of the MDP and then (2) finding an optimal policy based on the results of (1). In this work we skip (1) and directly perform policy synthesis in (2) with the same guarantees as (1) in the finite-state case. As we demonstrate in experiments, this drastically increases the convergence speed to the optimal policy and the scalability of the proposed framework over standard methods. Additionally, in the case of continuous-state MDPs, we introduce the first model-free RL policy synthesis algorithm. The proposed method solely relies on random experience samples gathered from the MDP and treats the MDP as a black box. We empirically show that our algorithm produces control strategies generating traces that satisfy the desired temporal property.

From a learning perspective, by employing LTL in an RL context, we can infuse structural knowledge into the learning procedure, whilst avoiding the bias otherwise introduced by a human teacher, as discussed above. This allows the expression of complex properties (such as safety, liveness and fairness guarantees) and can be extended with related techniques, such as sub-task decomposition and hierarchical learning. In particular, in order to show the enhancement of learning within the proposed architecture, we have picked the Atari 2600 game "Montezuma's Revenge" as one of our case studies, which is the only game in [72] that DQN fails to gain any score at.

Although drawing theoretical guarantees for uncountably infinite state-space models case is not possible in general, we prove that maximising an expected reward in a finite-state MDP with our RL algorithm is asymptotically equivalent to maximising the probability of satisfying the assigned LTL property. Additionally, we quantify this probability with a method based on asynchronous value iteration [11]. Conversely, we show that whenever the probability of

satisfying the given LTL property is zero, our algorithm produces "best available" policies in finite-state MDPs. Another contribution of this work to handle time-varying periodic environments, which are encoded as Kripke transition systems that are then synchronised with the LDBA.

In our setup, the LTL property acts as a high-level guide for the agent, whereas the low-level planning is handled by a native RL scheme. In order to synchronise this high-level guide with RL, we convert the LTL property into an automaton, namely a finite-state machine [8]. In general, however, LTL-to-automaton translation may result in a non-deterministic model, over which policy synthesis for MDPs is in general not semantically meaningful. A standard solution to this issue is to use Safra construction to determinise the automaton, which as expected can increase its size dramatically [80,92]. An alternative solution is to directly convert the given LTL formula into a Deterministic Rabin Automaton (DRA), which by definition rules out nondeterminism. Nevertheless, it is known that such conversion results, in the worst case, in automata that are doubly exponential in the size of the original LTL formula [5]. Conversely, in this paper we propose to express the given LTL property as a Limit Deterministic Büchi Automaton (LDBA) [95]. It is shown that this construction results in an exponential-sized automaton for LTL\GU¹, and it results in nearly the same size as a DRA for the rest of LTL. Furthermore, a Büchi automaton is semantically easier than a Rabin automaton in terms of its acceptance conditions, which makes policy synthesis algorithms much simpler to implement [96, 108]. However, we should emphasise that there exist a few LDBA construction algorithms for LTL, but not all of resulting LDBAs can be employed for quantitative model-checking, e.g. [56].

Once the LDBA is generated from the given LTL property, we construct on-the-fly² a synchronous product between the MDP and the resulting LDBA and then define a reward function that is synchronous with the accepting condition of the Büchi automaton over the state-action pairs of the MDP. Using this algorithmic reward shaping procedure, RL is able to generate a policy (or policies) that returns the maximum expected reward, or as we will show in the finite-state case, a policy (or policies) that satisfies the given LTL property with maximal probability. As mentioned above, we also propose a mechanism to determine this probability while the agent is learning the MDP: consequently, we can certify the generated policy by quantifying how safe it is with respect to the LTL property.

This work shows that the proposed architecture performs efficiently and is compatible with RL algorithms that are at the core of recent developments in the community, e.g. [71,72]. Thus, we believe that the proposed approach can open up to further research in the area.

¹ LTL\GU is a fragment of linear temporal logic with the restriction that no until operator occurs in the scope of an always operator

² On-the-fly here means that the algorithm tracks (or executes) the state of an underlying structure (or a function) without explicitly building the entire structure a-priori.

In short, in this paper we pursue the following objectives:

- Introducing the first model-free RL framework for LTL policy synthesis in both continuous-state and finite-state MDPs.
- Providing certificates for LTL satisfaction in RL when MDP state space is finite.
- Enhancing scalability and convergence rate of state-of-the-art LTL policy synthesis.
- Attaining automatic task decomposition in hierarchical RL.

Related Work: The problem of control synthesis in finite-state MDPs with temporal logic has been considered in numerous works. In [115], the property of interest is expressed in LTL, which is converted to a DRA using standard methods. A product MDP is then constructed with the resulting DRA and a modified DP is applied over the product MDP, maximising the worst-case probability of satisfying the specification over all transition probabilities. However, [115] assumes to know the MDP a priori. [29] assumes that the given MDP model has unknown transition probabilities and builds a Probably Approximately Correct MDP (PAC MDP), which is multiplied by the logical property after conversion to DRA. The overall goal is to calculate the finite-horizon T-step value function for each state, such that the obtained value is within an error bound from the probability of satisfying the given LTL property. The PAC MDP is generated via an RL-like algorithm, then value iteration is applied to update state values.

The problem of policy generation by maximising the probability of satisfying given unbounded reachability properties is investigated in [14]. The policy generation relies on an approximate DP, even when the MDP transition probabilities are unknown. This requires a mechanism to approximate these probabilities (much like PAC MDP above), and the quality of the generated policy critically depends on the accuracy of this approximation. Therefore, a sufficiently large number of simulations has to be executed to make sure that the probability approximations are accurate enough [14]. Furthermore, the algorithm in [14] assumes prior knowledge about the smallest transition probability. Via LTL-to-DRA conversion, [14] algorithm can be extended to the problem of control synthesis for LTL specifications, at the expense double exponential blow-up of the obtained automaton. Much in the same direction, [91] employs a learning-based approach to generate a policy that is able to satisfy a given LTL property. For this approach, as remarked before, LTL-to-DRA conversion is in general known to result in large automata, and the reward shaping is complicated, due to the accepting conditions of the DRA. As for [14], the algorithm in [91] hinges on approximating the transition probabilities, which limits the precision of the policy generation process.

Compared to the mentioned approaches, the proposed framework learns the dynamics of the MDP implicitly, whilst synthesising the optimal policy at the same time, hence without explicitly having to construct the transition probabilities or the MDP model first. Indeed, the proposed framework can be implemented completely "model-free", which means that we are able to synthesise policies (1) without knowing MDP graph and its transition probabilities (as opposed to DP); and (2) without preprocessing or constructing a model of the MDP (which is the base for, among other techniques, model-based RL). The second feature results in the synthesis of policies by direct interaction with the MDP. Moreover, unlike [91], the proposed algorithms are able to find the optimal policy even if the satisfaction probability is not equal to one. In the RL literature, model-free methods are very successful, since they learn a direct mapping from states and actions to the associated expected reward. Alternative approaches, known as model-based learning, are not as general as model-free methods [35], even though they have convenient theoretical guarantees [55,100]. Our work in [41] has been taken up more recently by [38], which has focused on model-free aspects of the algorithm in [41] and has employed a different LDBA structure and associated reward.

Moving away from RL and full LTL, the problem of synthesising a policy that satisfies a temporal logic specification and that at the same time optimises a performance criterion is considered in [19,65,104,114]. In [58], scLTL is proposed for mission specifications, which results in deterministic finite automata. A product MDP is then constructed and a linear programming solver is used to find optimal policies. [44] synthesises DFAs on-the-fly within a deep RL algorithm, when the scLTL property is not available. PCTL specifications are investigated in [60], where a linear optimisation solution is used to synthesise a control policy. In [79], an automated method is proposed to verify and repair the policies that are generated by RL with respect to a PCTL formula - the key engine runs by feeding the Markov chain induced by the policy to a probabilistic model checker. In [6], some practical challenges of RL are addressed by letting the agent plan ahead in real time using constrained optimisation.

In [114], the authors separate the problem into two sub-problems: extracting a (maximally) permissive strategy for the agent and then quantifying the performance criterion as a reward function and computing an optimal strategy for the agent within the operating envelope allowed by the permissive strategy. Similarly, [53] first computes safe, permissive strategies with respect to a reachability property. Then, under these constrained strategies, RL is applied to synthesise a policy that satisfies an expected cost criterion. The concept of shielding is employed in [4] to synthesise a policy that ensures that the agent remains safe during and after learning for a fully-deterministic reactive system. This approach is closely related to teacher-guided RL [106], since a shield can be considered as a teacher, which provides safe actions when absolutely necessary. To express the specification, [4] uses DFAs and then translates the problem into a safety game. The game is played by the environment and the agent. In every state of the game, the environment chooses an input, and then the agent selects an output. The game is won by the agent if only safe states are visited during the play. However, the generated policy always needs the shield to be online, as the shield maps every unsafe action to a safe action. The work in [52] extends [4] to probabilistic systems modelled as MDPs with adversarial uncontrollable agents. [52] assumes that the controllable agent acquires full observation over

the MDP and adversarial agents: unlike the proposed framework in this paper, the RL scheme used in [52] is model-based and requires the agent to first build a model of the stochastic MDP. [30,32] address safety-critical settings in the context of cyber-physical systems, where the agent has to deal with a heterogeneous set of models in model-based RL. [32] first generates a set of feasible models given an initial model and data on runs of the system. With such a set of feasible models, the agent has to learn how to safely identify which model is the most accurate one. [31] further employs differential dynamic logic [82], a first-order multimodal logic for specifying and proving properties of hybrid models.

Safe RL is an active area of research whose focus is on the efficient implementation of safety properties, and is mostly based on reward engineering [33]. Our proposed framework is related to work on safe RL, but cannot simply be reduced to it, due to its generality and to its inherent structural differences. By focusing on the safety fragment of LTL, the proposed framework does not require the reward function to be handcrafted. The reward function is automatically shaped by exploiting the structure of the LDBA and its generalised Büchi acceptance condition. However, for the safety fragment of LTL the proposed automatic reward shaping can be seen as a way of "modifying the optimization criterion," as in [33].

Our work cannot be considered a Constrained MDP (CMDP) method, as the LTL satisfaction is encoded in the expected return itself, while in CMDP algorithms the original objective is separated from the constraint. In a nutshell, the proposed method inherits reward engineering aspects that are standard in safe RL, however at the same time it infuses notions from formal methods that allow guiding exploration and certifying its outcomes.

Unfortunately, in the domain of continuous-state MDPs, to the best of our knowledge, no research has been done to enable RL to generate policies while respecting full LTL properties. The algorithm proposed in this paper is the first that can handle both finite-state and continuous-state MDPs in this context. More work has been done if the model of the MDP is known, as detailed next. Probabilistic reachability over a finite horizon for hybrid continuous-state MDPs is investigated in [1], where a DP-based algorithm is employed to produce safe policies. DFAs have been employed in [107] to find an optimal policy for infinite-horizon probabilistic reachability problems. FAUST² [98] deals with uncountable-state MDPs by generating a discrete-state abstraction based on the knowledge of the MDP model. Using probabilistic bi-simulation [37] showed that abstraction-based model checking can be effectively employed to generate control policies in continuous-state MDPs. Bounded LTL is proposed in [66] as the specification language, and a policy search method is used for synthesis.

Statistical Model Checking (SMC) techniques have also been studied for MDPs, however they are not well suited to models that exhibit non-determinism. This is due to the fact that SMC techniques often rely on generation of random paths, which are not well-defined for an MDP with non-determinism [13,64]. Some SMC approaches proposed to resolve the MDP non-determinism by using uniform distributions [20,61] and others proposed to consider all possible

strategies [45,62] and produced policies that are close to the optimal one. Unlike RL, which improves its exploration policy during learning, a constant random policy is expected to waste time and computational resources to generate sample traces. Also, a trace is "only" used to reinforce each state-action pair visited by the associated path, if the trace satisfies the property of interest. For this reason, SMC methods are not expected to scale as well as RL. Further, sampling and checking of traces needs to be computationally feasible: SMC techniques are effective with finite-horizon LTL properties, as opposed to the focus of this work on infinite-horizon properties and full LTL. The efforts on statistical model-checking of unbounded properties is limited to a few specifications [118]. However, there have been some recent developments, e.g. [45], that leverage RL to reduce the randomness in the policy that resolves the MDP non-determinism. Despite significant improvements, these SMC techniques are still limited to finite-horizon LTL and Monte Carlo search.

The rest of this article is organised as follow: Section 2 reviews basic concepts and definitions. In Section 3, we discuss the policy synthesis problem and we propose a method to constrain it. Case studies are provided in Section 4 to quantify the performance of the proposed algorithms.

2 Background

2.1 Problem Setup

Definition 1 (Continuous-state MDP) The tuple $\mathbf{M} = (\mathcal{S}, \mathcal{A}, s_0, P, \mathcal{AP}, L)$ is an MDP over a set of states $\mathcal{S} = \mathbb{R}^n$, where \mathcal{A} is a finite set of actions, s_0 is the initial state and $P : \mathcal{B}(\mathbb{R}^n) \times \mathcal{S} \times \mathcal{A} \to [0,1]$ is a Borel-measurable transition kernel which assigns to any pair of state and action a probability measure on the Borel space $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n))$ [10]. \mathcal{AP} is a finite set of atomic propositions and a labelling function $L : \mathcal{S} \to 2^{\mathcal{AP}}$ assigns to each state $s \in \mathcal{S}$ a set of atomic propositions $L(s) \subseteq 2^{\mathcal{AP}}$ [25].

A finite-state MDP is a special case of continuous-state MDP in which $|\mathcal{S}| < \infty$ and $P: \mathcal{S} \times \mathcal{A} \times \mathcal{S} \rightarrow [0,1]$ is the transition probability function. The transition function P induces a matrix, known as transition probability matrix.

Definition 2 (Path) In an MDP M, an infinite path ρ starting at s_0 is a sequence of states $\rho = s_0 \xrightarrow{a_0} s_1 \xrightarrow{a_1} \dots$ such that every transition $s_i \xrightarrow{a_i} s_{i+1}$ is possible in M, i.e. s_{i+1} belongs to the smallest Borel set B such that $P(B|s_i,a_i)=1$ (or in a finite-state MDP, s_{i+1} is such that $P(s_{i+1}|s_i,a_i)>0$). We might also denote ρ as s_0 .. to emphasize that ρ starts from s_0 .

Definition 3 (Stationary and Deterministic Policy) A stationary (randomized) policy $Pol: \mathcal{S} \times \mathcal{A} \to [0,1]$ is a mapping from any state $s \in \mathcal{S}$ to a probability distribution over actions. A deterministic policy is a degenerate case of a randomized policy which outputs a single action at a given state, that is $\forall s \in \mathcal{S}, \ \exists a \in \mathcal{A}, \ Pol(s,a) = 1$.

In an MDP **M**, we define a function $R: \mathcal{S} \times \mathcal{A} \to \mathbb{R}_0^+$ that denotes the immediate scalar bounded reward received by the agent from the environment after performing action $a \in \mathcal{A}$ in state $s \in \mathcal{S}$.

Definition 4 (Expected Infinite-Horizon Discounted Reward) For a deterministic policy $Pol: \mathcal{S} \to \mathcal{A}$ on an MDP \mathbf{M} , and given a reward function R, the expected discounted reward at state s is defined as [102]:

$$U^{Pol}(s) = \mathbb{E}^{Pol} \left[\sum_{n=0}^{\infty} \gamma^n \ R(s_n, Pol(s_n)) | s_0 = s \right], \tag{1}$$

where $\mathbb{E}^{Pol}[\cdot]$ denotes the expected value given that the agent follows policy Pol from state $s, \gamma \in [0,1)$ ($\gamma \in [0,1]$ when episodic, where episodes have a finite number of steps) is a discount factor, and $s_0, ..., s_n$ is the sequence of states generated by policy Pol up to time step n, initialised at $s_0 = s$.

Note that the discount factor γ is a hyper-parameter that can be tuned. In particular, there is standard work in RL on state-dependent discount factors [75, 81,113,117], which is shown to preserve convergence and optimality guarantees. A possible tuning strategy for our setup would let the discount factor be a state-dependent function, as:

$$\gamma(s) = \begin{cases} \eta & \text{if } R(s, a) > 0, \\ 1 & \text{otherwise,} \end{cases}$$
 (2)

where $0 < \eta < 1$ is a constant. Hence, (1) would reduce to the following [75]:

$$U^{Pol}(s) = \mathbb{E}^{Pol}\left[\sum_{n=0}^{\infty} \gamma(s_n)^{N(s_n)} R(s_n, Pol(s_n)) | s_0 = s\right], \ 0 \le \gamma \le 1, \quad (3)$$

where $N(s_n)$ is the number of times a positive reward has been observed at state s_n . Of course there might be alternatives to this tuning strategy: we do not pursue this direction as it is not central to our problem setup.

Definition 5 (Optimal Policy) An optimal policy Pol^* is defined as follows:

$$Pol^*(s) = \underset{Pol \in \mathcal{D}}{\operatorname{arg \, sup}} \ U^{Pol}(s),$$

where \mathcal{D} is the set of stationary deterministic policies over the state space \mathcal{S} .

Theorem 1 (From [18,86]) In any MDP M with a bounded reward function and a finite action space, if there exists an optimal policy, then that policy is stationary and deterministic.

As discussed before, an MDP \mathbf{M} is said to be solved if the agent discovers an optimal policy $Pol^*: \mathcal{S} \to \mathcal{A}$ that maximises the expected reward. Note that the reward function is assumed to be known in that we specify over which state-action pairs the agent will receive a given reward. More precisely, given an LTL property we know upon reaching which state in the automaton the

agent is going to receive a positive reward. There is no need to know the MDP a priori or to store a model of it, since at any given time the agent knows the exact automaton state, and the reward can be determined accordingly. Following this reward, the agent can generate an optimal policy in an unknown MDP.

In the following, we provide necessary background on model-free RL algorithms that we use in this work. We separate the presentation for finite-and the infinite-state MDPs. We emphasise that the infinite-state algorithm, which includes a generalisation step, can also handle the problem of policy synthesis in the finite-state case and can in particular be useful when the space cardinality is very large. However, if we require quantitative certificates and convergence guarantees in the finite-state case, we need to resort to the specific results that are provided for finite-state MDPs.

2.1.1 Finite-state MDPs

Q-learning (QL) is the most extensively used RL algorithm for synthesising optimal policies in finite-state MDPs [102]. For each state $s \in \mathcal{S}$ and for any available action $a \in \mathcal{A}$, QL assigns a quantitative value $Q: \mathcal{S} \times \mathcal{A} \to \mathbb{R}$, which is initialised with an arbitrary and finite value over all state-action pairs. As the agent starts receiving rewards and learning, the Q-function is updated by the following rule for taking action a at state s:

$$Q(s, a) \leftarrow Q(s, a) + \mu[R(s, a) + \gamma \max_{a' \in \mathcal{A}} (Q(s', a')) - Q(s, a)],$$
 (4)

where Q(s,a) is the Q-value corresponding to state-action (s,a), $0 < \mu \le 1$ is called learning rate or step size, R(s,a) is the reward obtained for performing action a in state s, $0 \le \gamma \le 1$ is the discount factor, and s' is the state obtained after performing action a. The Q-function for the rest of the state-action pairs remains unchanged.

Under mild assumptions over the learning rate, for finite-state and -action spaces QL converges to a unique limit³, call it Q^* , as long as every state action pair is visited infinitely often [112]. Once QL converges, the optimal policy $Pol^*: S \to \mathcal{A}$ can be generated by selecting the action that yields the highest Q^* , i.e.,

$$Pol^*(s) = \underset{a \in \mathcal{A}}{\operatorname{argmax}} \ Q^*(s, a).$$

Here Pol^* corresponds to the optimal policy that can be generated via DP. This means that when QL converges, we have

$$Q^*(s,a) = R(s,a) + \gamma \sum_{s' \in S} P(s,a,s') U^{Pol^*}(s'), \tag{5}$$

where s' is the agent new state after choosing action a at state s such that P(s'|s,a) > 0.

 $^{^3}$ This unique limit is the expected discounted reward by taking action a at state s, and following the optimal policy afterwards.

2.1.2 Continuous-state MDPs

In QL the agent stores the Q-values possibly over all state-action pairs, and updates them according to the rule in (4). When the MDP has a continuous state space it is not possible to directly use standard QL. Thus, as mentioned earlier we have to either finitely discretise the state space or to turn to function approximations, in order to interpolate the Q-function over the entire uncountably infinite state space.

Neural Fitted Q-iteration (NFQ) [89] is an algorithm that employs neural networks [49] to approximate the Q-function, namely to efficiently generalise or interpolate it over the entire state space, exploiting a finite set of experience samples. NFQ is also the core engine behind the well-known DQN [72] architecture.

Instead of the update rule in (4), NFQ introduces a loss function that measures the error between the current Q-values Q(s,a) and their target value $R(s,a) + \gamma \max_{a'} Q(s',a')$, namely

$$L = (Q(s,a) - R(s,a) + \gamma \max_{a'} Q(s',a'))^{2}.$$
 (6)

Gradient descent techniques [17] are then applied to adjust the weights of the neural network, so that this loss is minimised.

In classical QL, the Q-function is updated whenever a state-action pair is visited. In the continuous state-space case, we may update the approximation likewise, i.e., update the neural net weights once a new state-action pair is visited. However, in practice, a large number of trainings might need to be carried out until an optimal or near-optimal policy is found. This is due to the uncontrollable variations occurring in the Q-function approximation caused by unpredictable changes in the network weights when the weights are adjusted for a specific state-action pair [88]. More precisely, if at each iteration we only introduce a single sample point the training algorithm tries to adjust the weights of the entire neural network, such that the loss function is minimised at that specific sample point. This might result in some changes in the network weights such that the error between the network output and the output of previous sample points becomes large and thus fails to approximate the Qfunction correctly. Therefore, one needs to make sure that when the weights of the neural network are updated, we also consider all the previously generated samples: this technique is called "experience replay" [67], and is detailed next. The main idea underlying NFQ is to store all previous experiences and then reuse this data iteratively to update the neural Q-function. NFQ can thus be seen as a batch learning method in which there exists a training set that is repeatedly used to train the agent. In other words, experience gathering and learning happens separately.

NFQ exploits the positive effects of generalisation in neural nets as they are quite efficient in predicting Q-values for state-action pairs that have not been visited by interpolating between available data. This means that the

learning algorithm requires less experience and the learning process is thus data efficient.

2.2 Linear Temporal Logic Properties

In the proposed architecture, we use LTL formulae to express a wide range of properties (e.g., temporal, sequential, conditional), and to systematically and automatically shape a corresponding reward: such reward would otherwise be hard (if at all possible) to express and achieve by conventional methods in classical reward shaping. LTL formulae over a given set of atomic propositions \mathcal{AP} are syntactically defined as [83]

$$\varphi ::= true \mid \alpha \in \mathcal{AP} \mid \varphi \wedge \varphi \mid \neg \varphi \mid \bigcirc \varphi \mid \varphi \cup \varphi, \tag{7}$$

where the operators \bigcirc and U are called "next" and "until", respectively. The semantics of LTL formulae, as interpreted over MDPs, are discussed in the following.

Given a path ρ , the i-th state of ρ is denoted by $\rho[i]$, where $\rho[i] = s_i$. Furthermore, the i-th suffix of ρ is $\rho[i..]$ where $\rho[i..] = s_i \xrightarrow{a_i} s_{i+1} \xrightarrow{a_{i+1}} s_{i+2} \xrightarrow{a_{i+2}} s_{i+3} \xrightarrow{a_{i+3}} \dots$.

Definition 6 (LTL Semantics) For an LTL formula φ and for a path ρ , the satisfaction relation $\rho \models \varphi$ is defined as

```
\rho \models \alpha \in \mathcal{AP} \Leftrightarrow \alpha \in L(\rho[0]), 

\rho \models \varphi_1 \land \varphi_2 \Leftrightarrow \rho \models \varphi_1 \land \rho \models \varphi_2, 

\rho \models \neg \varphi \Leftrightarrow \rho \not\models \varphi, 

\rho \models \bigcirc \varphi \Leftrightarrow \rho[1..] \models \varphi, 

\rho \models \varphi_1 U \varphi_2 \Leftrightarrow \exists j \in \mathbb{N}_0 \text{ s.t. } \rho[j..] \models \varphi_2 \text{ and } \forall i, \ 0 \leq i < j, \ \rho[i..] \models \varphi_1.
```

The operator \bigcirc is read as "next" and requires φ to be satisfied starting from the next-state suffix of the path ρ . The operator U is read as "until" and is satisfied over ρ if φ_1 continuously holds until φ_2 becomes true. Through the until operator we are furthermore able to define two temporal modalities: (1) eventually, $\Diamond \varphi = true$ U φ ; and (2) always, $\Box \varphi = \neg \Diamond \neg \varphi$. The intuition for $\Diamond \varphi$ is that φ has to become true at some finite point in the future, whereas $\Box \varphi$ means that φ has to remain true forever. An LTL formula φ over \mathcal{AP} specifies the following set of words:

$$Words(\varphi) = \{ \sigma \in (2^{\mathcal{AP}})^{\omega} \text{ s.t. } \sigma \models \varphi \}.$$
 (8)

Definition 7 (Probability of Satisfying an LTL Formula) Starting from any state s and following a stationary deterministic policy Pol, we denote the probability of satisfying formula φ as

$$Pr(s..^{Pol} \models \varphi),$$

where $s..^{Pol}$ is the collection of all paths starting from s, generated under policy Pol. The maximum probability of satisfaction is also defined as:

$$Pr_{\max}(s_0.. \models \varphi) = \underset{Pol \in \mathcal{D}}{\operatorname{arg sup}} Pr(s_0..^{Pol} \models \varphi)$$

Definition 8 (Policy Satisfaction) In an MDP M, we say that a stationary deterministic policy Pol satisfies an LTL formula φ if:

$$Pr(s_0..^{Pol} \models \varphi) > 0,$$

where s_0 is the initial state of the MDP.

Using an LTL formula we can now specify a set of constraints (i.e., requirements, or specifications) over the traces of the MDP. Once a policy Pol is selected, it dictates which action has to be taken at each state of the MDP \mathbf{M} . Hence, the MDP \mathbf{M} is reduced to a Markov chain, which we denote by \mathbf{M}^{Pol} .

For an LTL formula φ , an alternative method to express the set $Words(\varphi)$ in (8) is to employ a limit-deterministic Büchi automaton (LDBA) [95]. We first define a Generalised Büchi Automaton (GBA), then we formally introduce the LDBA [95].

Definition 9 (Generalised Büchi Automaton) A GBA $\mathbf{N} = (\Omega, q_0, \Sigma, \mathcal{F}, \Delta)$ is a structure where Ω is a finite set of states, $q_0 \in \Omega$ is the initial state, $\Sigma = 2^{\mathcal{AP}}$ is a finite alphabet, $\mathcal{F} = \{F_1, ..., F_f\}$ is the set of accepting conditions, where $F_j \subset \Omega, 1 \leq j \leq f$, and $\Delta : \Omega \times \Sigma \to 2^{\Omega}$ is a transition relation.

Let Σ^{ω} be the set of all infinite words over Σ . An infinite word $w \in \Sigma^{\omega}$ is accepted by a GBA **N** if there exists an infinite run $\theta \in \mathbb{Q}^{\omega}$ starting from q_0 where $\theta[i+1] \in \Delta(\theta[i], \omega[i]), i \geq 0$ and for each $F_j \in \mathcal{F}$

$$inf(\theta) \cap F_j \neq \emptyset,$$
 (9)

where $inf(\theta)$ is the set of states that are visited infinitely often by the run θ .

Definition 10 (LDBA) A GBA $\mathbf{N} = (\Omega, q_0, \Sigma, \mathfrak{F}, \Delta)$ is limit-deterministic if Ω can be partitioned into two disjoint sets $\Omega = \Omega_N \cup \Omega_D$, such that [95]:

 $\begin{array}{l} -\ \varDelta(q,\alpha)\subset \mathfrak{Q}_D \ \text{and} \ |\varDelta(q,\alpha)|=1 \ \text{for every state} \ q\in \mathfrak{Q}_D \ \text{and for every} \ \alpha\in \varSigma, \\ -\ \text{for every} \ F_j\in \mathfrak{F}, \ F_j\subset \mathfrak{Q}_D. \end{array}$

Intuitively, an LDBA is a GBA that has two partitions: initial (Q_N) and accepting (Q_D) . The accepting part includes all the accepting states and has deterministic transitions. As an example, Fig. 1 shows the LDBA constructed for the formula $\varphi = a \wedge \bigcap (\Diamond \Box a \vee \Diamond \Box b)$.

Remark 1 The LTL-to-LDBA algorithm proposed in [95], which is used in this paper, results in an automaton with two parts (initial Ω_N and accepting Ω_D). Both initial and accepting parts comprise deterministic transitions, and additionally there are non-deterministic ε -transitions between them. According to Definition 10, the discussed structure is still an LDBA (the determinism

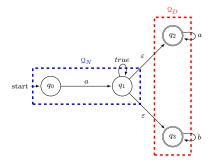


Fig. 1: LDBA for the formula $a \land \bigcirc (\Diamond \Box a \lor \Diamond \Box b)$.

in the initial part is stronger than that required in the LDBA definition). An ε -transition allows an automaton to change its state without reading an input symbol. In practice, during an episode of the RL algorithm, the ε -transitions between Ω_N and Ω_D reflect the agent's "guess" on reaching Ω_D : accordingly, if after an ε -transition the associated labels in the accepting set of the automaton cannot be read, or the accepting states cannot be visited, then the guess is deemed to be wrong, and the trace is disregarded.

3 Logically-Constrained Reinforcement Learning (LCRL)

We are interested in synthesising a policy (or policies) for an unknown MDP via RL such that the obtained structure satisfies a given LTL property. In order to explain the core ideas of the algorithm and for ease of exposition, we assume that the MDP graph and the associated transition probabilities are known. Later these assumptions are entirely removed, and we stress that the algorithm can be run model-free. We relate the MDP and the automaton by synchronising them, in order to create a new structure that is first of all compatible with RL and secondly that encompasses the given logical property.

Definition 11 (Product MDP) Given an MDP $\mathbf{M} = (S, A, s_0, P, AP, L)$ and an LDBA $\mathbf{N} = (Q, q_0, \Sigma, \mathcal{F}, \Delta)$ with $\Sigma = 2^{AP}$, the product MDP is defined as $(\mathbf{M} \otimes \mathbf{N}) = \mathbf{M}_{\mathbf{N}} = S^{\otimes}, A, s_0^{\otimes}, P^{\otimes}, AP^{\otimes}, L^{\otimes}, \mathcal{F}^{\otimes})$, where $S^{\otimes} = S \times Q$, $s_0^{\otimes} = (s_0, q_0), AP^{\otimes} = Q, L^{\otimes} : S^{\otimes} \to 2^{Q}$ such that $L^{\otimes}(s, q) = q$ and $\mathcal{F}^{\otimes} \subseteq S^{\otimes}$ is the set of accepting states $\mathcal{F}^{\otimes} = \{F_1^{\otimes}, ..., F_f^{\otimes}\}$, where $F_j^{\otimes} = S \times F_j$. The transition kernel P^{\otimes} is such that given the current state (s_i, q_i) and action a, the new state is (s_j, q_j) , where $s_j \sim P(\cdot|s_i, a)$ and $q_j \in \Delta(q_i, L(s_j))$. When the MDP \mathbf{M} has a finite state space, then $P^{\otimes} : S^{\otimes} \times A \times S^{\otimes} \to [0, 1]$ is the transition probability function, such that $(s_i \xrightarrow{a} s_j) \wedge (q_i \xrightarrow{L(s_j)} q_j) \Rightarrow P^{\otimes}((s_i, q_i), a, (s_j, q_j)) = P(s_i, a, s_j)$. Furthermore, in order to handle ε -transitions we make the following modifications to the above definition of product MDP:

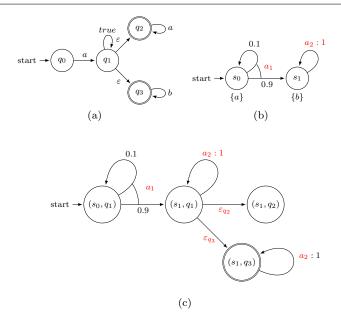


Fig. 2: Example of product MDP: the top figures are the LDBA in Fig. 1 and an instance MDP, and the bottom one is the product of this MDP with the LDBA according to Def. 11.

– for every potential ε -transition to some state $q \in \mathbb{Q}$ we add a corresponding action ε_q in the product:

$$\mathcal{A}^{\otimes} = \mathcal{A} \cup \{ \varepsilon_q, q \in \Omega \}.$$

- The transition probabilities corresponding to ε -transitions are given by

$$P^{\otimes}((s_i, q_i), \varepsilon_q, (s_j, q_j)) = \begin{cases} 1 & \text{if } s_i = s_j, \ q_i \xrightarrow{\varepsilon_q} q_j = q, \\ 0 & \text{otherwise.} \end{cases}$$

Recall that an ε -transitions between Ω_N and Ω_D indicates a guess on reaching Ω_D . Hence, if after an ε -transition the associated labels in the accepting set of the automaton cannot be read, or the accepting states cannot be visited, then the guess was wrong, and the trace is disregarded.

Intuitively, by constructing the product MDP we add an extra dimension to the state space of the original MDP. The role of the added dimension is to track automaton states and, hence, to synchronise the current state of the MDP with the state of the automaton: this allows to evaluate the (partial) satisfaction of the corresponding LTL property (or parts thereof). Fig. 2 illustrates the construction of a product MDP with the LDBA generated in Fig. 1.

 $Remark\ 2$ In order to clearly elucidate the role of different components in the proposed approach, we have employed model-dependent notions, such as

transition probabilities and the product MDP. However, we emphasise that the proposed approach can run "model-free", and as such it does not depend on these components. In particular, as per Definition 10, the LDBA is composed of two disjoint sets of states Ω_D (which is invariant) and Ω_N , where the accepting states belong to the set Ω_D . Since all transitions are deterministic within Ω_N and Ω_D , the automaton transitions can be executed "only" by reading the labels, which makes the agent aware of the automaton state without explicitly constructing the product MDP. We will later define a reward function "on-the-fly", emphasising that the agent does not need to know the model structure or the transition probabilities (or their product).

Before introducing a reward assignment for RL, we need to define the ensuing function. Recall that a generalised Büchi automaton accepts words that visit its accepting sets infinitely often.

Definition 12 (Accepting Frontier Function) Let $\mathbf{N} = (\mathfrak{Q}, q_0, \Sigma, \mathfrak{F}, \Delta)$, be an LDBA where $\mathfrak{F} = \{F_1, ..., F_f\}$ is the set of accepting conditions, and $F_j \subset \mathfrak{Q}, 1 \leq j \leq f$. Define the function $Acc : \mathfrak{Q} \times 2^{\mathfrak{Q}} \to 2^{\mathfrak{Q}}$ as the accepting frontier function, which executes the following operation over a given set $\mathbb{F} \subset 2^{\mathfrak{Q}}$ for every $F_j \in \mathfrak{F}$:

$$Acc(q, \mathbb{F}) = \begin{cases} \mathbb{F}_{\backslash F_j} & (q \in F_j) \wedge (\mathbb{F} \neq F_j), \\ \{F_k\}_{k=1}^f \rangle_{F_j} & (q \in F_j) \wedge (\mathbb{F} = F_j), \\ \mathbb{F} & \text{otherwise.} \end{cases}$$

Once the state $q \in F_j$ and the set \mathbb{F} are introduced to the function Acc, it outputs a set containing the elements of \mathbb{F} minus F_j . However, if $\mathbb{F} = F_j$, then the output is the family of sets of all accepting sets of the LDBA minus the set F_j . Finally, if the state q is not an accepting state then the output of Acc is \mathbb{F} . In short, the accepting frontier function excludes from \mathbb{F} the accepting set that is currently visited, unless it is the only remaining accepting set. Otherwise, the output of $Acc(q,\mathbb{F})$ is \mathbb{F} itself. What remains in \mathbb{F} are those accepting sets that still need to be visited in order to attain the generalised Büchi accepting condition, as per Definition 9. Note that there is no need to produce all the subsets of accepting sets thanks to the on-the-fly execution of the accepting frontier function.

The product MDP encompasses transition relations of the original MDP and the structure of the Büchi automaton, and it inherits characteristics of both. A proper reward function leads the RL agent to find a policy that is optimal, in the sense that it satisfies the LTL property φ with maximal probability. We employ an on-the-fly reward function that fits the RL architecture: when an agent observes the current state s^{\otimes} , implements action a and observes the subsequent state s^{\otimes} , the reward provides the agent with a scalar value,

according to the following reward:

$$R(s^{\otimes}, a) = \begin{cases} r_p & \text{if } q' \in \mathbb{A}, \ s^{\otimes'} = (s', q'), \\ r_n & \text{otherwise.} \end{cases}$$
 (10)

Here r_p is a positive reward and r_n is a neutral reward, which can be set to be close or equal to zero. A positive reward is assigned to the agent when it takes an action that leads to a state with a label in \mathbb{A} . The set \mathbb{A} is called the accepting frontier set, is initialised as the family of sets $\mathbb{A} = \{F_k\}_{k=1}^f$, and is updated by the following rule every time after the reward function is evaluated:

$$\mathbb{A} \leftarrow Acc(q', \mathbb{A}).$$

The set \mathbb{A} always contains those accepting states that are needed to be visited at a given time: in this sense the reward function is "synchronous" with the accepting condition set by the LDBA. Thus, the agent is guided by the above reward assignment to visit these states and once all of the sets F_k , k = 1, ..., f, are visited, the accepting frontier \mathbb{A} is reset. As such, the agent is guided to visit the accepting sets infinitely often, and consequently, to satisfy the given LTL property.

The reward structure follows $r_p = M + y \times m \times rand(s^{\otimes})$ and $r_n = y \times m \times rand(s^{\otimes})$. The parameter $y \in \{0,1\}$ is a constant, $0 < m \ll M$ are arbitrary positive values, and $rand: S^{\otimes} \to (0,1)$ is a function that generates a random number in (0,1) for each state s^{\otimes} each time R is being evaluated. The role of the function rand is to break the symmetry when neural nets are used for approximating the Q-function⁴. Also, note that parameter y acts as a switch to bypass the effect of the rand function on R when no neural net is used. Thus, this switch is active y = 1 when the MDP state space is continuous, and disabled in others y = 0.

Remark 3 Note that when running our algorithm there is no need to "explicitly build" the product MDP and to store all its states and transitions in memory. The automaton transitions can be executed on-the-fly as the agent reads the labels of the MDP states. Namely, the agent can track the automaton state by just looking at the trace that has been read so far. The agent only needs to store the current state of the automaton and observe the label at each step to check whether the automaton state has changed or not.

Definition 13 Given an LTL property φ and a set of G-sub-formulae \mathcal{G}^5 we define $\varphi[\mathcal{G}]$ the resulting formula when we substitute true for every G-subformula in \mathcal{G} and $\neg true$ for other G-sub-formulae of φ .

⁴ If all weights in a feedforward net start with equal values and if the solution requires that unequal weights be developed, the network can never learn. The reason is that the correlations between the weights within the same hidden layer can be described by symmetries in that layer, i.e. identical weights. Therefore, the neural net can generalise if such symmetries are broken and the redundancies of the weights are reduced. Starting with completely identical weights prevents the neural net from minimising these redundancies and from optimising the loss function [48].

⁵ A G-subformula is a subformula of φ of the form $\square(\cdot)$.

Proposition 1 Given an LTL formula φ and its associated LDBA $\mathbf{N} = (\mathbb{Q}, q_0, \Sigma, \mathbb{F}, \Delta)$, the accepting frontier set \mathbb{A} is history-independent, namely the members of \mathbb{A} only depend on the current state of the automaton and not on the sequence of automaton states that have been already visited.

Proof Let $\mathcal{G} = \{\Box \zeta_1, ..., \Box \zeta_f\}$ be the set of all G-sub-formulae of φ . Since elements of \mathcal{G} are sub-formulae of φ we can assume an ordering over \mathcal{G} , so that if $\Box \zeta_i$ is a subformula of $\Box \zeta_j$, then j > i. In particular, $\Box \zeta_f$ is not a subformula any G-subformula.

The accepting component of the LDBA Ω_D is a product of f of the DBAs $\{\mathbf{D}_1,....,\mathbf{D}_f\}$ called G-monitors, such that each $\mathbf{D}_i = (\Omega_i,q_{i0},\Sigma,F_i,\delta_i)$ expresses $\Box \zeta_i[\mathfrak{G}]$, where Ω_i is the state space of the i-th G-monitor, $\Sigma = 2^{\mathcal{AP}}$, and $\delta_i:\Omega_i\times\Sigma\to\Omega_i$ [95]. Note that $\zeta_i[\mathfrak{G}]$ has no G-subformula any more (Definition 13). The states of the G-monitor \mathbf{D}_i are pairs of formulae where at each state the the G-monitor only checks if the run satisfies $\Box \zeta_i[\mathfrak{G}]$ whilst putting the next G-subformula in the ordering of \mathfrak{G} on hold, assuming that it is true.

The product of G-monitor DBAs is a deterministic generalised Büchi automaton:

$$\mathbf{P}_{\mathbf{D}} = (Q_D, q_{D0}, \Sigma, \mathcal{F}, \delta)$$

where $\Omega_D = \Omega_1 \times ... \times \Omega_f$, $\Sigma = 2^{\mathcal{AP}}$, $\mathcal{F} = \{F_1, ..., F_f\}$, and $\delta = \delta_1 \times ... \times \delta_f$.

As shown in [95], while a word w is being read by the accepting component of the LDBA, the set of G-sub-formulae that hold is "monotonically" expanding. If $w \in Words(\varphi)$, then eventually all G-sub-formulae become true. Now, let the current state of the automaton be $q_D = (q_1, ..., q_i, ..., q_f)$ while the automaton is checking whether $\Box \zeta_i[\mathfrak{F}]$ is satisfied or not, assuming that $\Box \zeta_{i+1}$ is already true (though needs to be checked later), while all G-monitors $\Box \zeta_j[\mathfrak{F}]$, $1 \leq j \leq i-1$ have accepted w. At this point, the accepting frontier set $\mathbb{A} = \{F_i, F_{i+1}, ..., F_f\}$. Reasoning by contradiction, assume that the automaton returns to q_D but $\mathbb{A} \neq \{F_i, F_{i+1}, ..., F_f\}$, then at least one accepting set F_j , j > i has been removed from \mathbb{A} . This means that $\Box \zeta_j$ is a subformula of $\Box \zeta_i$, violating the ordering of check on \mathbb{G} . This is a contradiction with respect to the ordering of G-sub-formulae. Thus, when the automaton returns to a particular state in \mathfrak{Q}_D , the accepting frontier set \mathbb{A} is always the same.

In the following, we evaluate the proposed architecture in both finite- and continuous-state MDPs.

3.1 Finite-state MDPs: Logically-Constrained QL

Over finite-state MDPs, as introduced above we run QL over the product MDP $\mathbf{M_N}$ with the reward shaping proposed in (10), where we have set y=0. In order to handle also non-ergodic MDPs, we propose to employ a variant of standard QL that consists of several resets, at each of which the agent is forced to re-start from its initial state s_0 . Each reset defines an episode, as

such the algorithm is called "episodic QL". However, for the sake of simplicity, we omit the term "episodic" in the rest of the paper and we use the term Logically-Constrained QL (LCQL).

As stated earlier, since QL is proved to converge to the optimal Q-function [11,112], we can synthesise the optimal policy in the limit. The following result shows that the optimal policy produced by LCQL indeed satisfies the given LTL property (Definition 8).

Theorem 2 Let the MDP M_N be the product of a finite-state MDP M and of an LDBA N that is associated with the given LTL property φ . If a satisfying policy exists, then with a choice of $0 \le \gamma \le 1$, the LCQL algorithm will in the limit find one such policy.

Proof Assume that there exists a policy \overline{Pol} that satisfies φ . Policy \overline{Pol} induces a Markov chain $\mathbf{M}_{\mathbf{N}}^{\overline{Pol}}$ when it is applied over the MDP $\mathbf{M}_{\mathbf{N}}$. This Markov chain comprises a disjoint union between a set of transient states $T_{\overline{Pol}}$ and h sets of irreducible recurrent classes $R_{\overline{Pol}}^i$, i=1,...,h [25], namely:

$$\mathbf{M}_{\mathbf{N}}^{\overline{Pol}} = T_{\overline{Pol}} \sqcup R_{\overline{Pol}}^{1} \sqcup \ldots \sqcup R_{\overline{Pol}}^{h}.$$

From (9), policy \overline{Pol} satisfies φ if and only if:

$$\exists R_{\overline{Pol}}^{i} \text{ s.t. } \forall j \in \{1, ..., f\}, \ F_{j}^{\otimes} \cap R_{\overline{Pol}}^{i} \neq \emptyset.$$
 (11)

The recurrent classes that satisfy (11) are called accepting. From the irreducibility of the recurrent class R^i_{Pol} we know that all the states in R^i_{Pol} communicate with each other thus, once a trace ends up in such set, then all the accepting sets are going to be visited infinitely often. Therefore, from the definition of $\mathbb A$ and of the accepting frontier function (Definition 12), the agent receives a positive reward r_p ever after it has reached an accepting recurrent class R^i_{Pol} .

There are two other possibilities concerning the remaining recurrent classes that are not accepting. A non-accepting recurrent class, name it $R^k_{\overline{Pol}}$, either

1. has no intersection with any accepting set F_j^{\otimes} , i.e.

$$\forall j \in \{1, ..., f\}, \ F_j^{\otimes} \cap R_{\overline{Pol}}^k = \emptyset;$$

2. or has intersection with some of the accepting sets but not all of them, i.e.

$$\exists J \subset 2^{\{1,...,f\}} \setminus \{1,...,f\} \text{ s.t. } \forall j \in J, \ F_j^{\otimes} \cap R_{\overline{Pol}}^{\underline{k}} \neq \emptyset.$$

In the first instance, the agent does not visit any accepting set in the recurrent class and the likelihood of visiting accepting sets within the transient states $T_{\overline{Pol}}$ is zero since Q_D is invariant.

In the second case, the agent is able to visit some accepting sets but not all of them. This means that in the update rule of the frontier accepting set \mathbb{A} in Definition 12, the case where $(q \in F_j) \wedge (\mathbb{A} = F_j)$ will never happen since

there exist always at least one accepting set that has no intersection with R^k_{Pol} . Therefore, after a limited number of times, no positive reward can be obtained, and the reinitialisation of \mathbb{A} in Definition 12 is blocked.

Recall Definition 4, where the expected reward for the initial state $\bar{s} \in \mathbb{S}^{\otimes}$ is defined as:

$$U^{\overline{Pol}}(\bar{s}) = \mathbb{E}^{\overline{Pol}}[\sum_{n=0}^{\infty} \gamma^n \ R(S_n, \overline{Pol}(S_n))|S_0 = \bar{s}].$$

In both cases, from (10), for any arbitrary $r_p > 0$ (and $r_n = 0$), there always exists a γ such that the expected reward of a trace hitting R^i_{Pol} with unlimited number of successive times attaining positive reward, is higher than the expected reward of any other trace. Note that the discount factor can be state-dependent as in (2) and (3). With unlimited number of obtaining positive reward for the traces entering the accepting recurrent class R^i_{Pol} , and with a state-dependent discount factor, it can be shown that the expected reward is bounded and is higher than that for non-accepting traces, which have limited number of attainment of positive rewards.

In the following, by contradiction, we show that any optimal policy Pol^* which optimises the expected reward will satisfy the property. Suppose then that the optimal policy Pol^* does not satisfy the property φ . By this assumption:

$$\forall R_{Pol^*}^i, \ \exists j \in \{1, ..., f\}, \ F_j^{\otimes} \cap R_{Pol^*}^i = \emptyset.$$
 (12)

As we discussed in case 1 and case 2 above, the accepting policy \overline{Pol} has a higher expected reward than the optimal policy Pol^* due to limited number of positive rewards in policy Pol^* . This is, however, in direct contrast with Definition 5, leading to a contradiction.

Remark 4 Note that LCQL outputs its policy by choosing the maximum Q-value at any given state. Further, as we will show in Theorem 3, we can derive the probability of satisfying the LTL property from the Q-values. This means that, if there exists more than one optimal policy, i.e. if there is more than one satisfying policy corresponding to the same probability, then LCQL is able to find all of them by presenting the same Q-values to the agent for these policies. Thus, the agent is free to choose between these policies by arbitrarily choosing actions that have the same expected reward.

Definition 14 (Closeness to Satisfaction) Assume that two policies Pol_1 and Pol_2 do not satisfy the property φ . Accordingly, there are accepting sets in the automaton that have no intersection with runs of induced Markov chains \mathbf{M}^{Pol_1} and \mathbf{M}^{Pol_2} . We say that Pol_1 is closer to satisfying the property if runs of \mathbf{M}^{Pol_1} cross a larger number of distinct accepting sets of the automaton, than runs of \mathbf{M}^{Pol_2} .

Corollary 1 If no policy in the finite-state MDP M can be generated to satisfy the property φ , LCQL yields in the limit a policy that is closest (according to the previous Definition) to satisfying the given LTL formula φ . Proof Assume that there exists no policy in the MDP M that can satisfy the property φ . Construct the induced Markov chain $\mathbf{M}_{\mathbf{N}}^{Pol}$ for any arbitrary policy Pol and its associated set of transient states T_{Pol} and h sets of irreducible recurrent classes $R_{Pol}^i\colon \mathbf{M}_{\mathbf{N}}^{Pol}=T_{Pol}\sqcup R_{Pol}^1\sqcup \ldots\sqcup R_{Pol}^h$. By assumption, policy Pol cannot satisfy the property and we thus have that $\forall R_{Pol}^i,\ \exists j\in\{1,...,f\},\ F_j^\otimes\cap R_{Pol}^i=\emptyset$, which means that there are some automaton accepting sets like F_j that cannot be visited. Therefore, after a limited number of times no positive reward is given by the reward function $R(s^\otimes,a)$. However, the closest recurrent class to satisfying the property is the one that intersects with more distinct accepting sets.

By Definition 4, for any arbitrary $r_p > 0$ (and $r_n = 0$), the expected reward at the initial state for a trace with highest number of intersections with distinct accepting sets is maximum among other traces. Hence, by the convergence guarantees of QL, the optimal policy produced by LCQL converges to a policy whose recurrent classes of its induced Markov chain have the highest number of intersections with the accepting sets of the automaton.

Theorem 3 If the LTL property is satisfiable by a finite-state MDP M, then the optimal policy generated by LCQL, maximising the expected reward, maximises the probability of satisfying the property.

Proof Assume that the MDP M_N is obtained as the product of an MDP M and an automaton N, where N is the automaton associated with the given LTL property φ . In the MDP M_N , a directed graph induced by a pair (S^{\otimes}, A) , $S^{\otimes} \subseteq S^{\otimes}$, $A \subseteq \mathcal{A}$ is a Maximal End Component (MEC) if it is strongly connected and there exists no strongly connected pair $(S^{\otimes'}, A')$ such that $(S^{\otimes}, A) \neq (S^{\otimes'}, A')$ and $S^{\otimes} \subset S^{\otimes'}$ and $A \subset A'$ for all $s^{\otimes} \in S^{\otimes}$ [8]. A MEC is accepting if it contains accepting conditions of the automaton associated with the property φ . The set of all accepting MECs is denoted as the AMECs.

Let us first review how the property satisfaction probability is computed if the MDP was fully known, and then show that the LCQL optimal policy Pol^* maximises this probability. If the MDP graph and transition probabilities are known, the probability of property satisfaction can be calculated via DP-based methods, such as standard value iteration, over the product MDP $\mathbf{M_N}$ [8]. This allows to convert the problem of computing the satisfaction probability to a problem of computation of a reachability probability, where the goal in the related reachability problem is to find the maximum (or minimum) probability of reaching the AMECs [8,59]. For any state $s^{\otimes} \notin AMECs$, let us denote the maximum probability for this reachability predicate $Pr_{\max}(s^{\otimes}... \to AMECs)$, which is the maximum probability of satisfying the property φ (Definition 7).

The key to compare standard model-checking methods to LCQL is reduction of the probability computation of reachability predicate in the value iteration leading to $Pr_{max}(s^{\otimes}..\to AMECs)$ to a basic form [28]. More specifically, quantitative model-checking over an MDP with a reachability predicate can be converted to a model-checking problem with a related reward. This reduction is done by adding a one-off reward of 1 upon reaching the AMECs [28] (once the AMECs is entered, this reward is not accrued any longer). Let us call

this reward function $R'(s^{\otimes},a)$. Under this reduction, Bellman iterations are applied over the value function (which represents the satisfaction probability) to synthesise a policy that maximises the probability of satisfying the property. Therefore, for any state $s^{\otimes} \notin AMECs$, and for any stationary deterministic policy $Pol \in \mathcal{D}$ we define:

$$U'^{Pol}(s^{\otimes}) := \mathbb{E}^{Pol}\left[\sum_{n=0}^{\infty} R'(s_n^{\otimes}, Pol(s_n^{\otimes})) | s_0^{\otimes} = s^{\otimes}\right] = Pr(s^{\otimes}..^{Pol} \to AMECs).$$
(13)

Let us now revert to the LCQL scheme. As shown in Theorem 2, in view of the introduced adaptive structure of the reward function in LCQL, when an AMEC is reached following a policy Pol, i.e. when the agent enters an accepting recurrent class of $\mathbf{M}_{\mathbf{N}}^{Pol}$, an infinite number of positive rewards r_p will be accrued by the agent, as all of the accepting sets of the automaton will surely be visited infinitely often: notice that this is despite the fact that the MDP structure and AMECs are unknown to the agent (model free RL), which is the difference with the scheme above. Once in an AMEC, with probability one the MDP remains within it. In the following, we show that maximising the expected infinite number of discounted reward attained under R is indeed equivalent to maximising the expected undiscounted reward from R'. Observe that the probability of reaching the AMECs is the same. Assuming that γ is properly tuned, as discussed for Theorem 2, for any positive reward component r_p , the expected discounted reward is bounded, i.e.

$$U^{Pol}(s^{\otimes}) = \mathbb{E}^{Pol}\left[\sum_{n=0}^{\infty} \gamma^n R(s_n^{\otimes}, Pol(s_n^{\otimes})) | s_0^{\otimes} = s^{\otimes}\right] = C^{Pol}(s^{\otimes}), \tag{14}$$

where $0 < C^{Pol}(s^{\otimes}) < \infty$, $\forall s^{\otimes} \in \mathbb{S}^{\otimes}$, $\forall Pol \in \mathcal{D}$. Since the quantity $C^{Pol}(s^{\otimes})$ is bounded, then for any state $s^{\otimes} \notin AMECs$ there is a proportionality between the expected discounted reward above and the probability of the reachability predicate under policy Pol. Namely,

$$U^{Pol}(s^{\otimes}) = M(s^{\otimes}) \times Pr(s^{\otimes}..^{Pol} \to AMECs).$$

This means that the two maximisations over $\mathcal D$ are equivalent, as well as the corresponding policies, namely

$$\underset{Pol \in \mathcal{D}}{\arg\sup} \ U^{Pol}(s^{\otimes}) = M(s^{\otimes}) \times \underset{Pol \in \mathcal{D}}{\arg\sup} \ Pr(s^{\otimes}..^{Pol} \rightarrow AMECs),$$

The left-hand-side of the above equation is exactly the utility function optimisation attained by LCQL (Definition 5). Further, $\arg\sup_{Pol\in\mathcal{D}} Pr(s^{\otimes}..^{Pol}\to AMECs) = \arg\sup_{Pol\in\mathcal{D}} Pr(s^{\otimes}..^{Pol} \models \varphi)$, which denotes the policy yielding the maximum probability of satisfaction of the property (Definition 7). In conclusion, for any state s^{\otimes} the optimal policy Pol^* maximises the probability of satisfying the given LTL property.

Remark 5 Note that the projection of policy Pol^* onto the state space of the original MDP **M** yields a finite memory policy $Pol^*_{\mathbf{M}}$. Thus, if the generated traces under Pol^* maximise the LTL satisfaction probability, so do the traces of $Pol^*_{\mathbf{M}}$.

So far we have discussed an RL implementation that is capable of synthesising policies (when existing) that maximally satisfy an LTL formula over a finite-state MDP. In the following, we present an additional component, which allows to quantify the quality of the resulting policy by calculating the probability of satisfaction associated to the policy.

3.1.1 Probability of Satisfaction of a Property

The Probability of Satisfaction of a Property (PSP) can be calculated via standard DP, as implemented for instance in PRISM [59] and Storm [21]. However, as discussed before, DP is quite limited when the state space of the given MDP is large.

In this section we propose a local value iteration method as part of LCQL that calculates this probability in parallel with the RL scheme. RL guides the local update of the value iteration, such that it only focuses on parts of the state space that are relevant to the satisfaction of the property. This allows the value iteration to avoid an exhaustive search and thus to converge faster.

Recall that the transition probability function P^{\otimes} is not known. Further, according to Definition 11, for any two MDP states $s_i, s_j \in \mathcal{S}$ and any pair of automaton states $q_i, q_j \in \mathcal{Q}$, $P^{\otimes}((s_i, q_i), a, (s_j, q_j)) = P(s_i, a, s_j)$ if $(s_i \xrightarrow{a} s_j)$ and $(q_i \xrightarrow{L(s_j)} q_j)$, showing the intrinsic dependence of P^{\otimes} on P. This allows to apply the definition of α -approximation in MDPs [55] as follows.

Let us introduce two functions $\Psi: \mathbb{S} \times \mathcal{A} \to \mathbb{N}$ and $\psi: \mathbb{S} \times \mathcal{A} \times \mathbb{S} \to \mathbb{N}$ over the MDP \mathbf{M} . Function $\psi(s,a,s')$ represents the number of times the agent executes action a in state s, thereafter moving to state s', whereas $\Psi(s,a) = \sum_{s' \in \mathbb{S}} \psi(s,a,s')$. The maximum likelihood of P(s,a,s') is a Gaussian normal distribution with the mean $\bar{P}(s,a,s') = \psi(s,a,s')/\Psi(s,a)$, so that the variance of this distribution asymptotically converges to zero and $\bar{P}(s,a,s') = P(s,a,s')$. Function $\Psi(s,a)$ is initialised to be equal to one for every state-action pair (reflecting the fact that at any given state it is possible to take any action, and also avoiding division by zero), and function $\psi(s,a,s')$ is initialised to be equal to zero.

Definition 15 (Non-accepting Sink Component) A non-accepting sink component of the LDBA $\mathbf{N} = (\Omega, q_0, \Sigma, \mathcal{F}, \Delta)$ is a directed graph induced by a set of states $Q \subset \Omega$ such that (1) the graph is strongly connected; (2) it does not include all accepting sets F_k , k = 1, ..., f; and (3) there exist no other strongly connected set $Q' \subset \Omega$, $Q' \neq Q$ that $Q \subset Q'$. We denote the union of all non-accepting sink components as SINKs. Note that SINKs can be an empty set.

The set SINKs are those components in the automaton that are surely not accepting and impossible to escape from. Thus, reaching them is equivalent to not being able to satisfy the given LTL property. Now, consider a function $PSP: \mathbb{S}^{\otimes} \to [0,1]$. For a given state $s^{\otimes} = (s,q)$, the PSP function is initialised as $PSP(s^{\otimes}) = 0$ if q belongs to SINKs. Else, it is initialised as $PSP(s^{\otimes}) = 1$.

Definition 16 (Optimal PSP) The optimal PSP vector is denoted by $\underline{PSP}^* = (PSP^*(s_1), ..., PSP^*(s_{|S|}))$, where $PSP^* : S^{\otimes} \to [0,1]$ is the optimal PSP function and $PSP^*(s_i)$ is the optimal PSP value starting from state s_i such that

$$PSP^*(s_i) = \sup_{Pol \in \mathcal{D}} PSP^{Pol}(s_i),$$

where $PSP^{Pol}(s_i)$ is the PSP value of state s_i if we use the policy Pol to determine subsequent states.

In the following we prove that a proposed update rule that makes PSP converge to PSP^* .

Definition 17 (Bellman operation [11]) For any vector such as $\underline{PSP} = (PSP(s_1), ..., PSP(s_{|S|}))$ in the MDP $\mathbf{M} = (\mathcal{S}, \mathcal{A}, s_0, P, \mathcal{AP}, L)$, the Bellman DP operation T over the elements of \underline{PSP} is defined as:

$$T PSP(s_i) = \max_{a \in \mathcal{A}_{s_i}} \sum_{s' \in \mathcal{S}} P(s_i, a, s') PSP(s').$$
 (15)

If the operation T is applied over all the elements of \underline{PSP} , we denote it as T PSP.

Proposition 2 (From [11]) The optimal PSP vector \underline{PSP}^* satisfies the following equation:

$$PSP^* = T PSP^*,$$

and additionally, \underline{PSP}^* is the only solution of the equation $\underline{PSP} = T$ \underline{PSP} , i.e., the solution is unique.

In the standard value iteration method the value estimation is simultaneously updated for all states. However, an alternative method is to update the value for one state at a time. This method is known as asynchronous value iteration.

Definition 18 (Gauss-Seidel Asynchronous Value Iteration (AVI) [11]) We denote AVI operation by F and is defined as follows:

$$F \ PSP(s_1) = \max_{a \in \mathcal{A}} \{ \sum_{s' \in \mathcal{S}} P(s_1, a, s') PSP(s') \},$$
 (16)

where s_1 is the state that current state at the MDP, and for all $s_i \neq s_1$:

$$F PSP(s_i) = \max_{a \in \mathcal{A}} \left[\sum_{s' \in \mathcal{S}_L} P(s_i, a, s') F PSP(s') + \sum_{s' \in \mathcal{S}_R} P(s_i, a, s') PSP(s') \right],$$

$$(17)$$

where $S_L = \{s_1, ..., s_{i-1}\}$ and $S_R = \{s_i, ..., s_{|S|}\}$. By (17) we update the value of PSP state by state and use the calculated value for the next step.

Proposition 3 (From [11]) Let $k_0, k_1, ...$ be an increasing sequence of iteration indices such that $k_0 = 0$ and each state is updated at least once between iterations k_m and $k_{m+1} - 1$, for all m = 0, 1, ... Then the sequence of value vectors generated by AVI asymptotically converges to \underline{PSP}^* .

Lemma 1 (From [11]) F is a contraction mapping with respect to the infinity norm. In other words, for any two value vectors PSP and PSP':

$$||F \ \underline{PSP} - F \ \underline{PSP'}||_{\infty} \le ||\underline{PSP} - \underline{PSP'}||_{\infty}.$$

Proposition 4 (Convergence, [55]) From Lemma 1, and under the assumptions of Proposition 3, $\bar{P}(s, a, s')$ converges to P(s, a, s'), and from Proposition 3, the AVI value vector \underline{PSP} asymptotically converges to \underline{PSP}^* , i.e. the probability that could be alternatively calculated by DP-based methods if the MDP was fully known.

Algorithm 1: Logically-Constrained QL

```
input :LTL specification, it-threshold, \gamma, \mu
      output: Pol^* and \underline{PSP}^*
  1 initialize Q: \mathbb{S}^{\otimes} \times \mathcal{A}^{\otimes} \to \mathbb{R}_0^+
  2 initialize PSP: \mathbb{S}^{\otimes} \to [0,1]
 3 initialize ψ : S \times A \times S \rightarrow \mathbb{N}
  4 initialize \Psi: \mathbb{S} \times \mathcal{A} \to \mathbb{N}
     convert the desired LTL property to an LDBA {f N}
 6 initialize A
  7 initialize episode-number := 0
     initialize iteration-number := 0
 8
     while Q is not converged do
 9
             episode-number + +
10
             s^{\otimes} = (s_0, q_0)
11
             while (q \notin SINKs: s^{\otimes} = (s,q)) & (iteration-number < it_threshold) do
12
13
                    iteration-number + +
                    choose a_* = Pol(s^{\otimes}) = \arg \max_{a \in \mathcal{A}} Q(s^{\otimes}, a) \# \text{ or } \epsilon\text{-greedy}
14
                    \Psi(s^{\otimes}, a_*) + +
15
                    move to s_*^{\otimes} by a_*
16
                    if \Psi(s^{\otimes}, a_*) = 2 then
17
                            \psi(s^{\otimes}, a_*, s_*^{\otimes}) = 2
18
                     else
19
                      \psi(s^{\otimes}, a_*, s_*^{\otimes}) + +
20
                    end
21
                    receive the reward R(s^{\otimes}, a_*)
22
23
                    A \leftarrow Acc(s_*, A)
                    Q(s^{\otimes}, a_*) \leftarrow Q(s^{\otimes}, a_*) + \mu[R(s^{\otimes}, a_*) - Q(s^{\otimes}, a_*) + \gamma \max_{a'}(Q(s_*^{\otimes}, a'))]
24
                     \bar{P}^{\otimes}(s_{i}^{\otimes},a,s_{j}^{\otimes}) \leftarrow \psi(s_{i}^{\otimes},a,s_{j}^{\otimes})/\Psi(s_{i}^{\otimes},a), \ \forall s_{i}^{\otimes},s_{j}^{\otimes} \in \mathbb{S}^{\otimes} \ \text{and} \ \forall a \in \mathcal{A}
25
                    PSP(s^{\otimes}) \leftarrow \max_{a \in \mathcal{A}} \sum_{s \otimes' \in \mathcal{S}^{\otimes}} \bar{P}^{\otimes}(s^{\otimes}, a, s^{\otimes'}) \times PSP(s^{\otimes'})
26
                    s^{\otimes} = s_{*}^{\otimes}
27
             end
28
29 end
```

We conclude this section by presenting the overall procedure in Algorithm 1. The input of LCQL includes $it_threshold$, which is an upper bound on the number of iterations in each learning episode. Within each episode, the agent either ends up in SINKs, after which the LTL property cannot be satisfied and a new learning episode is required, or uses the iteration-number up to its upper bound $it_threshold$.

Recall that the function $\psi(s,a,s')$ represents the number of times the agent executes action a in state s, thereafter moving to state s', and $\Psi(s,a) = \sum_{s' \in \mathcal{S}} \psi(s,a,s')$. Therefore, at any given time the best estimate of the agent for $P_a(s,a,s')$ is the mean $\psi(s,a,s')/\Psi(s,a)$. Function $\Psi(s,a)$ is initialised to be 1 for every state-action pair, reflecting the fact that at any given state it is possible to take any action. The function $\psi(s,a,s')$ is initialised to 0. Once, the transition (s,a,s') is taken for the first time, $\Psi(s,a) \leftarrow 2$, and thus $\psi(s,a,s')$ has to be incremented to 2 to reflect the new belief $P_a(s,a,s') = 1$ (Algorithm 1, lines 17-21).

3.2 Continuous-state MDPs: Logically-Constrained NFQ

In this section, we propose the first RL algorithm based on Neural Fitted Q-iteration (NFQ) that can synthesise a policy satisfying a given LTL property when the given MDP has a continuous state space. We call this algorithm Logically-Constrained NFQ (LCNFQ).

In LCNFQ, the experience replay method is adapted to the product MDP structure, over which we let the agent explore the MDP and reinitialise it when a positive reward is received or when no positive reward is received after a given number th of iterations. The parameter th is set manually according to the state space of the MDP, allowing the agent to explore the MDP while keeping the size of the sample set limited. All the traces that are gathered within episodes, i.e. experiences, are stored in the form of $(s^{\otimes}, a, s^{\otimes'}, R(s^{\otimes}, a), q)$, where $s^{\otimes} = (s, q)$ is the current state in the product MDP, a is the selected action, $s^{\otimes'} = (s', q')$ is the subsequent state, and $R(s^{\otimes}, a)$ is the reward gained. The set of past experiences is called the sample set \mathcal{E} .

Once the exploration phase is completed and the sample set is created, learning is performed over the sample set. In the learning phase, we propose a hybrid architecture of n separate feedforward neural nets, each with one hidden layer, where $n = |\mathcal{Q}|$ and \mathcal{Q} is the finite cardinality of the automaton \mathbf{N}^6 . Each neural net is associated with a state in the LDBA and for each

 $^{^6}$ Different embeddings, such as the one hot encoding [40] and the integer encoding, have been applied in order to approximate the global Q-function with a single feedforward net. However, we have observed poor performance since these encodings allow the network to assume an ordinal relationship between automaton states. This means that by assigning integer numbers or one hot codes, automaton states are categorised in an ordered format, and can be ranked. Clearly, this disrupts Q-function generalisation by assuming that some states in product MDP are closer to each other. Consequently, we have turned to the use of n separate neural nets, which work together in a hybrid fashion, meaning that the agent can switch between these neural nets as it jumps from one automaton state to another.

Algorithm 2: LCNFQ

```
input : the set of experience samples \mathcal{E} output : approximated Q-function

1 initialize all neural nets B_{q_i} with (s_0, q_i, a) as the input and r_n as the output where a \in \mathcal{A} is a random action

2 repeat

3 | for q_i = |\mathfrak{Q}| to 1 do

4 | \mathfrak{P}_{q_i} = \{(input_l, target_l), \ l = 1, ..., |\mathcal{E}_{q_i}|)\}

5 | input_l = (s_l \otimes, a_l)

6 | target_l = R(s_l \otimes, a_l) + \gamma \max_{a'} Q(s_l \otimes', a')

7 | where (s_l \otimes, a_l, s_l \otimes', R(s_l \otimes, a_l), q_i) \in \mathcal{E}_{q_i}

8 | B_{q_i} \leftarrow \operatorname{Rprop}(\mathfrak{P}_{q_i})

9 | end

10 until end of trial
```

automaton state $q_i \in \Omega$ the associated neural net is called $B_{q_i}: \mathbb{S}^{\otimes} \times \mathcal{A} \to \mathbb{R}$. Once the agent is at state $s^{\otimes} = (s, q_i)$ the neural net B_{q_i} is used for the local Q-function approximation. The set of neural nets acts as a global hybrid Q-function approximator $Q: \mathbb{S}^{\otimes} \times \mathcal{A} \to \mathbb{R}$. Note that the neural nets are not fully decoupled. For example, assume that by taking action a in state $s^{\otimes} = (s, q_i)$ the agent is moved to state $s^{\otimes'} = (s', q_j)$ where $q_i \neq q_j$. According to (6) the weights of B_{q_i} are updated such that $B_{q_i}(s^{\otimes}, a)$ has minimum possible error to $R(s^{\otimes}, a) + \gamma \max_{a'} B_{q_j}(s^{\otimes'}, a')$. Therefore, the value of $B_{q_j}(s^{\otimes'}, a')$ affects $B_{q_i}(s^{\otimes}, a)$.

Let $q_i \in \mathcal{Q}$ be a state in the LDBA. Then define $\mathcal{E}_{q_i} := \{(\cdot, \cdot, \cdot, \cdot, \cdot, x) \in \mathcal{E} | x = q_i\}$ as the set of experiences within \mathcal{E} that are associated to state q_i , i.e. \mathcal{E}_{q_i} is the projection of \mathcal{E} onto q_i . Once the exploration phase is completed, each neural net B_{q_i} is trained based on the associated experience set \mathcal{E}_{q_i} . At each iteration of training, a pattern set \mathcal{P}_{q_i} is generated based on the experience set \mathcal{E}_{q_i} :

$$\mathcal{P}_{q_i} = \{(input_l, target_l), l = 1, ..., |\mathcal{E}_{q_i}|\},$$

where $input_l = (s_l^{\otimes}, a_l)$ and $target_l = R(s_l^{\otimes}, a_l) + \gamma \max_{a'} Q(s_l^{\otimes'}, a')$ such that $(s_l^{\otimes}, a_l, s_l^{\otimes'}, R(s_l^{\otimes}, a_l), q_i) \in \mathcal{E}_{q_i}$. In each cycle of LCNFQ (Algorithm 2), the pattern set \mathcal{P}_{q_i} is used as the input-output set to train the neural net B_{q_i} . In order to update the weights in each neural net, we use Rprop [90] for its efficiency in batch learning [89]. The training schedule in the hybrid network starts from individual networks that are associated with accepting states of the automaton. The training sequence goes backward until it reaches the networks that are associated to the initial states. By doing so, we allow the Q-value to back-propagate through the connected networks. In Algorithm 2, without loss of generality we assume that the automaton states are ordered and hence the back-propagation starts from $q_i = |\mathcal{Q}|$.

Algorithm 3: Episodic VQ

```
input : minimum resolution \Delta
     \mathbf{output}: \mathbf{approximated} \ \mathbf{Q}\text{-function} \ \mathbf{Q}
 1 initialize c_1 = c = initial state
 2 initialize Q(c_1, a) = 0, \forall a \in \mathcal{A}
 з repeat
          set \mathcal{C} = c_1
          \alpha = \arg \max_{a \in \mathcal{A}} Q(c,a)
 5
 6
          repeat
                execute action \alpha and observe the next state (s',q)
                if \mathbb{C}^q is empty then
 8
                      append c_{new} = (s', q) to \mathfrak{C}^q
 9
10
                      initialize Q(c_{new}, a) = 0, \ \forall a \in \mathcal{A}
                else
11
                      determine the nearest neighbour c_{new} within C^q
12
13
                      if c_{new} = c then
                           if ||c - (s', q)||_2 > \Delta then
14
                                 append c_{new} = (s', q) to \mathcal{C}^q
15
                                 initialize Q(c_{new}, a) = 0, \ \forall a \in \mathcal{A}
16
                           end
17
                      else
18
                           Q(c,\alpha) = (1-\mu)Q(c,\alpha) + \mu[R(c,\alpha) + \gamma \max_{a'}(Q(c_{new},a'))]
19
20
                      end
                end
21
22
                c = c_{new}
          until end of trial
23
24 until end of trial
```

3.3 Alternatives to LCNFQ

In the following, we discuss the most popular alternative approaches to solving infinite-state MDPs, namely the Voronoi Quantiser (VQ) and Fitted Value Iteration (FVI). They will be benchmarked against LCNFQ in Section 4.

3.3.1 Voronoi Quantiser

VQ can be classified as a discretisation algorithm which abstracts the continuous-state MDP to a finite-state MDP, allowing classical RL to be run. However, most of discretisation techniques are usually done in an ad-hoc manner, disregarding one of the most appealing features of RL: autonomy. In other words, RL is able to produce the optimal policy with regards to the reward function, with minimum supervision. Therefore, the state space discretisation should be performed as part of the learning task, instead of being fixed at the start of the learning process.

Inspired by [63], we propose a version of VQ that is able to discretise the state space of the product MDP S^{\otimes} , while allowing RL to explore the MDP. VQ maps the state space onto a finite set of disjoint regions called Voronoi cells [111]. The set of centroids of these cells is denoted by $\mathcal{C} = \{c_i\}_{i=1}^m$, $c_i \in S^{\otimes}$,

where m is the number of the cells. With C, we are able to use QL and find an approximation of the optimal policy for a continuous-state MDP.

In the beginning, \mathcal{C} is initialised to consist of just one c_1 , which corresponds to the initial state. This means that the agent views the entire state space as a homogeneous region when no a-priori knowledge is available. Assuming that states are represented by vectors, when the agent explores this unknown state space, the Euclidean norm of the distance between each newly visited state and its nearest neighbour can calculated. If this norm is greater than a threshold value Δ called "minimum resolution", or if the new state s^{\otimes} comprises an automaton state that has never been visited, then the newly visited state is appended to \mathcal{C} . Therefore, as the agent continues to explore, the size of \mathcal{C} would increase until the "relevant" parts of the state space are partitioned. In our algorithm, the set \mathcal{C} has $|\mathcal{Q}|$ disjoint subsets where \mathcal{Q} is the finite set of states of the automaton. Each subset \mathcal{C}^{q_j} , $j=1,...,|\mathcal{Q}|$ contains the centroids of those Voronoi cells that have the form of $c_i^{q_j}=(\cdot,q_j)$, i.e. $\bigcup_i^m c_i^{q_j}=\mathcal{C}^{q_j}$ and $\mathcal{C}=\bigcup_{j=1}^{|\mathcal{Q}|} \mathcal{C}^{q_j}$. Therefore, a Voronoi cell

$$\{(s,q_j) \in \mathbb{S}^{\otimes}, ||(s,q_j) - c_i^{q_j}||_2 \leq ||(s,q_j) - c_{i'}^{q_j}||_2\},$$

is defined by the nearest neighbour rule for any $i' \neq i$. The proposed VQ algorithm is presented in Algorithm 3.

3.3.2 Fitted Value Iteration

FVI is an approximate DP algorithm for continuous-state MDPs, which employs function approximation techniques [34]. In standard DP the goal is to find a mapping, i.e. value function, from the state space to \mathbb{R} , which can generate the optimal policy. The value function in our setup is the expected reward in (1) when Pol is the optimal policy, i.e. U^{Pol^*} . Over continuous state spaces, analytical representations of the value function are in general not available. Approximations can be obtained numerically through approximate value iterations, which involve approximately iterating a Bellman operator on a an approximate value function [99].

We propose a modified version of FVI that can handle the product MDP. The global value function $v: \mathbb{S}^{\otimes} \to \mathbb{R}$, or more specifically $v: \mathbb{S} \times \mathbb{Q} \to \mathbb{R}$, consists of $|\mathbb{Q}|$ number of components. For each $q_j \in \mathbb{Q}$, the sub-value function $v^{q_j}: \mathbb{S} \to \mathbb{R}$ returns the value the states of the form (s, q_j) . Similar to the LCNFQ algorithm, the components are not decoupled.

Let $P^{\otimes}(dy|s^{\otimes},a)$ be the distribution over S^{\otimes} for the successive state given that the current state is s^{\otimes} and the selected action is a. For each state (s,q_j) , the Bellman update over each component of value function v^{q_j} is defined as:

$$\tau v^{q_j}(s) = \sup_{a \in \mathcal{A}} \{ \int v(y) P^{\otimes}(dy|(s, q_j), a) \},$$
(18)

where τ is the Bellman operator [46]. The update in (18) is different than the standard Bellman update in DP, as it does not comprise a running reward, and

Algorithm 4: FVI

as the (terminal) reward is replaced by the following function initialization:

$$v(s^{\otimes}) = \begin{cases} r_p & \text{if } s^{\otimes} \in \mathbb{A}, \\ r_n & \text{otherwise.} \end{cases}$$
 (19)

Here r_p and r_n are defined in (10) with y=0. The main hurdle in executing the Bellman operator in continuous state MDPs, as in (18), is that no analytical representations of the value function v and of its components v^{q_j} , $q_j \in \Omega$ are in general available. Therefore, we employ an approximation method, by introducing a new operator L.

The operator L provides an approximation of the value function, denoted by Lv, and of its components v^{q_j} , which we denote by Lv^{q_j} . For each $q_j \in \Omega$ the approximation is based on a set of points $\{(s_i, q_j)\}_{i=1}^k \subset S^{\otimes}$ which are called centres. For each q_j , the centres i = 1, ..., k are distributed uniformly over S.

In the proposed FVI algorithm, we employ the kernel averager method [99], which can be represented by the following expression for each state (s, q_j) :

$$Lv(s,q_j) = Lv^{q_j}(s) = \frac{\sum_{i=1}^k K(s_i - s)v^{q_j}(s_i)}{\sum_{i=1}^k K(s_i - s)},$$
 (20)

where the kernel $K: S \to \mathbb{R}$ is a radial basis function, such as $e^{-|s-s_i|/h'}$, and h' is smoothing parameter. Each kernel is characterised by the point s_i , and its value decays to zero as s diverges from s_i . This means that for each $q_j \in \mathcal{Q}$ the approximation operator L in (20) is a convex combination of the values of the centres $\{s_i\}_{i=1}^k$ with larger weight given to those values $v^{q_j}(s_i)$ for which s_i is close to s. Note that the smoothing parameter h' controls the weight assigned to more distant values.

In order to approximate the integral in the Bellman update (18) we use a Monte Carlo sampling technique [94]. For each centre (s_i, q_j) and for each action a, we sample the next state $y_a^z(s_i, q_j)$ for z = 1, ..., Z times and append

these samples to the set of Z subsequent states $\mathcal{Y}_a^Z(s_i, q_j)$. We then replace the integral with

$$I_a(s_i, q_j) = \frac{1}{Z} \sum_{z=1}^{Z} Lv(y_a^z(s_i, q_j)).$$
 (21)

The approximate value function Lv is initialised according to (19). In each loop in FVI, the Bellman update approximation is first executed over those sub-value functions that are linked with the accepting states of the LDBA, i.e. those that have initial value of r_p . The approximate Bellman update then goes backward until it reaches those sub-value functions that are linked with the initial states of the automaton. This allows the state values to back-propagate through the product MDP transitions that connects the sub-value function via (21). Without loss of generality we assume that the automaton states are ordered and hence the back-propagation starts from $q_i = |\Omega|$. Once we have the approximated value function, we can generate the optimal policy by following the maximum value (Algorithm 4).

We conclude this section by emphasising that Algorithms 3 and 4 are proposed to be benchmarked against LCNFQ, later in Section 4. Further, MDP abstraction techniques such as [98] failed to scale and to find an optimal policy. In the following we describe another contribution of this work in dealing with time-varying MDPs that show periodic behaviours. Such behaviours can be seen in a number of applications such as physical systems and video games.

3.4 Transfer Learning for Time-Varying MDPs

The classical RL setting dealing with static (time-invariant) MDPs is not particularly representative of real-world situations where the environment is time varying. To this end, we consider MDPs that exhibit time-dependent behaviours. This was inspired by the initial chamber of Atari 2600 Montezuma's Revenge, where a skull rolls periodically on a platform. Such time-varying obstacle can easily render QL useless, as the method is memory-less and only takes into consideration the current state when choosing the best action.

Periodic behaviour can be encompassed in the MDP dynamics by extending its state space with a time variable. However, this approach is in general not computationally viable due to state-space explosion, which is caused by adding the extra time dimension. More specifically, for each time-step in the period of the MDP dynamics, the agent finds itself in a completely new environment and has to learn everything anew.

To overcome this limitation we model the periodically moving obstacle as a Kripke structure. The structure over \mathcal{AP}^{\otimes} , which comprises the possible positions of the obstacle, when unfolded to account for directionality (as shown in Fig. 3), represents the obstacle positions. It can be defined as $\mathbf{D}(\mathcal{K}, k_0, \Delta', L')$ where \mathcal{K} is the state space with transition relation $\Delta' \subseteq \mathcal{K} \otimes \mathcal{K}$ and labelling function $L': \mathcal{K} \to 2^{\mathbb{N}}$. In this paper, for the sake of simplicity, we assume that the labelling function assigns a natural number to each state.

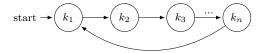


Fig. 3: Kripke structure capturing the time-varying behaviour of the MDP.

We propose to first take the cross product with the generated LDBA N (Definition 11) and Kripke structure D (notice again that we do not explicitly product the Kripke structure with the MDP). The resulting structure is a time-varying automaton with which we can synchronise the original MDP M on-the-fly (see Remark 3). Thanks to this new automaton and the fact that no explicit product MDP is constructed and stored in memory, the proposed approach can handle time-dependent behaviour of the MDP much more efficiently as opposed to explicit encoding of time as a lifting to the MDP. Furthermore, thanks to the local asynchronous update of model-free RL we do not need to execute the Bellman operator over the whole state space as in DP.

A related idea has been recently discussed in [54], where a Kripke-like structure has been proposed to synthesise a controller for partially-observable MDPs: however, whereas the finite-state machine in [54] is designed to act as a memory for the sequence of observations, the Kripke structure in this work is employed to capture the periodic dynamics of the MDP. The final product captures the time-varying parts of the original MDP, and maps it to a static MDP including **D**. The following definition formalises the intuition:

Definition 19 (Periodic Product MDP) Given an MDP $\mathbf{M}(\mathbb{S}, \mathcal{A}, s_0, P, \mathcal{AP}, L)$, an LDBA $\mathbf{N}(\mathbb{Q}, q_0, \Sigma, \mathcal{F}, \Delta)$ with $\Sigma = 2^{\mathcal{AP}}$, and a Kripke structure $\mathbf{D}(\mathcal{K}, k_0, \Delta', L')$, the product MDP is defined as $\mathbf{M}_{\mathbf{ND}}(\mathbb{S}^{\boxtimes}, \mathcal{A}, s_0^{\boxtimes}, P^{\boxtimes}, \mathcal{AP}^{\boxtimes}, L^{\boxtimes}, \mathcal{F}^{\boxtimes})$, where $\mathbb{S}^{\boxtimes} = \mathbb{S} \times (\mathbb{Q} \times \mathcal{K})$, $s_0^{\boxtimes} = (s_0, q_0, k_0)$, $\mathcal{AP}^{\boxtimes} = \mathbb{Q}$, $L^{\boxtimes} : \mathbb{S}^{\boxtimes} \to 2^{\mathbb{Q}}$ such that $L^{\boxtimes}(s, q, k) = q$ and $\mathcal{F}^{\boxtimes} \subseteq \mathbb{S}^{\boxtimes}$ is the set of accepting states $\mathcal{F}^{\boxtimes} = \{F_1^{\boxtimes}, ..., F_f^{\boxtimes}\}$ where $F_j^{\otimes} = \mathbb{S} \times F_j \times \mathcal{K}$. The intuition behind the transition kernel P^{\boxtimes} is that given the current state (s_i, q_i, k_i) and action a, the new state is (s_j, q_j, k_j) where $s_j \sim P(\cdot|s_i, a)$, $q_j \in \Delta(q_i, L(s_j))$, and $k_j \in \Delta'(k_i)$. When the MDP \mathbf{M} is finite-state then $P^{\boxtimes} : \mathbb{S}^{\boxtimes} \times \mathcal{A} \times \mathbb{S}^{\boxtimes} \to [0, 1]$ is the transition probability function such that $(s_i \xrightarrow{a} s_j) \wedge (q_i \xrightarrow{L(s_j)} q_j) \wedge (k_i \to k_j) \Rightarrow P^{\boxtimes}((s_i, q_i, k_i), a, (s_j, q_j, k_j)) = P(s_i, a, s_j)$.

The curse of dimensionality related to the alternative explicit encoding of the periodicity within the MDP is now turned into slowness of the learning process. To speed up the process we can use the observation that the agent, and inherently the Q-values, are only affected by the time-varying parts of the original MDP when they are in close proximity. In other words, the optimal strategy can be learnt more quickly by sharing the state-action values across the dimension defined by $\mathfrak K$.

Recall the classical update rule in QL, when the agent executes action a at state $s^{\boxtimes} = (s, q, k)$ is as follows:

$$Q(s^{\boxtimes}, a) \leftarrow Q(s^{\boxtimes}, a) + \mu[R(s^{\boxtimes}, a) + \gamma \max_{a' \in \mathcal{A}} (Q(s^{\boxtimes'}, a')) - Q(s^{\boxtimes}, a)],$$

Once a positive behaviour is learned in dealing with the time-varying part, it is propagated along the $\mathcal K$ dimension to allow the agent to do the same behaviour in states that are in close proximity of the time-varying part. Technically speaking, when the agent executes action a at state $s^{\boxtimes} = (s, q, k)$ and updates the Q-value for s^{\boxtimes} , a, then

$$\forall k' \in \mathcal{K} \setminus \{k\}, \ Q(s, q, k', a) \leftarrow \max\{Q(s, q, k, a), Q(s, q, k', a)\}.$$

This update rule, once combined with QL classic update rule, allows the positive behaviours to be echoed in S^{\boxtimes} and significantly reduces the learning time.

In other words, the knowledge that the agent has gained while solving one time instance is transferred and applied to different but related times instances. The insight behind the use of transfer learning in this work is to generalise over components of the LTL task, i.e. the automaton states, and across time. Namely, the Q-value update for a given state-action pair affects the Q-values of distinct but related state-action pairs. Transfer learning is used to improve the learning process for one specific time instance in the automaton by transferring information from other instances. The general idea of transfer learning has been applied over different domains in supervised [23, 39, 57] and unsupervised learning [27, 51, 54].

4 Experimental Results

We discuss a number of planning experiments dealing with policy synthesis problems around temporal specifications that are extended with safety requirements, both when the state space is finite and continuous.

4.1 Finite-state MDPs

The first experiment is an LTL-constrained control synthesis problem for a robot in a slippery grid-world. Let the grid be an $L \times L$ square over which the robot moves. In this setup, the robot location is the MDP state $s \in \mathcal{S}$. At each state $s \in \mathcal{S}$ the robot has a set of actions $\mathcal{A} = \{left, right, up, down, stay\}$ by which the robot is able to move to other states (e.g. s') with the probability of $P(s, a, s'), a \in \mathcal{A}$. At each state $s \in \mathcal{S}$, the actions available to the robot are either to move to a neighbour state $s' \in \mathcal{S}$ or to stay at the state s. In this example, if not otherwise specified, we assume for each action the robot chooses, there is a probability of 85% that the action takes the robot to the correct state and 15% that the action takes the robot to a random state in its neighbourhood (including its current state). This example is a well-known

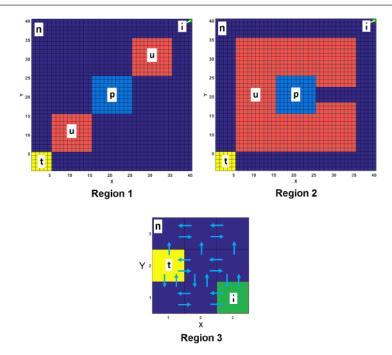


Fig. 4: Slippery grid-world with |S| = 1600 - green: initial state (i); dark blue: neutral (n); red: unsafe (u); light blue: pre-target (p); yellow: target (t).

benchmark and is often referred to as "slippery grid-world". This experiment has 1600 states, with 5 enabled actions at each state.

A labelling function $L: \mathbb{S} \to 2^{\mathcal{AP}}$ assigns to each state $s \in \mathbb{S}$ a set of atomic propositions $L(s) \subseteq \mathcal{AP}$. We assume that in each state s the robot is aware of the labels of the neighbouring states. We consider two 40×40 regions and one 3×3 region with different labels as in Fig. 4. In Region 3 and in the state target, the subsequent state after performing action stay is always the state target itself. Note that all the actions are not active in Region 3 and the agent has to avoid the top row otherwise it gets trapped.

In the first experiment, we consider the following LTL properties. The first two properties (22) and (23) focus on safety and reachability, while the third property (24) requires a sequential visit to states with label p and then to target t:

$$\Diamond t \wedge \Box (t \to \Box t) \wedge \Box (u \to \Box u), \tag{22}$$

$$\Diamond \Box t,$$
 (23)

and

$$\Diamond(p \land \Diamond t) \land \Box(t \to \Box t) \land \Box(u \to \Box u), \tag{24}$$

where t stands for "target", u stands for "unsafe", and p refers to the area that has to be visited before visiting the area with label t. Property (22) asks

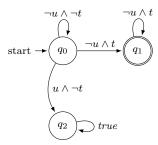


Fig. 5: LDBA for the specification in (22) with removed transitions labelled $t \wedge u$ (since it is impossible to be at target and unsafe at the same time).

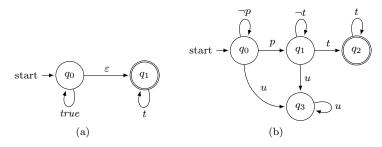


Fig. 6: (a) LDBA for the specification in (23) - (b) LDBA for property in (24).

the agent to eventually find the target $\Diamond t$ and to stay there $\Box(t \to \Box t)$, while avoiding the unsafe - otherwise it is going to be trapped there $\Box(u \to \Box u)$. Specification (23) requires the agent to eventually find the target and to stay there. The intuition behind (24) is that the agent has to eventually first visit p and then visit t at some point in the future $\Diamond(p \land \Diamond t)$ and stay there $\Box(t \to \Box t)$ while avoiding unsafe areas $\Box(u \to \Box u)$.

The LDBAs associated with (22), (23) and (24) are in Fig. 5, and Fig. 6 respectively. Note that the LDBA expressing (22) in Fig. 5 is deterministic and only needs the state set Ω_D as in Definition 10 while the LDBA in Fig. 6. a needs both Ω_D and Ω_N to express (23).

The second experiment is the well-known Atari 2600 game Pacman, which is initialised in a tricky configuration (Fig. 7). In order to win the game the agent has to collect all available tokens without being caught by moving ghosts. The ghost dynamics is stochastic: a probability p_g for each ghost determines if the ghost is chasing Pacman (often referred to as "chase mode") or if it is executing a random action ("scatter mode"). Notice that, unlike the first experiment, in this setup the actions of the ghosts and of the agent result in a deterministic transition, i.e. the world is not "slippery". Each combination of (Pacman, ghost1, ghost2, ghost3, ghost4) represents a state in the experiment, resulting in a state-space cardinality in excess of 80,000.

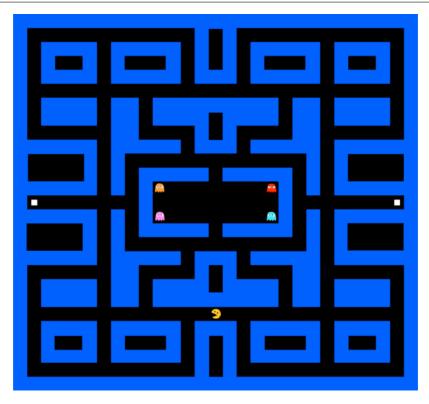


Fig. 7: Pacman environment with $|\mathcal{S}| > 80,000$ - initial condition: the square on the left is labelled as food 1 (f_1) and the one on the right as food 2 (f_2) , the state of being caught by a ghost is labelled as (g) and the rest of the state space is neutral (n).

In the second experiment, in order to win the game, Pacman is required to choose between one of the two available foods and then find the other one $(\lozenge[(f_1 \land \lozenge f_2) \lor (f_2 \land \lozenge f_1)])$ while avoiding ghosts $(\Box \neg g)$. These clauses are what a human can perceive just by looking at the game screen and we feed a conjunction of these associations to the agent by using the following LTL formula:

$$\Diamond [(f_1 \land \Diamond f_2) \lor (f_2 \land \Diamond f_1)] \land \Box \neg g, \tag{25}$$

The constructed LDBA is shown in Fig. 8.

The third experiment deals with the complex environment of Atari 2600 Montezuma's Revenge. To win the game the agent needs to descend down the ladders, to jump over the skull, to fetch the key and to return to the top and to open one of the doors. In this experiment, we assume that for each action that the agent selects, there is a 90% that the chosen action is executed and a 10% that a random action is instead performed.

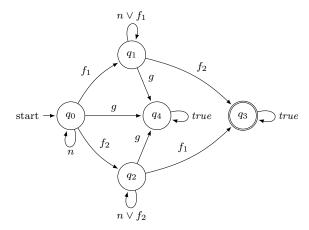


Fig. 8: LDBA for the specification in (25).



Fig. 9: Initial condition in the first level of Montezuma's Revenge.

Using the OpenAI gym environment [15] we set as our test-bed the first chamber of Montezuma's Revenge (Fig. 9). In order to enable a tabular approach, we reduce the size of the state-action space: This simplification is only a means of expediting the training process, but no generality is lost. The goal is to achieve a better score overall than some modern algorithms, such as the DQN approach, which on average has achieved a score of zero [72].

In the following, we describe the methodology of simplifying the environment to make the testing feasible. The game simulator is very general and therefore comes with 18 possible actions, many of which do not apply in our environment, e.g. "FIRE". We observe that only 6 actions, out of the 18 native ones, are active in the Montezuma's Revenge environment, whilst the remaining ones produce

no change to the environment, so exploring them is a waste of exploration time. As such, the algorithm could work just as well with the full set of actions, except that it would require additional time. We extract and work with pixel matrix to identify and locate different elements of the state space. Hence, we treat the state space as being discrete with over 700,000 states.

Montezuma's Revenge is a rather more complicated environment, where the probability of winning the game by randomly exploring the state space is close to zero. However, a human player can derive the logical property behind the game by simply looking at the map and associating the acquiring of the key to the ability of opening the door $\Diamond(k \land \Diamond d)$ and staying at the door to win the first chamber $\Box(d \to \Box d)$, while avoiding the moving skull $\Box(s \to \Box s)$. Here k represent the key, d is the door, and s is the skull. We can then combine these constraints and express them as an LTL formula, such as:

$$\Diamond(k \land \Diamond d) \land \Box(d \to \Box d) \land \Box(s \to \Box s), \tag{26}$$

Note that this LTL formula is equivalent to (24) and therefore we employ the LDBA in Fig. 6, however with different labels. The LDBA built from the formula encompasses the safety and the goal of the agent, however to deal with the moving skull we represent the location and direction of the skull as a Kripke structure, which allows the agent to learn Q-values that generate policies avoiding the danger.

As mentioned earlier, the probability of randomly reaching the key and moving back to the door is very low, and even advanced algorithms, such as DQN [72], fail to achieve the overall goal. Of course, human intuition can solve this game and synthesise a successful policy – the advantage of our automated synthesis technique is that it does not require complete end-to-end examples, and thus it may avoid local optima that the human may believe to be global.

Note that the agent also loses a life when it falls from a high enough altitude, but this is not something that we can concretely assume and as such, it will not be penalised. Since we do not control the game engine, the agent will continue to lose its life upon falling, but rather than actively avoiding these moves, the agent will simply learn that the Q-value is null and there are better actions to be chosen.

4.1.1 Simulation Results

In the first experiment (slippery grid-world), the simulation parameters are set as $\mu=0.9$ and $\gamma=0.9$. Fig. 11 gives the results of the learning for the expression (24) in Region 1 and Region 2 after 400,000 iterations and 200 learning episodes. Again, according to (24) the robot has to avoid the red (unsafe) regions, visit the light-blue (pre-target) area at least once and then go to the yellow (target) region. Recall that selected action is executed with a probability of 85%. Thus, there might be some undesired deviations in the robot path.

Fig. 10 gives the results of the learning for the LTL formula (22) in Region 1 and Region 2 after 400,000 iterations and 200 learning episodes. The intuition

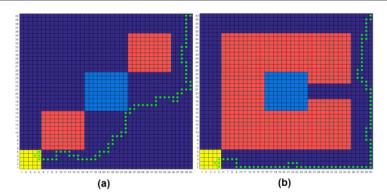


Fig. 10: Simulation results for specification (22) in (a) Region 1 and in (b) Region 2.

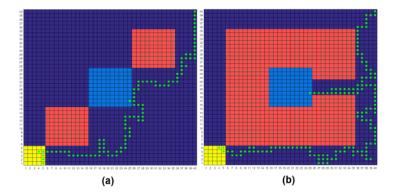


Fig. 11: Simulation results for specification (24) in (a) Region 1 and (b) Region 2.

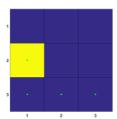


Fig. 12: Simulation results for (23) in Region 3.

behind the LTL formula in (22) is that the robot has to avoid red (unsafe) areas until it reaches the yellow (target) region, otherwise the robot is going to be stuck in the red (unsafe) area.

Finally, in Fig. 12 the learner tries to satisfy the LTL formula $\Diamond \Box t$ in (23). The learning takes 1000 iterations and 20 learning episodes.

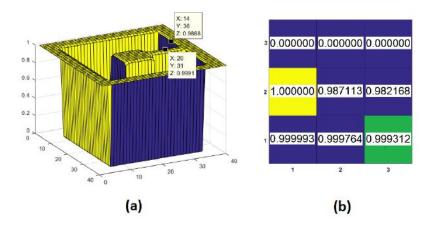


Fig. 13: PSP in (a) Region 2 with property (24) and in (b) Region 3 with specification (23). The results generated by LCQL are identical to the outcomes from PRISM.

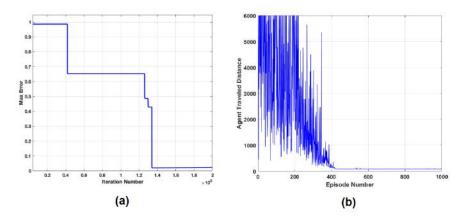


Fig. 14: In Region 2 under specification (24): (a) Maximum error between PSP computed with LCQL and with PRISM (b) The distance that agent traverses from initial state to final state with LCQL.

Fig. 13 gives the result of our proposed value iteration method for calculating the maximum PSP in Region 2 with (24) and Region 3 with (23). In both cases our method was able to accurately calculate the maximum probability of satisfying the LTL property. We observed a monotonic decrease in the maximum error between the correct PSP calculated by PRISM and the probability calculation by LCQL (Fig. 14.a). Fig. 14.b shows the distance that agent traverses from initial state to final state at each learning episode in Region 1 under (24). After almost 400 episodes of learning the agent converges to the final optimal policy and the travelled distance stabilizes. It is worth mentioning

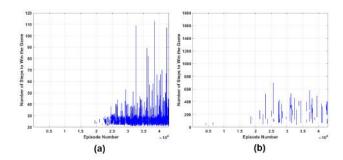


Fig. 15: Results of learning in Pacman with LCQL (classical QL with positive reward for winning the game failed to converge and score even once).

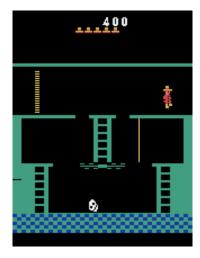


Fig. 16: Montezuma's Revenge - The agent successfully unlocks the door (notice reward).

that the application of standard QL has failed to find an optimal and stable policy for this experiment.

In the second experiment (Pacman), the simulation parameters are set as $\mu=0.9$ and $\gamma=0.9$. The stochastic behaviour of the ghosts is also captured by $p_g=0.9$. Fig. 15 gives the results of learning with LCQL⁷ for (8). After almost 80,000 episodes, LCQL finds a stable policy to win the game even with ghosts playing probabilistically. On the other hand, standard RL (in this case, classical QL with positive reward for winning the game) fails to find a stable policy.

 $^{^7}$ Please visit https://www.cs.ox.ac.uk/conferences/lcrl to watch the videos of the agent playing Pacman. The code is adaptive and can be run under new configurations.

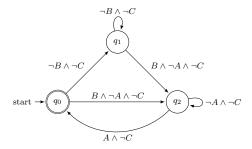


Fig. 17: LDBA expressing the LTL formula in (27) with removed transitions labelled $A \wedge B$ (since it is impossible to be at A and B at the same time).

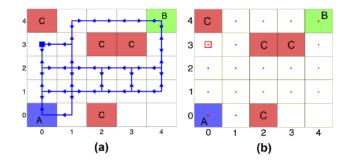


Fig. 18: (a) Example considered in [91]. (b) Trajectories under the policy generated by LCQL in [91].

In the third experiment (Montezuma's Revenge) the agent succeeds in reaching the set target after relatively short training (10000 episodes), which on a machine with a 3.2GHz Core i5 processor and 8GB of RAM, running Windows 7 took over a day, producing the results shown on Figure 16. The simulation parameters are set as $\mu = 0.75$, $\gamma = 0.9$.

4.1.2 Comparison with a DRA-based Learning Algorithm

The problem of LTL-constrained learning is also investigated in [91], where the authors propose to translate the LTL property into a DRA and then to construct a product MDP. A 5×5 grid world is considered and starting from state (0,3) the agent has to visit two regions infinitely often (areas A and B in Fig. 18). The agent has to also avoid the area C. This property can be encoded as the following LTL formula:

$$\Box \Diamond A \wedge \Box \Diamond B \wedge \Box \neg C. \tag{27}$$

The product MDP in [91] contains 150 states, which means that the Rabin automaton has 6 states. Fig. 18.a shows the trajectories under the optimal policy generated by [91] algorithm after 600 iterations. However, by employing

LCQL we are able to generate the same trajectories with only 50 iterations (Fig. 18.b). The automaton that we consider is an LDBA with only 3 states as in Fig. 17. This result in a smaller product MDP and a much more succinct state space (only 75 states) for the algorithm to learn, which consequently leads to a faster convergence.

In addition, the reward shaping in LCQL is significantly simpler thanks to the Büchi acceptance condition. In a DRA $\mathbf{R}(\Omega, \Omega_0, \Sigma, \mathcal{F}, \Delta)$, the set $\mathcal{F} = \{(G_1, B_1), \ldots, (G_{n_F}, B_{n_F})\}$ represents the acceptance condition in which G_i , $B_i \in \Omega$ for $i = 1, \ldots, n_F$. An infinite run $\theta \in \Omega^{\omega}$ starting from Ω_0 is accepting if there exists $i \in \{1, \ldots, n_F\}$ such that

$$inf(\theta) \cap G_i \neq \emptyset$$
 and $inf(\theta) \cap B_i = \emptyset$.

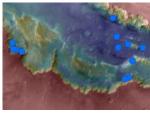
Therefore for each $i \in \{1, ..., n_F\}$ a separate reward assignment is needed in [91] which complicates the implementation and increases the required calculation costs. This complicated reward assignment is not needed by employing the accepting frontier function in our framework.

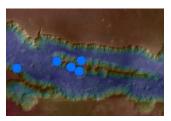
More importantly, LCQL is a model-free learning algorithm that does not require an approximation of the transition probabilities of the underlying MDP. This even makes LCQL more easier to employ. We would like to emphasize that LCQL convergence proof solely depends on the structure of the MDP and this allows LCQL to find satisfying policies even if they have probability of less than one.

4.2 Continuous-state MDPs

In this section, we describe a mission planning architecture for an autonomous Mars-rover that uses LCNFQ to follow a mission on Mars. We start with a satellite image from the surface of Mars, and add the desired labels from $2^{\mathcal{AP}}$, e.g. safe or unsafe, to that image. Next we express the desired mission task by an LTL formula defined over \mathcal{AP} , and then we run LCNFQ on the labelled image. We would like the rover to satisfy the given LTL property with the highest probability possible starting from any random initial state (as we assume we cannot predict the landing location precisely). We compare LCNFQ with Voronoi quantizer and FVI and we show that LCNFQ outperforms these methods.

In this numerical experiment we focus on Coprates quadrangle, in which there exist a significant number of signs of water. We consider two parts of Valles Marineris, a canyon system in Coprates quadrangle (Fig. 19). The blue dots, provided by NASA, indicate locations of recurring slope lineae (RSL) in the canyon network. RSL are seasonal dark streaks regarded as the strongest evidence for the possibility of liquid water on the surface of Mars. RSL extend down-slope during a warm season and then disappear in the colder part of the Martian year [70]. The two areas mapped in Fig. 19, Melas Chasma and Coprates Chasma, have the highest density of known RSL.





(a) Melas Chasma

(b) Coprates Chasma

Fig. 19: Melas Chasma and Coprates Chasma, in the central and eastern portions of Valles Marineris. Map colour spectrum represents elevation, where red is high and blue is low. (Image courtesy of NASA, JPL, Caltech and University of Arizona.)

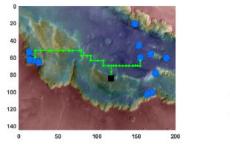
For each case, let the entire area be our MDP state space S, where the rover location is a single state $s \in S$. At each state $s \in S$, the rover has a set of actions $A = \{left, right, up, down, stay\}$ by which it is able to move to other states: at each state $s \in S$, when the rover takes an action $a \in \{left, right, up, down\}$ it is moved to another state (e.g., s') towards the direction of the action with a range of movement that is randomly drawn from (0, D] unless the rover hits the boundary of the area which forces the rover to remain on the boundary. In the case when the rover chooses action a = stay it is again moved to a random place within a circle centred at its current state and with radius $d \ll D$. Again, d captures disturbances on the surface of Mars and can be tuned accordingly.

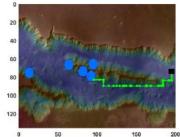
With S and A defined we are only left with the labelling function $L: S \to 2^{A\mathcal{P}}$ which assigns to each state $s \in S$ a set of atomic propositions $L(s) \subseteq 2^{A\mathcal{P}}$. With the labelling function, we are able to divide the area into different regions and define a logical property over the traces that the agent generates. In this particular experiment, we divide areas into three main regions: neutral, unsafe and target. The target label goes on RSL (blue dots), the unsafe label lays on the parts with very high elevation (red coloured) and the rest is neutral. In this example we assume that the labels do not overlap each other.

Note that when the rover is deployed to its real mission, the precise landing location is not known. Therefore, we should take into account the randomness of the initial state s_0 . The dimensions of the area of interest in Fig. 19.a are 456.98×322.58 km and in Fig. 19.b are 323.47×215.05 km. The diameter of each RSL is 19.12 km. Other parameters in this numerical example have been set as D=2 km, d=0.02 km, the reward function parameter y=1 for LCNFQ and y=0 for VQ and FVI, M=1, m=0.05 and $\mathcal{AP}=\{\text{neutral}, \text{unsafe}, \text{target_1}, \text{target_2}\}.$

The first control objective in this numerical example is expressed by the following LTL formula over Melas Chasma (Fig. 19.a):

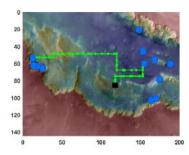
$$\Diamond(p \land \Diamond t) \land \Box(t \to \Box t) \land \Box(u \to \Box u), \tag{28}$$

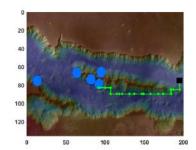




- (a) Melas Chasma and landing location (black rectangle) (118, 85)
- (b) Coprates Chasma and landing location (black rectangle) (194, 74)

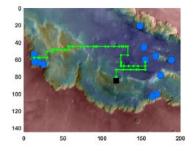
Fig. 20: Generated paths by LCNFQ.

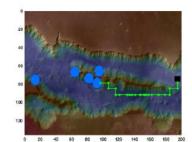




- (a) Melas Chasma and landing location (black rectangle) (118, 85)
- (b) Coprates Chasma and landing location (black rectangle) (194, 74)

Fig. 21: Generated paths by episodic VQ.





- (a) Melas Chasma and landing location (black rectangle) (118, 85)
- (b) Coprates Chasma and landing location (black rectangle) (194, 74)

Fig. 22: Generated paths by FVI.

Melas Chasma					
Algorithm	Sample Complexity	$U^{Pol^*}(s_0)$	Success Rate †	Training Time*(s)	Iteration Num.
LCNFQ	7168 samples	0.0203	99%	95.64	40
$VQ~(\Delta=0.4)$	27886 samples	0.0015	99%	1732.35	2195
$VQ \ (\Delta = 1.2)$	7996 samples	0.0104	97%	273.049	913
$VQ (\Delta = 2)$	=	0	0%	=	=
FVI	40000 samples	0.0133	98%	4.12	80
Coprates Chasma					
Algorithm	Sample Complexity	$U^{Pol}^*(s_0)$	Success Rate †	Training Time*(s)	Iteration Num.
LCNFQ	2680 samples	0.1094	98%	166.13	40
$VQ \ (\Delta = 0.4)$	8040 samples	0.0082	98%	3666.18	3870
$VQ \ (\Delta = 1.2)$	3140 samples	0.0562	96%	931.33	2778
$VQ \ (\Delta = 2)$	=	0	0%	=	-
FVI	25000 samples	0.0717	97%	2.16	80

Table 1: Simulation results for Continuous-State MDPs

where n stands for "neutral", p stands for "target 1", t stands for "target 2" and u stands for "unsafe". Target 1 are the RSL (blue bots) on the right with a lower risk of the rover going to unsafe region and the target 2 label goes on the left RSL that are a bit riskier to explore. Conforming to (28) the rover has to visit the target 1 (any of the right dots) at least once and then proceed to the target 2 (left dots) while avoiding unsafe areas. Note that according to $\Box(u \to \Box u)$ in (28) the agent is able to go to unsafe area u (by climbing up the slope) but it is not able to come back due to the risk of falling. Note that the LDBA expressing (28) is as in Fig. 6.a.

The second formula focuses more on safety and we are going to employ it in exploring Coprates Chasma (Fig. 19.b), where a critical unsafe slope exists in the middle of this region:

$$\Diamond t \wedge \Box (t \to \Box t) \wedge \Box (u \to \Box u) \tag{29}$$

Here, t refers to the "target", i.e. RSL in the map, and u stands for "unsafe". According to this LTL formula, the agent has to eventually reach the target $(\lozenge t)$ and stays there $(\square(t \to \square t))$. However, if the agent hits the unsafe area it can never comes back and remains there forever $(\square(u \to \square u))$. With (29) we can again build the associated Büchi automaton as in Fig. 6.b. Having the Büchi automaton for each formula, we are able to use Definition 11 to build product MDPs and run LCNFQ on both.

4.2.1 Simulation Results

This section presents the simulation results. All simulations are carried on a machine with a 3.2GHz Core i5 processor and 8GB of RAM, running Windows 7. LCNFQ has four feedforward neural networks for (24) and three feedforward neural networks for (22), each associated with an automaton state in Fig. 6.a

[†] Testing the trained agent (for 100 trials)

^{*} Average for 10 trainings

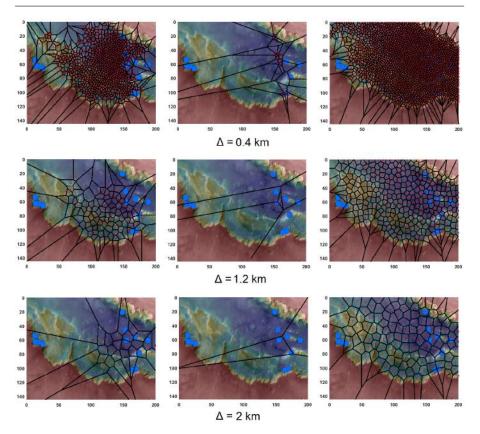


Fig. 23: VQ – generated cells in Melas Chasma for different resolutions.

and Fig. 6.b. We assume that the rover lands on a random safe place and has to find its way to satisfy the given property in the face of uncertainty. The learning discount factor γ is also set to be equal to 0.9.

Fig. 20 gives the results of learning for LTL formulae (24) and (22). At each state s^{\otimes} , the robot picks an action that yields highest $Q(s^{\otimes}, \cdot)$ and by doing so the robot is able to generate a control policy Pol^{\otimes^*} over the state space S^{\otimes} . The control policy Pol^{\otimes^*} induces a policy Pol^* over the state space S^{\otimes} and its performance is shown in Fig. 20.

Next, we investigate the episodic VQ algorithm as an alternative solution to LCNFQ. Three different resolutions ($\Delta=0.4,\ 1.2,\ 2$ km) are used to see the effect of the resolution on the quality of the generated policy. The results are presented in Table 1, where VQ with $\Delta=2$ km fails to find a satisfying policy in both regions, due to the coarseness of the resulted discretisation. A coarse partitioning result in the RL not to be able to efficiently back-propagate the reward or the agent to be stuck in some random-action loop as sometimes the agent current cell is large enough that all actions have the same value. In Table

1, training time is the empirical time that is taken to train the algorithm and travel distance is the distance that agent traverses from initial state to final state. We show the generated policy for $\Delta=1.2$ km in Fig. 21. Additionally, Fig. 23 depicts the resulted Voronoi discretisation after implementing the VQ algorithm. Note that with VQ only those parts of the state space that are relevant to satisfying the property are accurately partitioned.

Finally, we present the results of FVI method in Fig 22 for the LTL formulae (24) and (22). The FVI smoothing parameter is h'=0.18 and the sampling time is Z=25 for both regions where both are empirically adjusted to have the minimum possible value for FVI to generate satisfying policies. The number of basis points also is set to be 100, so the sample complexity of FVI is 8 equal to $100 \times Z \times |\mathcal{A}| \times (|\mathcal{Q}|-1)$. Note that in Table 1, in terms of timing, FVI outperforms the other methods. However, we have to remember that FVI is an approximate DP algorithm, which inherently needs an approximation of the transition probabilities. Therefore, as we have seen in (21), for the set of basis points we need to perform Monte Carlo sampling for the subsequent states. This reduces the FVI applicability, as this sampling is not possible when dealing with a black-box model. In this numerical example, for the sake of comparison we have assumed that FVI is able to perform Monte Carlo sampling, so that it can be benchmarked against LCNFQ.

Additionally, both FVI and episodic VQ need careful hyper-parameter tuning to generate a satisfying policy, i.e., h' and Z for FVI and Δ for VQ. The big merit of LCNFQ is that it does not need any external intervention. Further, as in Table 1, LCNFQ succeeds to efficiently generate a better policy compared to FVI and VQ. LCNFQ has less sample complexity while at the same time produces policies that are more reliable and also has better expected reward, i.e. higher probability of satisfying the given property.

5 Conclusions

In this paper we have proposed a framework to guide an RL agent, by expanding the agent domain knowledge about the environment by means of an LTL property. This additional knowledge, as we have observed in experiments, boosts the agent learning of the global optimal policy. Further we have shown that we can calculate the probability that is associated with the satisfaction of the LTL property that enables us to quantify the safety of the generated optimal policy at any given state.

We have argued that converting the LTL property to an LDBA results in a significantly smaller automaton than DRA alternatives, which increases the convergence rate of RL. In addition to the more succinct product MDP and

⁸ We do not sample the states in the product automaton that are associated to the accepting state of the automaton since when we reach the accepting state the property is satisfied and there is no need for further exploration. Hence, the last term is $(|\Omega|-1)$. However, if the property of interest produces an automaton that has multiple accepting states, then we need to sample those states as well.

faster convergence, our algorithm is easier to implement as opposed to standard methods that convert the LTL property to a DRA due to the simpler accepting conditions of LDBA. Much like the way we synchronised the states of LDBA with the states of the MDP, we have shown that synchronising a Kripke structure with the LDBA allows us to handle time-varying periodic environments on-the-fly. This particularly becomes important when we employed this synchronised LDBA-Kripke automaton as an infrastructure for the agent to transfer its learning over the dimension of time and to overcome the curse of dimensionality.

Last but not least, LCNFQ is the first RL algorithm that can do LTL policy synthesis in a continuous-state MDP. LCNFQ is model-free, meaning that the learning only depends on the sample experiences that the agent gathered by interacting and exploring the MDP. Further, the sample set can be small thanks to the generalisation that neural nets offer. The core engine in LCNFQ is very flexible and can be extended to the most recent developments in RL literature.

For future work we are currently looking into a multi-agent setup, in which a heterogeneous set of agents attempts to satisfy an LTL formula (or set thereof). Further, we would like to extend this approach to partially observable MDPs to limit the knowledge of the agent even more.

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