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# Learning Algorithms for Verification of Markov Decision Processes

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**ABSTRACT.** We present a general framework for applying learning algorithms and heuristical guidance to the verification of Markov decision processes (MDPs). The primary goal of our techniques is to improve performance by avoiding an exhaustive exploration of the state space, instead focussing on particularly relevant areas of the system, guided by heuristics. Our work builds on the previous results of Brázdil et al., significantly extending it as well as refining several details and fixing errors.

The presented framework focuses on probabilistic reachability, which is a core problem in verification, and is instantiated in two distinct scenarios. The first assumes that full knowledge of the MDP is available, in particular precise transition probabilities. It performs a heuristic-driven partial exploration of the model, yielding precise lower and upper bounds on the required probability. The second tackles the case where we may only sample the MDP without knowing

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the exact transition dynamics. Here, we obtain probabilistic guarantees, again in terms of both the lower and upper bounds, which provides efficient stopping criteria for the approximation. In particular, the latter is an extension of statistical model checking (SMC) for unbounded properties in MDPs. In contrast to other related approaches, we do not restrict our attention to time-bounded (finite-horizon) or discounted properties, nor assume any particular structural properties of the MDP.

# 1. Introduction

Markov decision processes (MDP) [86, 67, 118] are a well established formalism for modelling, analysis and optimization of probabilistic systems with non-determinism, with a large range of application domains [16, 104]. For example, MDPs are used as models for concurrent probabilistic systems [54] or probabilistic systems operating in open environments [123]. See [140, 139, 138] for further applications.

In essence, MDP comprise three major parts, namely states, actions, and probabilities. Intuitively, the system evolves as follows: In any state, there is a set of actions to choose from. This corresponds to the *non-determinism* of the system. After choosing an action, the system then transitions into the next state according to the probability distribution associated with that action. For example, we may use MDP to represent a robot moving around in a 2D world (sometimes called "gridworld"). The states then are (bounded, integer) coordinates, representing the current position of the robot. In each state the robot can choose to move in one of the four cardinal directions or carry out some task depending on the current location. To illustrate the randomness, consider a "move east" action. Choosing this action may move the robot to the next position component of the robot fails and we instead end up in a state north of our current position. Given such a system, the general goal is to optimize a given *objective* by choosing optimal actions. For example, we may want to control the robot such that it reaches an interesting research site with maximal probability. We additionally may be interested in minimizing time or power consumption and avoiding dangerous terrain on our way to the site.

This example hints at one of the simplest, yet important objectives, namely *reachability*. A reachability problem is specified by an MDP together with a set of designated target states. The task is to compute the maximal probability with which the system can reach this set of states. Reachability is of particular interest since in the infinite horizon setting many other objectives, e.g., LTL or long-run average reward, can be reduced to variants of reachability. A variety of approaches has been established to solve this problem. In theory, linear programming [53, 68] is the most suitable approach, as it provides exact answers (rational numbers with no representation imprecision) in polynomial time. See [19] for an application. Unfortunately, LP

turns out to be quite inefficient in practice for classical reachability. For systems with more than a few thousand states, linear programming often falls behind other approaches, see, e.g., [68, 7, 77]. As an alternative, one can apply iterative methods. Here, value iteration (VI) [86] is the most prominent variant. See [49] for a detailed survey of VI. Notably, variations of VI are the default method in the state-of-the-art probabilistic model checkers PRISM [104] and Storm [62], even though it only provides an approximate solution, converging in the limit. In contrast, strategy iteration (SI) (also known as policy iteration, PI) [86, 118, 99] yields precise answers, but is also used to a lesser extent due to scalability issues. See for example [24] for an overview of both methods, [77, 78] for recent comparisons of practical implementations of LP, VI, and SI for MDP, [102] for a similar comparison on *stochastic games* (MDP with two antagonistic players), and [4] for in-depth practical comparison of modern probabilistic model checkers.

**Interval Iteration** Surprisingly, until about a decade ago, standard value iteration as applied in popular model checkers only yielded *lower bounds* on the true value, without any *sound stopping criterion*. Concretely, this meant that the model checker might conclude that the computation is finished and stop it, despite still being far off from the true result. We note that there exists a tight, exponential a-priori bound on the number of steps VI requires until convergence, see e.g. [49]. This could be used as "stopping criterion", by simply iterating for this number of steps. However, this is far too pessimistic on most models.

In [73, 33], a correct and *adaptive* stopping criterion was discovered independently. This bound follows from under- and (newly obtained) over-approximations converging to the true value, yielding a straightforward stopping criterion: iterate until upper and lower bound are close enough. This criterion is adaptive in the sense that if the iteration should converge faster than the naive a-priori bound, we can detect this case and stop early. Subsequent works included this stopping criterion in model checkers [18] and developed further sound approaches [119, 79]. (Some more developments are discussed in the related work.)

However, despite value iteration scaling much better than linear programming, systems with more than a few million states remain out of reach, not only because of time-outs, but also memory-outs. Several approaches have been devised to deal with such large state spaces, which we extensively survey in the related work section. Now, we outline a variant of VI, called *asynchronous VI*. The central idea is to perform the iterative computations in an asynchronous manner, i.e. apply the iteration operation to some states more often than to others, or even not at all to some states. This allows to obtain speed-ups of several orders of magnitude. However, since states are evaluated at different paces and, potentially, a set of states is omitted completely, convergence is unclear and even its rate is unknown and hard to analyse. Yet, by exploiting the discussed lower and upper bounds, we obtain a correct and efficient algorithm, inspired by *bounded real-time dynamic programming* (BRTDP) [112]. This algorithm interleaves construction of the model, analysis, and bound approximation. For example, we can sample a path through

the system (constructing states that we have not seen so far on the fly) and apply the bound update mechanism only on these paths. For some models, this allows to obtain tight bounds on the true value while only constructing a small fraction of the complete state space.

**Limited Information** The methods discussed above (and most which are introduced in the related work) rely on an exact formalization of the system being available. In particular they require that the transition probabilities are known precisely. We call this situation the *white box* or *complete information* setting. This is a common, valid assumption when verifying, e.g., formally defined protocols, but not so much when working with real-world systems comprising difficult dynamics, where the effects of an action can be approximated at most. As such, these systems can be treated as a *black box*, which accept a next action to take as input and output the subsequent state, sampled from the associated underlying, unknown distribution.

Here *statistical model checking* (SMC) [144, 82] is applicable. The general idea of SMC is to repeatedly sample the system in order to obtain strong statistical guarantees. Thus, SMC approaches can (at most) be probably approximately correct (PAC), i.e. yield an answer close to the true value with high probability, but there always is a small chance for a significant error. By itself, SMC algorithms are restricted to systems without non-determinism, e.g., Markov chains [142, 126]. A number of approaches tackling the issue of non-determinism have been presented (see related work). However, these methods deal with non-determinism by either resolving it uniformly at random or sample several schedulers, both of which can lead to surprising results in certain scenarios [28]. Additionally, note that both approaches can only give a statistical estimate of a lower bound of the true achievable maximal reachability. In particular, they do not give any guarantees on the maximal achievable performance (i.e. an upper bound). Based on the ideas of *delayed Q-learning (DQL)* [129] (which also only yields lower bounds) we present a PAC model-free algorithm, yielding statistical upper and lower bounds on the maximal reachability. (Model-free intuitively means that our algorithm only stores a fixed number of values per state-action pair, independent of how many transitions are associated with that action; further discussion can be found in Remark 5.1.) This approach is similar in spirit to the BRTDP approach discussed above, however much more involved due to the underlying statistical arguments. The main contribution of this algorithm is to prove the possibility of obtaining such a result, exploring the boundaries of what exactly is necessary to obtain guarantees.

**Algorithm Outline** To provide the reader with a preliminary overview of our approach, we present a high-level pseudo-code in Algorithm 1. As already mentioned, the fundamental idea is to compute lower and upper bounds on the true probability of reaching the target in each state (Line 2 to Line 6). Essentially, we want to iteratively update these bounds in a converging and correct manner. In the complete information setting, this can be achieved by directly computing the weighted average of the successor bounds. For the limited information setting, we instead

**Input:** MDP  $\mathcal{M}$ , target states T, precision  $\varepsilon$ . **Output:** Values (l, u) which are  $\varepsilon$ -optimal. while difference between upper and lower bound in initial state is 1: larger than  $\varepsilon$  do Obtain a set of states to update by, e.g., sampling a path. 2: foreach state and action in this set do if this state is a target state then 3: Set its bounds to 1. 4: else 5: Update action bounds based on the weighted average of 6: its successors. Detect end components in the relevant area of the system. 7: return lower and upper bound of the initial state. 8:

Algorithm 1. High-level overview of the structure of our algorithms.

aggregate many successor samples. This yields a good approximation of this weighted average with high probability.

The details of how the set of states to be updated is obtained in Line 2 are abstracted in the complete information setting and we only require some basic properties. One possibility is a sampling-based approach, which is guided by the currently computed bounds. We discuss several alternatives later on. In contrast, the limited information setting requires a particular kind of sampling approach in order to ensure correctness. We highlight these differences in the respective sections.

Now, while it is rather simple to prove correctness of the computed bounds, the tricky part is to obtain convergence. In particular, for general MDP, this approach would not converge. To solve this, in the past many algorithms working with MDP often made assumptions about the structure of the model. For example, it was sometimes required that the model is "strongly connected" or free of *end components* [61] (except trivial ones). Instead, one of the main contributions of [73, 33] is to identify end components as the sole "culprits" and devising methods to deal with them in a general manner, obtaining convergence. While [73] tackles the problem in a "global" manner (assuming to have access to the complete MDP at once), we present an asynchronous way of treating end components. This treatment is "on-the-fly" and can be interleaved with the iterative construction of the system.

In the white box setting, we solve this problem by adapting exiting graph analysis algorithms and incorporating them with our main procedure. However, with limited information we again need to employ statistical methods. In essence, if we remain inside a particular region of the system for a long enough time, there is a high probability that this region is an end component. This overall process then is repeated until the computed bounds in the initial state are close enough.

### 1.1 Related Work

We present a number of related ideas, all attempting, in one way or another, to make the analysis of (large or black box) probabilistic system tractable.

*Compositional* techniques aim to first analyse parts of the system separately and combine the sub-results to obtain an overall result, e.g. [42, 63, 83, 21, 45, 22]. Then, there are *abstraction* approaches which try to merge states with equivalent or sufficiently similar behaviour w.r.t. the objective in question, e.g. [57, 84, 75, 92, 75]. *Reduction* approaches try to eliminate states from the system and restrict computation to a sub-system through structural properties, e.g. [15, 14, 52, 64, 66, 30]. *Guessing* [50] tries to guess and verify the value of certain states, which can lead to theoretical speed-ups when the guesses decompose the system into independent parts. Another approach is *symbolic computation*, where the model and value functions are compactly represented using *BDD* [35] and *MTBDD* / *ADD* [13, 70]. See [17, 105, 145, 141, 29, 96] for further details and applications of symbolic methods.

In related fields such as planning and artificial intelligence, many learning-based and heuristic-driven approaches for MDP have been proposed. In the complete information setting, RTDP [20] and BRTDP [112] use very similar approaches, but have no stopping criterion or do not converge in general, respectively. [117] uses upper and lower bounds in the setting of *partially observable MDP* (POMDP). Many other algorithms rely on certain assumptions to ensure convergence, for example by including a *discount factor* [93] or restricting to the *Stochastic Shortest Path* (SSP) problems, whereas we deal with arbitrary MDP without discounting. This is addressed by an approach called FRET [97], but this only yields a lower bound. Others similarly only provide convergence in the limit [32, 89], which is usually satisfactory for applications to planning or robotics, where systems have intractably large or even uncountable state spaces. We are not aware of any attempts at generally applicable methods in the context of probabilistic verification prior to [33]. An earlier, related paper is [3], where heuristic methods are applied to MDP, but for generating counterexamples.

As mentioned, **[73]** independently discovered a stopping criterion for value iteration on general MDP. The idea behind this criterion is very similar to **[33]**, but they construct and analyse the whole system at once. The underlying idea of "interval iteration", spawned by these two papers, is further developed in, e.g., **[18, 72, 8]**.

Additionally, the idea of *optimistic* value iteration (OVI) [79, 11] emerged. Here, instead of *always* updating both lower and upper bound, only the lower bound is iterated (as in classical value iteration). Then, based on heuristics, the algorithm *optimistically* conjectures that the values actually converged. To verify that conjecture, a (potential) upper bound is guessed based on the current lower bound (e.g. by incrementing all bounds by  $\varepsilon$ ) and then checked for consistency by applying a few steps of VI. This approach turns out to be quite efficient in practice when dealing with MDP in a "global" manner, however is incompatible with our guided sampling approach, since we continuously use upper bounds for guidance. Similarly, *sound* value iteration (SVI) [119] also works with lower and upper bounds, however they derive bounds based on *k*-step reachability probabilities. These fundamentally require a global and synchronous value iteration, which is precisely what we aim to avoid.

**Statistical Methods** There are two primary motivations to use statistical approaches. Firstly, the model might be large, even too large to fit into memory, and analysing it by standard approaches becomes infeasible, yet generating samples may be quick and easy. In this case, one can decide to "only" aim for a statistical guarantee, which often comes with tremendous speed-ups and space savings. Secondly, as explained above, the model might be an unknown black box – we do not know how it works internally, only that it is some Markov process. If we can observe and control the system, we can gather samples and from that derive statistical guarantees for the considered value.

As mentioned, our approach focuses on the latter, however most statistical methods focus on the former. Indeed, many of the following methods are *only* applicable to the "full knowledge" setting, i.e. knowing the internals of the system. Here, significant improvements can be observed: Several SMC algorithms have sub-linear or even constant space requirements (often called *model-free* algorithms). Appropriately, SMC is an active area of research with extensive tool support [87, 27, 31, 41, 60, 142, 126, 40] but also a lot of subtle pitfalls [103]. See also [98, 2, 109] for extensive surveys and [121] for an application of SMC to a complex real world problem. In contrast to our work, most algorithms focus on *time-bounded* or discounted properties, e.g., step-bounded reachability, rather than truly unbounded properties. Several approaches try to bridge this gap by transforming unbounded properties into testing of bounded properties, for example [143, 80, 120, 124]. However, these approaches target models without nondeterminism and as such are not applicable to MDP. As a slight extension, [26] considers MDP with *spurious nondeterminism*, where the resolution of nondeterminism does not influence the value of interest.

Adapting SMC techniques to models with (true) nondeterminism such as MDP is an important topic, with several recent papers. See [43, 128] and [136, Chapter 4.1.5] for a survey on simulation-based algorithms in this context. One approach is to give nondeterminism a probabilistic interpretation, e.g., resolving it uniformly, as is done in PRISM for MDP [104]

and Uppaal SMC for timed automata [60, 59, 107]. A second approach, taken for example by recent versions of the modes tool [76, 56, 37], is to repeatedly sample schedulers, using for example *lightweight scheduler sampling* (LSS) [110, 55], and then estimate the performance of these controllers using existing SMC methods. Uppaal Stratego [58] synthesizes a "good" scheduler and uses it for subsequent SMC analysis. All of the above methods only yield a lower bound on the true reachability and the quality of this bound is highly dependent on the model. Others aim to indeed quantify over all strategies and approximate the true maximal value, for example [108, 81]. The work in those papers deals with the setting of discounted or bounded properties, respectively. In [81], candidates for optimal schedulers are generated and gradually improved, which does not give upper bounds on the convergence. The nearly simultaneously published [69] essentially tackles the same problem. In contrast to our work, their approach is model-based, i.e. the transition probabilities are learned, and is not guided by a heuristic, requiring to learn the whole transition matrix.

In summary, most approaches are only applicable to the first case, or, if they can work in the "limited information" setting, they require a purely probabilistic system, finite or discounted properties, or only give lower bounds on the optimal value. Our focus explicitly lies on the limited information case, and, similar to many approaches from statistical model checking [144, 82, 125, 69], we aim to provide PAC guarantees, however on the optimal value of an infinite horizon objective in models with nondeterminism.

Another issue of statistical methods is the analysis of *rare events*. This is, of course, very relevant for SMC approaches in general. They can be addressed using for example importance sampling **[87, 80]** or importance splitting **[88, 36]**. We take a rather conservative approach towards rare events and delegate more sophisticated handling of this issue to future work.

### **1.2 Differences to the Published Article**

This work is a significant extension of [33]. Numerous details are refined and errors discovered and fixed. We discuss major changes in the following. Notably, in the process of resolving some of the issues of [33], we also discovered several problems in [129], on which the DQL method of [33] is based, both conceptually and in terms of proof structure.

- A complete rewrite, only retaining parts of the proof strategies.
- The related work is updated with recent advances and work based on [33].
- The BRTDP approach and related proofs are extended significantly to a generic template, allowing for a variety of implementations of the sampling methods.
- Both variants of the DQL algorithm have been restructured and simplified.
- The proofs, especially those related to DQL, are more modular and easier to adapt / re-use for similar endeavours in these directions.
- Several technical issues of the original paper are fixed. Firstly, the proofs in the appendix proved properties of slightly different algorithms, only to conclude with a brief, imprecise

argument that the presented algorithms are not too different from the algorithms proven correct. Some proofs were only given implicitly or assumed to be common knowledge, in particular treatment of collapsed end components and similar. Moreover, several small mistakes have been corrected.

- Lemma 16 of the original paper both has a flawed proof and an erroneous statement, which is now fixed: Firstly, the Algorithm as presented potentially never follows an  $\varepsilon$ optimal strategy, as exemplified in Example 3.7. Secondly, the proof applies the multiplicative Chernoff bound to variables  $X_i$ , which indicate whether the algorithm performed a particular action during a time interval. To apply this bound, the variables would need to be independent, but the  $X_i$  are dependent. This is elaborated in detail later on. Interestingly, a similar, yet slightly different error already is present in [129]. Firstly, their Theorem 1 claims that the algorithm eventually follows an  $\varepsilon$  optimal strategy, which does not hold due to the same reasons. Secondly, in the corresponding proof the authors apply
  - the Hoeffding bound to similar dependent variables. This happens at same location in the overall proof layout as in [33], however the applied bound is different. Our alternative approach to proving the statements is also applicable to the proof of [129].

### 1.3 Impact of the Presented Work

Since its publications about a decade ago, the two approaches introduced by [33], i.e. BRTDP for complete information and DQL for limited information, have directly inspired a number of subsequent works, of which we provide a (non-exhaustive) list. Firstly, the BRTDP approach has been extended to settings with long-run average reward [7], continuous time Markov chains [6], continuous space MDP [71], and stochastic games [65]. Notably, taking inspiration from [33] and subsequent works, [101] recently provided a unified approach to value iteration for stochastic games. Concretely, this work extends the central ideas required to obtain convergence guarantees in MDP to stochastic games in a unified way, subsuming and extending, among others, the ideas and algorithms of [33, 73, 7, 65]. In particular, this explains how to extend the BRTDP approach to further objectives, such as safety, expected total reward, or mean payoff. In an orthogonal direction, [100] modifies the approach of [33] to determine *cores* of probabilistic systems, which intuitively describe "most" possible behaviours of the given system. (This can also be viewed as a probabilistic generalization of the set of reachable states.)

Secondly, the DQL approach (and its proof strategy) inspired a *model-based* variant [10], which improved scalability. (Note that, as remarked in [10, Appendix D], the convergence of their "fast" variant is not proven.) Subsequently, this lead to a surge of papers considering model-based SMC, for example adapting to MDP with reachability [9] or mean payoff objective [1], continuous state-spaces [12], dynamic information flow tracking games [137], or changing environments [130].



**Figure 1.** An example Markov decision process. Boxes represent states, dots represent actions, and arrows correspond to transitions (with the respective probabilities as labels). For simplicity, actions with a single successor are depicted as a single, direct arrow and the probability 1 is omitted. We use this notation throughout the paper.

Thirdly, for practical impact, we highlight the tool PET [113, 115], which directly implements and extends the BRTDP approach in a highly efficient manner. As seen in several evaluations, the relevance of partial exploration in practice highly depends on the structure of the model (as with many other approaches). In some cases, effectively the entire model has to be explored and there is no improvement possible. However, for several families of models orders-of-magnitude or even *arbitrary* speed-ups can be observed. This tool has also participated in several iterations of the *Comparison of Tools for the Analysis of Quantitative Formal Models* (QComp), a friendly competition of quantitative model checking tools, namely in 2019 [74] (as PRISM-TUMheuristic), 2020 [39], and 2023 [4].

### 1.4 Contributions and Structure

In Section 2 we set up notation and introduce some known results. We then present our contributions as follows.

- We introduce an extensible framework for efficient reachability on "complete information"
   MDP without end components in Section 3 and extend it to arbitrary MDP in Section 4.
- We introduce a model-free PAC learning algorithm for reachability on "limited information"
   MDP without end components in Section 5 and extend it to arbitrary MDP in Section 6.

We conclude in Section 7. We intentionally omit an experimental evaluation and instead refer to tools based on these ideas, see e.g. the works in Section 1.3.

# 2. Preliminaries

As usual,  $\mathbb{N}$  and  $\mathbb{R}$  refers to the (positive) natural numbers and real numbers, respectively. Given two real numbers  $a, b \in \mathbb{R}$  with  $a \leq b$ ,  $[a, b] \subseteq \mathbb{R}$  denotes the set of all real numbers between a and b inclusively. For a set S,  $\overline{S}$  denotes its complement, while  $S^*$  and  $S^{\omega}$  refers to the set of finite and infinite sequences comprising elements of S, respectively. We often explicitly name sub-claims in the form of [Fact I], and reference them by [I]. In the digital version, the references are clickable. We assume familiarity with basic notions of probability theory, e.g., probability spaces and probability measures. A probability distribution over a countable set X is a mapping  $d : X \rightarrow [0, 1]$ , such that  $\sum_{x \in X} d(x) = 1$ . Its support is denoted by  $\operatorname{supp}(d) = \{x \in X \mid d(x) > 0\}$ .  $\mathcal{D}(X)$  denotes the set of all probability distributions on X. Some event happens almost surely (a.s.) if it happens with probability 1. For readability, we omit detailed treatment of probability measures on uncountable sets and instead direct the reader to appropriate literature, e.g. [25].

# 2.1 Markov Systems

Markov decision processes (MDPs) are a widely used formalism to capture both non-determinism (for, e.g., control, concurrency) and probability. For a "complete" introduction to Markov systems, we direct the interested reader to [118, 90]. A lighter, more recent introduction can be found in [114, Chapter 2].

First, we introduce Markov chains (MCs), which are purely stochastic.

**DEFINITION 2.1.** A *Markov chain* (MC) is a tuple  $M = (S, \delta)$ , where S is a (countable) set of *states*, and  $\delta : S \to \mathcal{D}(S)$  is a *transition function* that for each state s yields a probability distribution over successor states.

Note that we do not require the set of states of a Markov chain to be finite. This is mainly due to technical reasons, which become apparent later.

Next, we define MDP, which extend Markov chains with non-determinism.

**DEFINITION 2.2.** A Markov decision process (MDP) is a tuple  $\mathcal{M} = (S, Act, Av, \Delta)$ , where S is a finite set of *states*, Act is a finite set of actions,  $Av : S \rightarrow 2^{Act} \setminus \{\emptyset\}$  assigns to every state a non-empty set of available actions, and  $\Delta : S \times Act \rightarrow \mathcal{D}(S)$  is a *transition function* that for each state s and (available) action  $a \in Av(s)$  yields a probability distribution over successor states.

A state  $s \in S$  is called *terminal*, if  $\Delta(s, a)(s) = 1$  for all enabled actions  $a \in Av(s)$ .

**REMARK 2.3.** We assume w.l.o.g. that actions are unique for each state, i.e.  $Av(s) \cap Av(s') = \emptyset$  for  $s \neq s'$  and denote the unique state associated with action a in  $\mathcal{M}$  by state $(a, \mathcal{M})$ . This can be achieved in general by replacing *Act* with  $S \times Act$  and adapting Av and  $\Delta$ .

Note that we assume the set of available actions to be non-empty in all states. This means that a run can never get "stuck" in a degenerate state without successors. See Figure 1 for an example of an MDP.

For ease of notation, we overload functions mapping to distributions  $f : Y \to \mathcal{D}(X)$  by  $f : Y \times X \to [0,1]$ , where  $f(y,x) \coloneqq f(y)(x)$ . For example, instead of  $\delta(s)(s')$  and  $\Delta(s,a)(s')$  we write  $\delta(s,s')$  and  $\Delta(s,a,s')$ , respectively. Furthermore, given a distribution  $d \in \mathcal{D}(X)$  and a function  $f : X \to \mathbb{R}$  mapping elements of a set X to real numbers, we write  $d\langle f \rangle \coloneqq \sum_{x \in X} d(x)f(x)$  to denote the weighted sum of f with respect to d. For example,  $\delta(s)\langle f \rangle$  and

 $\Delta(s, a)\langle f \rangle$  denote the weighted sum of f over the successors of s in MC and s with action a in MDP, respectively.

### **State-Action Pairs**

Throughout this work, we often speak about *state-action pairs*. This refers to tuples of the form (s, a) where  $s \in S$  and  $a \in Av(s)$  or equivalently  $a \in Act$  and s = state(a, M). Due to our restriction that each action is associated with exactly one state, denoting both the state and action is superfluous, strictly speaking. We keep the terminology for consistency with other works. In Section 6 this notation would however introduce significant overhead and we only speak about actions there.

Given a set of states  $S' \subseteq S$  and an available-action function  $Av' : S' \to \mathcal{P}(Act) \setminus \emptyset$  we write, slightly abusing notation,  $S' \times Av' = \{(s, a) \mid s \in S', a \in Av'(s)\}$  to denote the set of state-action pairs obtained in S' using Av'. In particular,  $S \times Av$  denotes the set of all state-action pairs in an MDP. Moreover, for a set of state-action pairs K we also write  $s \in K$  if there exists an action asuch that  $(s, a) \in K$ . Dually, we also write  $a \in K$  if an appropriate state s exists.

Note that there are two isomorphic representations of sets of state-action pairs, namely as a set of pairs  $X \subseteq S \times Av$  or as a pair of sets  $(R, B) \in 2^S \times 2^{Act}$ . We make use of both views and note explicitly when switching from one to another.

### **Paths & Strategies**

An *infinite path*  $\rho$  in a Markov chain is an infinite sequence  $\rho = s_1 s_2 \dots \in S^{\omega}$ , such that for every  $i \in \mathbb{N}$  we have that  $\delta(s_i, s_{i+1}) > 0$ . A *finite path* (or *history*)  $\varrho = s_1 s_2 \dots s_n \in S^*$  is a non-empty, finite prefix of an infinite path of length  $|\varrho| = n$ , ending in some state  $s_n$ , denoted by  $last(\varrho)$ . For simplicity, we define  $|\rho| = \infty$  for infinite paths  $\rho$ . We use  $\rho(i)$  and  $\varrho(i)$  to refer to the *i*-th state  $s_i$  in a given (in)finite path. A state *s occurs* in an (in)finite path  $\rho$ , denoted by  $s \in \rho$ , if there exists an  $i \leq |\rho|$  such that  $s = \rho(i)$ . We denote the set of all finite (infinite) paths of a Markov chain M by FPaths<sub>M</sub> (Paths<sub>M</sub>). Further, we use FPaths<sub>M,s</sub> (Paths<sub>M,s</sub>) to refer to all (in)finite paths starting in state  $s \in S$ . Observe that in general FPaths<sub>M</sub> and Paths<sub>M</sub> are proper subsets of  $S^*$  and  $S^{\omega}$ , respectively, as we imposed additional constraints.

An *infinite path* in an MDP is an infinite sequence  $\rho = (s_1, a_1)(s_2, a_2) \cdots \in (S \times Av)^{\omega}$ , such that for every  $i \in \mathbb{N}$ ,  $a_i \in Av(s_i)$  and  $s_{i+1} \in \text{supp}(\Delta(s_i, a_i))$ , setting the length  $|\rho| = \infty$ . *Finite paths*  $\varrho$  and *last*( $\varrho$ ) are defined analogously as elements of  $(S \times Av)^* \times S$  and the respective last state. Again,  $\rho(i)$  and  $\varrho(i)$  refer to the *i*-th state in an (in)finite path with an analogous definition of a state occurring,  $|\varrho|$  denotes the length of a finite path, we refer to the set of (in)finite paths of an MDP  $\mathcal{M}$  by FPaths<sub> $\mathcal{M}$ </sub> (Paths<sub> $\mathcal{M}$ </sub>), and write FPaths<sub> $\mathcal{M},s$ </sub> (Paths<sub> $\mathcal{M},s$ </sub>) for all such paths starting in a state  $s \in S$ . Further, we use  $\rho^a(i)$  and  $\varrho^a(i)$  to denote the *i*-th action in the respective path. We

say that a state-action pair (*s*, *a*) is in an (in)finite path  $\varrho$  if there exists an  $i < |\varrho|$  with  $s = \varrho(i)$ and  $a = \varrho^a(i)$ .

A Markov chain together with a state  $s \in S$  naturally induces a unique probability measure  $Pr_{M,s}$  over infinite paths [16, Chapter 10]. For MDP, we first need to eliminate the non-determinism in order to obtain such a probability measure. This is achieved by *strategies* (also called *policy*, *controller*, or *scheduler*).

**DEFINITION 2.4.** A strategy on an MDP  $\mathcal{M} = (S, Act, Av, \Delta)$  is a function mapping finite paths to distributions over available actions, i.e.  $\pi$  : FPaths<sub> $\mathcal{M}$ </sub>  $\rightarrow \mathcal{D}(Act)$  where supp $(\pi(\varrho)) \subseteq Av(last(\varrho))$  for all  $\varrho \in FPaths_{\mathcal{M}}$ .

Intuitively, a strategy is a "recipe" describing which step to take in the current state, given the evolution of the system so far. Note that the strategy may yield a distribution on the actions to be taken next.

A strategy  $\pi$  is called *memoryless* (or *stationary*) if it only depends on  $last(\varrho)$  for all finite paths  $\varrho$  and we identify it with  $\pi : S \to \mathcal{D}(Act)$ . Similarly, it is called *deterministic*, if it always yields a Dirac distribution, i.e. picks a single action to be played next, and we identify it with  $\pi$ : FPaths<sub>M</sub>  $\to$  Act. Together, *memoryless deterministic* strategies can be treated as functions  $\pi : S \to Act$  mapping each state to an action. We write  $\Pi_M$  to denote the set of all strategies of an MDP  $\mathcal{M}$ ,  $\Pi^{\mathsf{M}}_{\mathcal{M}}$  for memoryless strategies, and  $\Pi^{\mathsf{MD}}_{\mathcal{M}}$  for all memoryless deterministic strategies.

Fixing a strategy  $\pi$  induces a Markov chain  $\mathcal{M}^{\pi} = (\text{FPaths}_{\mathcal{M}}, \delta^{\pi})$ , where for a state  $\varrho = s_1 a_1 \dots s_n \in \text{FPaths}_{\mathcal{M}}$ , action  $a_{n+1} \in Av(s_n)$ , and successor state  $s_{n+1} \in \text{supp}(\Delta(s_n, a_{n+1}))$ , the successor distribution is given by  $\delta^{\pi}(\varrho, \varrho a_{n+1}s_{n+1}) = \pi(\varrho, a_{n+1}) \cdot \Delta(s, a_{n+1}, s_{n+1})$ . In particular, for any MDP  $\mathcal{M}$ , strategy  $\pi \in \Pi_{\mathcal{M}}$ , and state s, we obtain a measure over paths<sup>1</sup>  $\Pr_{\mathcal{M}^{\pi},s}$ , which we refer to as  $\Pr_{\mathcal{M},s}^{\pi}$ . Observe that all these measures operate on the same probability space, namely the set of all infinite paths  $\operatorname{Paths}_{\mathcal{M}}$ . (See e.g. [118, Section 2.1.6] for further details.) Consequently, given a measurable event A, we can define the maximal probability of this event starting from state  $\hat{s}$  under any strategy by

$$\mathsf{Pr}^{\sup}_{\mathcal{M},\hat{s}}[A] \coloneqq \sup_{\pi \in \Pi_{\mathcal{M}}} \mathsf{Pr}^{\pi}_{\mathcal{M},\hat{s}}[A].$$

Note that depending on the structure of A it may be the case that no optimal witness exists, thus we have to resort to the supremum instead of the maximum. We lift this restriction for our particular use case later on. For a memoryless strategy  $\pi \in \Pi^{\mathsf{M}}_{\mathcal{M}}$ , we can identify  $\mathcal{M}^{\pi}$  with a Markov chain over the states of  $\mathcal{M}$ .

Given an MDP  $\mathcal{M}$ , memoryless strategy  $\pi \in \Pi^{\mathsf{M}}_{\mathcal{M}}$ , and a function assigning a value to each state-action pair  $f : S \times Av \to \mathbb{R}$ , we define  $\pi[f] : S \to \mathbb{R}$  as the expected value of taking one

<sup>1</sup> Technically, this measure operates on infinite sequences of finite paths, as each state of  $M^{\pi}$  is a finite path. But this measure can easily be projected directly on finite paths.

step in state *s* following the strategy  $\pi$ , i.e.

$$\pi[f](s) \coloneqq \sum_{a \in Av(s)} \pi(s, a) \cdot f(s, a).$$

### Strongly Connected Components and End Components

A non-empty set of states  $C \subseteq S$  in a Markov chain is *strongly connected* if for every pair  $s, s' \in C$  there is a non-trivial path from s to s'. Such a set C is a *strongly connected component* (SCC) if it is inclusion maximal, i.e. there exists no strongly connected C' with  $C \subsetneq C'$ . Thus, each state belongs to at most one SCC. An SCC is called *bottom strongly connected component* (BSCC) if additionally no path leads out of it, i.e. for all  $s \in C, s' \in S \setminus C$  we have  $\delta(s, s') = 0$ . The set of SCCs and BSCCs in an MC M is denoted by SCC(M) and BSCC(M), respectively.

The concept of SCCs is generalized to MDPs by so called *(maximal) end components* [61]. Intuitively, an end component describes a set of states in which the system can remain forever.

**DEFINITION 2.5.** Let  $\mathcal{M} = (S, Act, Av, \Delta)$  be an MDP. A pair (R, B), where  $\emptyset \neq R \subseteq S$  and  $\emptyset \neq B \subseteq \bigcup_{s \in R} Av(s)$ , is an *end component* of an MDP  $\mathcal{M}$  if

- (i) for all  $s \in R$ ,  $a \in B \cap Av(s)$  we have supp $(\Delta(s, a)) \subseteq R$ , and
- (ii) for all  $s, s' \in R$  there is a finite path  $\varrho = sa_0 \dots a_n s' \in \mathsf{FPaths}_{\mathcal{M}} \cap (R \times B)^* \times R$ , i.e. the path stays inside R and only uses actions in B.

An end component (R, B) is a *maximal end component* (MEC) if there is no other end component (R', B') such that  $R \subseteq R'$  and  $B \subseteq B'$ .

We identify an end component with the respective set of states, e.g.  $s \in E = (R, B)$  means  $s \in R$ . Observe that given two overlapping ECs  $(R_1, B_1)$  and  $(R_2, B_2)$  with  $R_1 \cap R_2 \neq \emptyset$ , their union  $(R_1 \cup R_2, B_1 \cup B_2)$  also is an EC. Consequently, each state belongs to at most one MEC. Again, a MEC is *bottom* if there are no outgoing transitions. The set of ECs of an MDP  $\mathcal{M}$  is denoted by EC( $\mathcal{M}$ ), the set of MECs by MEC( $\mathcal{M}$ ). For the MDP in Figure 1, the set of MECs is given by  $(\{s_1, s_2\}, \{a_1, b_1, b_2\}), (\{s_+\}, \{a_+\}), \text{ and } (\{s_-\}, \{a_-\}).$ 

**REMARK 2.6.** For a Markov chain M, the computation of SCC(M), BSCC(M) and a topological ordering of the SCCs can be achieved in linear time w.r.t. the number of states and transitions by, e.g., Tarjan's algorithm [133]. Similarly, the MEC decomposition of an MDP can be computed in polynomial time [54]. For improved algorithms on general MDP and various special cases see [48, 46, 47].

These components fully capture the limit behaviour of any Markov chain and decision process, respectively. Intuitively, both of the following statements say that a run of such systems eventually remains inside one BSCC or MEC forever, respectively. The measurability of the sets in the following two lemmas is well known, see, e.g. [16, Chapter 10].

**LEMMA 2.7 (MC almost-sure absorption).** *For any MC* M *and state s, we have that*  $Pr_{M,s}[\{\rho \mid \exists R_i \in BSCC(M). \exists n_0 \in \mathbb{N}. \forall n > n_0. \rho(n) \in R_i\}] = 1.$ 

**PROOF.** Follows from [16, Theorem 10.27].

**LEMMA 2.8 (MDP almost-sure absorption).** For any MDP  $\mathcal{M}$ , state s, and strategy  $\pi$ , we have that

$$\mathsf{Pr}_{\mathcal{M},s}^{\pi}[\{\rho \mid \exists (R_i, B_i) \in \operatorname{MEC}(\mathcal{M}) . \exists n_0 \in \mathbb{N} . \forall n > n_0 . \rho(n) \in R_i\}] = 1.$$

**PROOF.** Follows from [61, Theorem 3.2].

### 2.2 Reachability

For an MDP  $\mathcal{M} = (S, Act, Av, \Delta)$  and a set of *target states*  $T \subseteq S$ , *bounded reachability* for step k, denoted by  $\diamond^{\leq k}T = \{\rho \in \mathsf{Paths}_{\mathcal{M}} \mid \exists i \in \{1, \ldots, k+1\}. \rho(i) \in T\}$ , is the set of all infinite paths that reach a state in T within k steps. Analogously, *(unbounded) reachability*  $\diamond T = \{\rho \in \mathsf{Paths}_{\mathcal{M}} \mid \exists i \in \mathbb{N}. \rho(i) \in T\}$  are all paths which eventually reach the target set T. We overload the  $\diamond$  operator to also accept sets of state-action pairs and sets of actions, with analogous semantics. The sets of paths produced by  $\diamond$  are measurable for any MDP, target set, and step bound [16, Section 10.1.1].<sup>2</sup> Note that for a set T, both  $\diamond \overline{T}$  and  $\overline{\diamond T}$  are well-defined, however they refer to two different concepts. The former denotes the set of all paths reaching a state not in T, whereas the latter is the set of all paths which never reach T (also called *co-reachability* or *safety*).

Now, it is straightforward to define the *maximal reachability problem* of a given set of states. Given an MDP  $\mathcal{M}$ , target set T, and state s, we are interested in computing the maximal probability of eventually reaching T, starting in state s. Formally, we want to compute the *value* of state s, defined as

$$\mathcal{V}(s) \coloneqq \mathsf{Pr}^{\sup}_{\mathcal{M},s}[\Diamond T] = \sup_{\pi \in \Pi_{\mathcal{M}}} \mathsf{Pr}^{\pi}_{\mathcal{M},s}[\Diamond T].$$

For an example, suppose we have  $T = \{s_+\}$  in Figure 1. This can be reached from  $\hat{s}$  with probability 0.5 by always choosing action  $a_1$  in  $s_1$  and  $a_2$  in  $s_2$ , and this value is optimal. In general, an optimal strategy always exists and memoryless deterministic strategies are sufficient to achieve the optimal value [61, Theorem 3.10], i.e.

$$\mathcal{V}(s) = \mathsf{Pr}_{\mathcal{M},s}^{\max}[\diamond T] = \max_{\pi \in \Pi_{\mathcal{M}}} \mathsf{Pr}_{\mathcal{M},s}^{\pi}[\diamond T] = \max_{\pi \in \Pi_{\mathcal{M}}^{\mathsf{MD}}} \mathsf{Pr}_{\mathcal{M},s}^{\pi}[\diamond T].$$

This state value function satisfies a straightforward fixed point equation, namely

$$\mathcal{V}(s) = \begin{cases} 1 & \text{if } s \in T, \\ \max_{a \in Av(s)} \Delta(s, a) \langle \mathcal{V} \rangle & \text{otherwise.} \end{cases}$$
(1)

2 Recall that we defined MDP to have finite state and action sets.

Moreover,  $\mathcal{V}$  is the *smallest* fixed point of this equation [118]. In our approach, we also deal with values of state-action pairs  $(s, a) \in S \times Av$ , where

$$\mathcal{V}(s,a) \coloneqq \Delta(s,a) \langle \mathcal{V} \rangle = \sum_{s' \in S} \Delta(s,a,s') \cdot \mathcal{V}(s').$$

Intuitively,  $\mathcal{V}(s, a)$  is the value in state *s* when playing action *a* and then acting optimally (note that *a* might be a suboptimal action). The overall value of *s*,  $\mathcal{V}(s)$ , is obtained by choosing an optimal action, i.e.  $\mathcal{V}(s) = \max_{a \in Av(s)} \mathcal{V}(s, a)$ .

**REMARK 2.9.** Our algorithms primarily work by approximating these state-action values and derive state-values by the above equation. This may seem counter-intuitive at first, since we could as well directly work with state values and derive state-action values as described above, saving memory. However, our approaches are inspired by *reinforcement learning* [131], explained later, which traditionally assigns values to actions. Thus, we stick with this convention in our algorithms as well. Finally, in the limited information setting of Sections 5 and 6, the algorithms do not have access to the exact transition probabilities and hence cannot exploit the above equation.

See [68, Section 4] for an in-depth discussion of reachability on finite MDP.

### **Approximate Solutions**

The value of a state  $\mathcal{V}(s)$  can, for example, be determined using *linear programming* [53, 68]<sup>3</sup> in polynomial time [95, 91]. Unfortunately, this approach turns out to be inefficient in practice [73, 7]. One way to potentially ease the task is by only considering *approximate solutions*. Concretely, on top of an MDP  $\mathcal{M}$ , starting state  $\hat{s}$ , and target set T, we assume that we are given a precision requirement  $\varepsilon > 0$ . We say a strategy  $\pi$  is  $\varepsilon$ -optimal, if  $\Pr_{\mathcal{M},\hat{s}}^{\pi}[\diamond T] + \varepsilon > \mathcal{V}(\hat{s})$ . Analogously, a tuple of values (l, u) is  $\varepsilon$ -optimal if  $0 \le u - l < \varepsilon$  and  $\mathcal{V}(\hat{s}) \in [l, u]$ , i.e. l and u are lower and upper bounds on the value, respectively. All algorithms in this work are designed to efficiently compute such  $\varepsilon$ -optimal values. We omit computation of a witness strategy due to the technical difficulties this would entail in the general cases. The general idea of obtaining the witness strategies moreover is not specific to our approach, as such the related discussion may in turn distract from the central results.

Note that requiring to find a single value v such that  $|v - V(\hat{s})| < \varepsilon$  is similar, however slightly stricter. In particular, if we find (l, u) with  $0 \le u - l < 2\varepsilon$  where  $V(\hat{s}) \in [l, u]$ , we know that v = (u + l)/2 would satisfy this requirement (i.e. be at most  $\varepsilon$  away from the true value).

#### 3 See [122] for details on linear programming in general.

## 2.3 Probabilistic Learning Algorithms

In order to obtain such approximate solutions, we study a class of *learning-based* algorithms that (stochastically) approximate the value function, inspired by approaches from the field of machine learning. Let us fix an MDP  $\mathcal{M} = (S, Act, Av, \Delta)$ , starting state  $\hat{s}$ , and target set  $T \subseteq S$ . Recall that by approximating the state-action values, we approximate the overall value of a state. Inspired by *BRTDP* (bounded real-time dynamic programming) [112]<sup>4</sup>, we consider algorithms which maintain and update Upper bounds Up :  $S \times Av \rightarrow [0, 1]$  and Lower bounds Lo :  $S \times Av \rightarrow [0, 1]$  of these sate-action values  $\mathcal{V}(s, a)$ . The functions Up and Lo are initialised to appropriate values such that  $Lo(s, a) \leq \mathcal{V}(s, a) \leq Up(s, a)$  for all  $s \in S$  and  $a \in Av(s)$ . This is clearly satisfied by  $Lo(\cdot, \cdot) = 0$  and  $Up(\cdot, \cdot) = 1$ , but non-trivial bounds obtained by previous computations or domain knowledge can be incorporated. We define the state-bounds by

 $\mathsf{Up}(s) \coloneqq \max_{a \in Av(s)} \mathsf{Up}(s, a), \quad \text{and} \quad \mathsf{Lo}(s) \coloneqq \max_{a \in Av(s)} \mathsf{Lo}(s, a).$ 

It may seem counter-intuitive at first that both sides are maximized. One can think of Up(s) as "an upper bound on the best this state can offer" (maximization) and Lo(s) as "at least this value can be obtained in this state" (also maximization).

Now, we clearly have  $Lo(s) \leq \mathcal{V}(s) \leq Up(s)$ , thus we can determine the value of a state  $\varepsilon$ -precise when these respective bounds are sufficiently close. In particular, if we have that

$$\mathsf{Up}(\hat{s}) - \mathsf{Lo}(\hat{s}) = \max_{a \in Av(\hat{s})} \mathsf{Up}(\hat{s}, a) - \max_{a \in Av(\hat{s})} \mathsf{Lo}(\hat{s}, a) < \varepsilon,$$

the values  $(Lo(\hat{s}), Up(\hat{s}))$  are  $\varepsilon$ -optimal.

Our *learning algorithms* update the upper and lower bounds by repeatedly selecting "interesting" / promising state-action pairs of the system  $\mathcal{M}$ , usually by sampling the system beginning in the starting state  $\hat{s}$ . As such, they are similar to *Q-learning* [135] approaches, a commonly used reinforcement learning technique. By following appropriate sampling heuristics the algorithm learns "important" areas of the system and focuses computation there, potentially omitting irrelevant parts of the state space without sacrificing correctness. For example, given a state *s* we propose to select an action *a* with maximal upper bound Up(*s*, *a*), as such an action is the most "promising" one. Then, either this action keeps up to its promise, which will eventually be reflected by an increasing lower bound, or the algorithm finds that the upper bound is too high and lowers it. As such, this idea is very similar to *optimism in the face of uncertainty* [132, Section 4.2], [106]: We only know that the exact value lies between the upper and lower bound, thus we are optimistic and assume the best value (= the upper bound) during sampling. As it turns out, this will lead us to either (i) proving that the upper bound is indeed correct (so following it was the "correct" move all along) or (ii) proving that the bound is too optimistic, i.e. leading us to lower it (so following it was "required" to realize this fact).

<sup>4</sup> See [20] for the "non-bounded" case *RTDP*.

The algorithms repeatedly experience (learning) *episodes*, where each episode consists of several *steps*. One episode corresponds to sampling a path of some length in the system, while one step corresponds to sampling the successor state, i.e. each episode comprises several steps. Throughout this paper, we use  $e \in \mathbb{N}$  exclusively to refer to the e-th episode of some algorithm execution. Later we also refer to distinct steps within episodes by  $t \in \mathbb{N}$ . In particular, t denotes the t-th overall step. Finally,  $t_e$  denotes the first step of the e-th episode, i.e. its starting step. These variables also appear in the algorithms.

The considered algorithms make heavy use of randomness during their execution. Thus, in order to reason about them, we model them as a stochastic process over an appropriate measure space  $(\mathfrak{A}, \mathcal{A}, \mathbb{P}_A)$ . The entire state of our algorithms at the beginning of episode e only depends on the sequences of state-action pairs considered until episode e.<sup>5</sup> Hence, we use episodes as our primitive objects. We need to consider both finite and infinite episodes, since (i) a single episode might in theory comprise infinitely many state-action pairs and (ii) we could see infinitely many episodes, each of finite length. (In both cases, the algorithm does not terminate.) Thus, we set  $\mathfrak{A} = ((S \times Av \times S)^{\times})^{\times}$ , where  $S^{\times} = S^{\star} \cup S^{\omega}$ . (Note that this can be encoded into a single sequence space by introducing a fresh symbol to separate the individual episodes.) The tuples  $S \times Av \times S$  correspond to the current state, chosen action, and sampled successor state, respectively. The  $\sigma$ -field  $\mathcal{A}$  is obtained analogously to the  $\sigma$ -field for Markov chains by considering cylinder sets induced by finite prefixes, see [118, Section 2.1.6]. For a given prefix, its probability can be obtained by computing the probability of each episode occurring in the MDP given the current state of the algorithm.

Now that we defined the probability space these algorithms operate in, we can define notions like almost sure convergence.

**DEFINITION 2.10.** Denote by  $A(\varepsilon)$  the instance of learning algorithm A with precision  $\varepsilon$ . We say that A *converges (almost) surely* if, for every MDP  $\mathcal{M}$ , starting state  $\hat{s}$ , target set T, and precision  $\varepsilon > 0$ , the computation of  $A(\varepsilon)$  terminates (almost) surely (w.r.t.  $\mathbb{P}_A$ ) and yields  $\varepsilon$ -optimal values l and u.

We consider a symbolic input encoding, where the MDP's properties are specified implicitly. In particular, we design our algorithms such that they are applicable when the available actions Av and transition function  $\Delta$  are given as oracles. This means that given a state *s* we can compute Av(s), and given a state-action pair (s, a) we obtain the successor distribution  $\Delta(s, a)$ . This allows us to achieve sub-linear runtime for some classes of MDP w.r.t. their number of states and transitions. Note that most practical modelling languages such as the PRISM language [104] or JANI [38] describe models in such a way.

<sup>5</sup> Due to their "template"-structure, Algorithms 2 and 3 are allowed to introduce some further side effects. For example, they may keep a round-robin counter on actions or other heuristics that are used to sample paths in the system. We assume w.l.o.g. that these side effects are either deterministic or can be properly incorporated into the above measure space.

Since our learning algorithms in essence only rely on being able to repeatedly sample the system, we can drastically reduce the knowledge needed about the system. In particular, we consider the setting of *limited information*, where the algorithm only has very restricted access to the system in question. There, we are only provided with bounds on some properties of the MDP, e.g., the number of states, together with a minimal interaction mechanism. Concretely, we only get an oracle revealing the currently available actions and a "sampling" oracle, which upon choosing one of the available actions moves the system into a successor state, sampled according to the underlying, hidden distributions. The algorithm thus can only simulate an execution of the MDP starting from the initial state *ŝ*, repeatedly choosing an action from the set of available actions and querying the sampling oracle for a successor. This corresponds to a "black-box" setting, where we can easily interact with a system and observe the current state, but have very limited knowledge about its internal transition structure, as might be the case with complex physical systems.

Here, we cannot directly apply the ideas of Q-learning, since the value of the sampled successor might not correspond to the actual value of the action. Instead, the algorithm remembers the result of recent visits, *delaying* the learning update. Intuitively, by seeing many sampling results, we can get a stochastic estimate of the distribution of successor values. In particular, the average of these observations corresponds to the true value with high confidence. This idea is exploited by *delayed Q-learning* [129]. In this setting, we inherently cannot guarantee almost sure convergence, instead we demand that the algorithm terminates correctly with sufficiently high probability, specified by the *confidence*  $\delta > 0$ .

**DEFINITION 2.11.** Denote by  $A(\varepsilon, \delta)$  the instance of learning algorithm A with precision  $\varepsilon$  and confidence  $\delta$ . We say that A is *probably approximately correct* (PAC) if for every MDP  $\mathcal{M}$ , starting state  $\hat{s}$ , target set T, precision  $\varepsilon > 0$ , and confidence  $\delta > 0$ , with probability at least  $1 - \delta$  the computation of  $A(\varepsilon, \delta)$  terminates and yields  $\varepsilon$ -optimal values l and u. In other words, we require that the set of correct and terminating executions has a measure of at least  $1 - \delta$  under  $\mathbb{P}_A$ .

Note that the "confidence" parameter  $\delta$  sometimes is used to refer to the probability of error and sometimes for the probability of correct results. We deliberately use  $\delta$  for the probability of error to slightly simplify notation. See [134, 5, 129, 127] for several, slightly different variants of PAC. Some (but not all) definitions also require that the result is obtained within a particular time-bound (called *efficient PAC-MDP* in [127]). We prove appropriate bounds for both variants of our PAC approach.

**REMARK 2.12.** We assume the system to be "observable" in both settings, i.e. the algorithm can access the *precise* current state of the system and the set of available actions. Extending our methods to *partially observable* systems, e.g. POMDP, is left for future work. Moreover, we also assume that the system can be repeatedly "reset" into the initial configuration  $\hat{s}$ .

# 3. Complete Information – MDP without End Components

In this section, we treat the case of complete information, i.e. the algorithm has full access to the system, in particular its transition function  $\Delta$ . Additionally, we assume that the system has no MECs except two distinguished terminal states. This greatly simplifies the reachability problem and allows us to gradually introduce our approach. In Section 4, we explain the issue of MECs (see Example 4.1) and extend our approach to general MDP.

### 3.1 The Ideas of Value Iteration

Our approach is based on ideas related to *value iteration* (VI) [86]. Thus, we first explain the basic principles of VI. Value iteration is a technique to solve, among others, reachability queries on MDP. It essentially amounts to applying *Bellman iteration* [23] corresponding to the fixed point equation in Equation (1) [68, Section 4.2]. In particular, starting from an initial value vector  $v_0$  with  $v_0(s) = 1$  if  $s \in T$  and 0 otherwise, we apply the iteration

$$v_{n+1}(s) = \begin{cases} 1 & \text{if } s \in T, \\ \max_{a \in Av(s)} \Delta(s, a) \langle v_n \rangle & \text{otherwise.} \end{cases}$$

It is known that this iteration converges to the true value  $\mathcal{V}$  in the limit from below, i.e. for all states *s* we have (i)  $\lim_{n\to\infty} v_n(s) = \mathcal{V}(s)$  and (ii)  $v_n(s) \leq v_{n+1}(s) \leq \mathcal{V}(s)$  for all iterations *n* [118, Theorem 7.2.12]<sup>6</sup>. It is not difficult to construct a system where convergence up to a given precision takes exponential time [73], but in practice VI often is much faster than methods based on *linear programming* (LP)<sup>7</sup> [77], which in theory has worst-case polynomial runtime and yields precise answers [91]. An important practical issue of VI is the absence of a *stopping criterion*, i.e. a straightforward way of determining in general whether the current values  $v_n(s)$ are close to the true value function  $\mathcal{V}(s)$ , as discussed in, e.g., [68, Section 4.2]. As already hinted at, we solve this problem by additionally computing upper bounds, converging to the true value from above.

While the classical value iteration approach updates all states synchronously, the iteration can also be executed *asynchronously*. This means that we do not have to update the values of all states (or state-action pairs) simultaneously. Instead, the update order may be chosen by heuristics, as long as fairness constraints are satisfied, i.e. eventually all states get updated. This observation is essential for our approach, since we want to focus our computation on "important" areas.

<sup>6</sup> Note that reachability is a special case of *expected total reward*, obtained by assigning a one-time reward of 1 to each goal state.

<sup>7</sup> See [16, Theorem 10.105] for an LP-based solution of reachability.

```
MDP \mathcal{M}, state \hat{s}, precision \varepsilon, and initial bounds Up<sub>1</sub> and
          Input:
                          Lo<sub>1</sub>.
          Output: \varepsilon-optimal values (l, u), i.e., \mathcal{V}(\hat{s}) \in [l, u] and 0 \le u - l < \varepsilon.
          e ← 1
1:
                                                                                                                                   > Initialize
          while Up_{e}(\hat{s}) - Lo_{e}(\hat{s}) \geq \varepsilon do
2:
                   \varrho_{e} \leftarrow \text{SamplePairs}(\mathcal{M}, \hat{s}, Up_{e}, Lo_{e}, \varepsilon)
                                                                                                               > Sample pairs to update
3:
                   Up_{e+1} \leftarrow Up_e, Lo_{e+1} \leftarrow Lo_e
4:
                   forall (s, a) \in \rho_e do
                                                                                               > Update the upper and lower bounds
5:
                           Up_{e+1}(s, a) \leftarrow \Delta(s, a) \langle Up_e \rangle
6:
                           Lo_{e+1}(s, a) \leftarrow \Delta(s, a) \langle Lo_e \rangle
7:
                   e \leftarrow e + 1
8:
          return (Lo_e(\hat{s}), Up_e(\hat{s}))
9:
```

Algorithm 2. The BRTDP learning algorithm for MDPs without ECs.

# 3.2 The No-EC BRTDP Algorithm

With these ideas in mind, we are ready to present our first algorithm. Throughout this section, fix a required precision  $\varepsilon > 0$ , an MDP  $\mathcal{M} = (S, Act, Av, \Delta)$  with two distinguished states  $s_+, s_- \in S$ , target set  $T = \{s_+\}$ , and a starting state  $\hat{s}$ . We assume that  $\mathcal{M}$  has no MECs except the two terminal states  $s_+$  and  $s_-$ .

**Assumption 1.** *MDP*  $\mathcal{M}$  *has no MECs, except two trivial ones comprising the target state*  $s_+$  *and sink state*  $s_-$ , *respectively. Formally, we require that* MEC( $\mathcal{M}$ ) = {({ $s_+$ },  $Av(s_+)$ ), ({ $s_-$ },  $Av(s_-)$ )}.

Observe that with Assumption 1 and  $T = \{s_+\}$ , we have  $\mathcal{V}(s_+) = 1$  and  $\mathcal{V}(s_-) = 0$ .

We present our *BRTDP* approach in Algorithm 2. As already mentioned in the introduction, the algorithm repeatedly samples sets of state-action pairs from the system. Based on these experiences, it updates the upper and lower bounds using *Bellman updates* (or *Bellman backups*), corresponding to Equation (1), until convergence. (Recall that  $Up(s) = \max_{a \in Av(s)} Up(s, a)$  and Lo(s) analogously.)

To allow for practical optimization, we leave the sampling method SAMPLEPAIRS undefined and instead only require some generic properties. A simple implementation is given by sampling a path starting in the initial state and following random actions. However, SAMPLEPAIRS may use randomization and sophisticated guidance heuristics, as long as it satisfies certain conditions in the limit (formally defined in Assumption 3). **REMARK 3.1.** We highlight that SAMPLEPAIRS is not even required to return paths. Instead, it can yield any set of state-action pairs. However, when dealing with the limited information setting, we require sampling paths. Thus, it may be instructive to already think of SAMPLEPAIRS as a procedure returning paths.

# 3.3 Proof of Correctness

In this section, we prove correctness of the algorithm, i.e. that the returned result is correct and that the algorithm terminates. We now first establish correctness of the result, assuming that the received input is sane.

Assumption 2. We have that (i) the given initial bounds  $Up_1$  and  $Lo_1$  are correct, i.e.  $Lo_1(s, a) \le V(s, a) \le Up_1(s, a)$  for all  $(s, a) \in S \times Av$ , and (ii)  $Lo_1(s_+) = 1$  and  $Up_1(s_-) = 0$ .

**LEMMA 3.2.** Assume that Assumption 2 holds. Then, during any execution of Algorithm 2 we have for every episode e and all state-action pairs (s, a) that

$$Lo_e(s, a) \le Lo_{e+1}(s, a) \le \mathcal{V}(s, a) \le Up_{e+1}(s, a) \le Up_e(s, a).$$

**PROOF.** Initially, we have that  $Lo_1(s, a) \leq \mathcal{V}(s, a) \leq Up_1(s, a)$  by Assumption 2. The updates in Lines 6 and 7 clearly preserve these inequalities by Equation (1). A simple inductive argument concludes the proof.

**LEMMA 3.3.** Assume that Assumption 2 holds. Then, the result (l, u) of Algorithm 2 is correct, *i.e.* (i)  $0 \le u - l < \varepsilon$ , and (ii)  $\mathcal{V}(\hat{s}) \in [l, u]$ .

**PROOF.** Clearly, (i) immediately follows from Lemma 3.2 and the main loop condition in Line 2. Similarly, (ii) also follows from Lemma 3.2.

In order to prove (almost sure) convergence of Algorithm 2, we need some assumptions on SAMPLEPAIRS. Intuitively, SAMPLEPAIRS may not neglect actions which might be the optimal ones. In order to allow for a wide range of implementations for SAMPLEPAIRS, we present the rather liberal but technical condition of *fairness* in Assumption 3. We further explain each part of this assumption in the following proof of convergence.

Before we continue to the assumption, we introduce a concept, namely the set of Upoptimal actions, which is also used in the proof. We define the set of actions optimal w.r.t. Up<sub>e</sub> in state *s* during episode e as  $MaxA_e(s) \coloneqq arg max_{a \in Av(s)} Up_e(s, a)$ . If the algorithm does not converge, the set  $MaxA_e(s)$  may change infinitely often. For example, two equivalent actions may get updated in an alternating fashion. Thus, for each state *s*, we also define the set of actions that are optimal infinitely often as  $MaxA_{\infty}(s) \coloneqq \bigcap_{k=1}^{\infty} \bigcup_{e=k}^{\infty} MaxA_e(s)$ . This set is non-empty, since there are only finitely many actions and  $MaxA_e(s)$  is non-empty for any episode e. Assumption 3. Let  $\{Up_e\}_{e=1}^{\infty}$  and  $\{Lo_e\}_{e=1}^{\infty}$  be consistent sequences of upper and lower bounds, i.e.  $Lo_1(s, a) \leq Lo_2(s, a) \leq \cdots \leq \mathcal{V}(s, a) \leq \cdots \leq Up_2(s, a) \leq Up_2(s, a)$  for all state-action pairs (s, a). Assume that each call SAMPLEPAIRS $(\mathcal{M}, \hat{s}, Up_e, Lo_e, \varepsilon)$  terminates in finite time and let  $\varrho_1, \varrho_2, \cdots \in \mathcal{P}(S \times Act) \setminus \emptyset$  the infinite sequence of non-empty state-action sets obtained from it.

Set  $S_{\infty} = \bigcap_{k=1}^{\infty} \bigcup_{e=k}^{\infty} \{s \in S \mid s \in \varrho_e\}$  the set of all states which occur infinitely often, analogous for the set of actions occurring infinitely often, denoted  $Act_{\infty}$ . Then

- 1. the initial state is sampled infinitely often, i.e.  $\hat{s} \in S_{\infty}$ ,
- 2. all actions which are optimal infinitely often are also sampled infinitely often, i.e.  $MaxA_{\infty}(s) \subseteq Act_{\infty}$  for every  $s \in S_{\infty}$ , and
- 3. all successors of optimal actions are sampled infinitely often, i.e. for every  $s \in S_{\infty}$  and  $a \in MaxA_{\infty}(s)$  we have that  $supp(\Delta(s, a)) \subseteq S_{\infty}$ .

We say SAMPLEPAIRS almost surely satisfies Assumption 3, if all of its conditions hold with probability 1.

In essence, the assumption requires that all states which are reachable by following optimal actions are indeed reached infinitely often in the limit: Starting from the initial state (Item 1), we select each optimal action infinitely often (Item 2) and explore all successors of these actions (Item 3). For each of these successors, we again select all optimal actions, etc. This insight directly yields an implementation for SAMPLEPAIRS, namely to repeatedly sample a path, starting in the initial state and in each state selecting any optimal action from  $MaxA_e(s)$  uniformly at random, until  $s_+$  or  $s_-$  are reached. Variants of this implementation can, for example, select actions in a round-robin fashion or sample from the optimal actions in a weighted manner. Similarly, naively selecting all state-action pairs in every iteration (effectively classical value iteration) or selecting a single pair at random would also satisfy the assumption.

**LEMMA 3.4.** Algorithm 2 terminates under Assumptions 1 to 3. It terminates almost surely if Assumption 3 is satisfied almost surely.

**PROOF.** We prove the second case, i.e. almost sure termination, by contradiction. Assume that Assumptions 1 and 2 hold, and that Assumption 3 holds a.s. Further, assume for contradiction that the set of non-terminating executions of Algorithm 2 has non-zero measure. Since we assume that each call to SAMPLEPAIRS terminates in finite time (Assumption 3) a.s., the only way Algorithm 2 does not terminate is when the central while-loop is executed infinitely often, i.e. the bounds never converge.

Given some execution of Algorithm 3, define  $\text{Diff}_{e}(s, a) := \text{Up}_{e}(s, a) - \text{Lo}_{e}(s, a)$ . Fix an arbitrary action  $a_{e}^{\max}(s) \in \text{MaxA}_{e}(s)$  for each episode e. Clearly, for any such action  $a_{e}^{\max}(s)$  we have  $\text{Diff}_{e}(s, a_{e}^{\max}(s)) = \text{Up}_{e}(s) - \text{Lo}_{e}(s, a_{e}^{\max}) \ge \text{Up}_{e}(s) - \text{Lo}_{e}(s)$ . By Lemma 3.2, the limits  $\text{Up}_{\infty}(s, a) := \lim_{e \to \infty} \text{Up}_{e}(s, a)$  and  $\text{Lo}_{\infty}(s, a) := \lim_{e \to \infty} \text{Lo}_{e}(s, a)$  are well-defined and finite for any state-action pair (s, a). Thus,  $\text{Diff}(s, a) := \lim_{e \to \infty} \text{Diff}_{e}(s, a)$  and Diff(s) :=  $\limsup_{e\to\infty} \text{Diff}_{e}(s, a_{e}^{\max}(s))$  is also well-defined and finite. We prove that  $\text{Diff}(\hat{s}) = 0$  for almost all executions, contradicting the assumption, as then necessarily  $Up_{e}(\hat{s}) - Lo_{e}(\hat{s}) \leq \text{Diff}_{e}(\hat{s}) < \varepsilon$  for some e a.s.

Observe that the preconditions of Assumption 3 are satisfied through Lemma 3.2 and Assumption 2, hence we have  $\hat{s} \in S_{\infty}$  a.s. [Fact I]. Let  $S_{\infty}$  the set of states seen infinitely often as defined in Assumption 3. By the assumption, we also have that  $\operatorname{supp}(\Delta(s, a)) \subseteq S_{\infty}$  for all  $s \in S_{\infty}, a \in \operatorname{MaxA}_{\infty}(s)$  a.s. [Fact II].

Now, we identify a witness action  $a_{\text{Diff}}(s)$  for the lim sup of Diff(s), i.e. an action  $a_{\text{Diff}}(s)$  such that  $\text{Diff}_{\infty}(s) = \lim_{e \to \infty} \text{Diff}_{e}(s, a_{\text{Diff}}(s))$  and then derive a fixed-point equation. We have  $Up_{\infty}(s, a) = Up_{\infty}(s, a')$  for all  $s \in S_{\infty}$  and  $a, a' \in \text{MaxA}_{\infty}(s)$ , as otherwise one of the two actions would not be optimal eventually. Consequently,  $\lim_{e \to \infty} Up_{e}(s, a_{e}^{\max})$  is well-defined and equals  $Up_{\infty}(s, a)$  for any  $a \in \text{MaxA}_{\infty}(s)$ . Equally,  $\lim_{e \to \infty} Up_{e}(s, a_{e}^{\max})$  also is well-defined, since  $Lo_{e}$  is bounded. Hence the lim sup of Diff(s) distributes over the minus. Recall that for each state-action pair, the limit of  $Lo_{\infty}(s, a)$  is well-defined. As there are only finitely many actions, the sequence  $Lo_{e}(s, a_{e}^{\max})$  only has finitely many accumulation points and there necessarily exists an action  $a_{\text{Diff}}(s) \in \text{MaxA}_{\infty}(s)$  such that  $\limsup_{e\to\infty} Lo_{e}(s, a_{e}^{\max}) = Lo_{\infty}(s, a_{\text{Diff}}(s))$ . Together, we have that Diff(s) =  $Up_{\infty}(s, a_{\text{Diff}}(s)) - Lo_{\infty}(s, a_{\text{Diff}}(s))$ . Since all states  $S_{\infty}$  and all optimal actions  $MaxA_{\infty}$  are visited infinitely often, we have that  $Up_{\infty}(s, a) = \Delta(s, a) \langle Up_{\infty} \rangle$  and  $Lo_{\infty}(s, a) = \Delta(s, a) \langle Lo_{\infty} \rangle$  for all  $s \in S_{\infty}$  and  $a \in MaxA_{\infty}(s)$  by the back-propagation in Lines 6 and 7—if not, they would get updated. Consequently, Diff(s) =  $\Delta(s, a_{\text{Diff}}(s)) \langle Diff \rangle$  for all  $s \in S_{\infty}$ , since  $a_{\text{Diff}}(s) \in MaxA_{\infty}(s)$  [Fact III].

Finally, we use Assumption 1 together with the above equation to show that  $\text{Diff}(\hat{s}) = 0$ . Let the maximal difference  $\text{Diff}_{\max} = \max_{s \in S_{\infty}} \text{Diff}(s)$  and define the witness states  $S_{\text{Diff}} = \{s \in S_{\infty} \mid \text{Diff}(s) = \text{Diff}_{\max}\}$ . Assume for contradiction that Diff > 0 (a.s.). Then, clearly  $s_+, s_- \notin S_{\text{Diff}}$ , as  $\text{Diff}(s_+) = \text{Diff}(s_-) = 0$  by Lemma 3.2 (the bounds of the special states are both set to 1 or 0 initially, respectively) and Assumption 2 (bounds are monotone). Consequently,  $S_{\text{Diff}}$  cannot contain any EC by Assumption 1 (the MDP is MEC-free). Since  $S_{\text{Diff}}$  does not contain an EC, there exists some state  $s \in S_{\text{Diff}}$  such that for all  $a \in Av(s)$  we have  $\text{supp}(\Delta(s, a)) \notin S_{\text{Diff}}$ . In other words, for each action  $a \in Av(s)$ , there exists a state  $s_a$  with both  $s_a \notin S_{\text{Diff}}$  and  $\Delta(s, a, s_a) > 0$ . By definition of  $S_{\text{Diff}}$  (all states with maximal difference), we have that  $\text{Diff}(s_a) < \text{Diff}_{\max}$ . In particular,  $\text{Diff}(s, a_{\text{Diff}}(s)) < \text{Diff}(s)$  [Fact IV]. We abbreviate the witness action from [III] by  $\overline{a} := a_{\text{Diff}}(s)$ . Then

$$\operatorname{Diff}(s) \stackrel{[\operatorname{IIII}]}{=} \Delta(s, \overline{a}) \langle \operatorname{Diff}_{\max} \rangle = \sum_{s' \in S} \Delta(s, \overline{a}, s') \cdot \operatorname{Diff}(s')$$

$$\stackrel{[\operatorname{III}]}{=} \sum_{s' \in S_{\infty}} \Delta(s, \overline{a}, s') \cdot \operatorname{Diff}(s')$$

$$= \sum_{s' \in S_{\infty} \setminus \{s_{\overline{a}}\}} \Delta(s, \overline{a}, s') \cdot \operatorname{Diff}(s') + \Delta(s, \overline{a}, s_{\overline{a}}) \cdot \operatorname{Diff}(s_{\overline{a}})$$

$$\leq \sum_{s' \in S_{\infty} \setminus \{s_{\overline{a}}\}} \Delta(s, \overline{a}, s') \cdot \operatorname{Diff}_{\max} + \Delta(s, \overline{a}, s_{\overline{a}}) \cdot \operatorname{Diff}(s_{\overline{a}})$$





$$\stackrel{[IV]}{\leq} \sum_{s' \in S_{\infty} \setminus \{s_{\overline{a}}\}} \Delta(s, \overline{a}, s') \cdot \text{Diff}_{\max} + \Delta(s, \overline{a}, s_{\overline{a}}) \cdot \text{Diff}_{\max}$$
$$= \text{Diff}_{\max},$$

contradicting  $s \in S_{\text{Diff}}$ , i.e.  $\text{Diff}(s) = \text{Diff}_{\max}$ , and we have that  $\text{Diff}_{\max} = 0$ . To conclude the proof, observe that  $S_{\text{Diff}} = S_{\infty}$  a.s., as  $0 \leq \text{Diff}(s) \leq \text{Diff}_{\max} = 0$  for all  $s \in S_{\infty}$ , and  $\text{Diff}(\hat{s}) = 0$  a.s., since  $\hat{s} \in S_{\infty}$  a.s. by **[I]**.

Guaranteed convergence (instead of "only" almost sure) follows analogously.

As an immediate consequence of Lemma 3.3 (correctness) and Lemma 3.4 (termination), we get the desired result.

**THEOREM 3.5.** Assume that Assumptions 1 and 2, and (almost surely) Assumption 3 hold. Then Algorithm 2 is correct and converges (almost surely).

**REMARK 3.6.** If an implementation of SAMPLEPAIRS satisfies Assumption 3 only almost surely, we can easily obtain a surely terminating variant by interleaving it with a deterministic sampling procedure, e.g., a round-robin method.

**EXAMPLE 3.7.** Interestingly, following the optimal upper bound does not necessarily yield an  $\varepsilon$ -optimal strategy, as shown by the MDP in Figure 2. Assume that initially we take action  $a_1$ , setting Up<sub>2</sub>( $\hat{s}, a_1$ ) = Lo<sub>2</sub>( $\hat{s}, a_1$ ) =  $\frac{1}{2}$ . Then, Up<sub>2</sub>( $\hat{s}, b_1$ ) = 1 > Up<sub>2</sub>( $\hat{s}, a_1$ ) and we sample  $b_1$ , updating Up<sub>3</sub>( $\hat{s}, b_1$ ) =  $\frac{3}{4}$ , Up<sub>4</sub>( $\hat{s}, b_1$ ) =  $\frac{3}{4} \cdot \frac{3}{4}$ , etc. This continues until the upper bound of  $b_1$ is  $\varepsilon$ -close to  $\frac{1}{2}$ , when the algorithm terminates. Now, suppose that instead of  $\Delta(\hat{s}, b_1, s_-) = \frac{1}{4}$ exactly, we have  $\Delta(\hat{s}, b_1, s_-) = p$ . Then, Up<sub>*i*</sub>( $\hat{s}, b_1$ ) =  $(1 - p)^{i-1}$ . For a fixed  $\varepsilon$ , choose p such that  $\frac{1}{2} < (1 - p)^k < \frac{1}{2} + \varepsilon$  for some k. This means that in episode e = k + 1 (where the algorithm terminates) we have Up<sub>e</sub>( $\hat{s}, b_1$ ) > Up<sub>e</sub>( $\hat{s}, a_1$ ). Yet, following  $b_1$  yields a (highly) suboptimal value, namely 0 instead of  $\frac{1}{2}$ .

It is straightforward to also apply this example to our DQL approach and as a counterexample to [33, Lemma 16].

Following the maximal *lower* bound yields a strategy achieving at least this value, using results on asynchronous VI [118]. We omit formal treatment of this claim, since we are not



Figure 3. Example MDP with an EC where Algorithm 2 does not converge.

concerned with extracting a witness strategy to avoid distraction from the main result. (Note that it is in general not correct to choose an arbitrary *value-optimal* action, i.e. any action  $\arg \max_{a \in Av(s)} \mathcal{V}(s, a)$ .)

# 4. Complete Information – General Case

In this section, we deal with the case of general MDP, in particular, we allow for arbitrary ECs. We first illustrate with an example the additional difficulties arising when considering general MDPs with non-trivial ECs. In particular, Algorithm 2 does not converge, even on a small example.

**EXAMPLE 4.1.** Consider the MDP depicted in Figure 3. Clearly, we can reach the goal  $T = \{s_+\}$  with probability  $\frac{1}{2}$  by playing  $a_0$  in  $\hat{s}$  and then  $b_1$  in  $s_1$ . But the EC  $(\{\hat{s}, s_1\}, \{a_0, a_1\})$  causes issues for Algorithm 2. When running the algorithm on this example MDP, we eventually have that  $Up(s_1, b_1) = Lo(s_1, b_1) = \frac{1}{2}$ , but  $Up(s_1, a_1) = 1$ , since  $Up(\hat{s}) = 1$ . Similarly, we keep  $Up(\hat{s}, a_0) = 1$ , as  $Up(s_1) = 1$ . Informally,  $\hat{s}$  and  $s_1$  "promise" each other that the target state might still be reachable with probability 1, but these promises depend on each other cyclically. Removing the internal behaviour of this EC and "merging"  $\hat{s}$  and  $s_1$  into a single state (with only action  $b_1$ ) solves this issue.

In general, by definition of ECs, every state inside an EC can be reached from any other state with probability 1. Since we are interested in (unbounded) reachability, this means that for an EC there can only be two cases. Either, the EC contains a target state. Then, reaching any state of the EC is (a.s.) equivalent to reaching the target already and we do not need to treat the internal transitions of the EC further. Otherwise, i.e. when the EC does not contain a target state, we can also omit treatment of its internal behaviour and only consider its interaction with outside states. For the remainder of the section, fix an arbitrary MDP  $\mathcal{M} = (S, Act, Av, \Delta)$ , starting state  $\hat{s}$ , target set T, and precision  $\varepsilon > 0$ .

**LEMMA 4.2.** Let  $(R, B) \in EC(\mathcal{M})$  be an EC of  $\mathcal{M}$ . Then,  $\Pr_{\mathcal{M},s}^{\max}[\diamondsuit\{s'\}] = 1$  for any states  $s, s' \in R$  and consequently  $\Pr_{\mathcal{M},s}^{\max}[\diamondsuit T] = \Pr_{\mathcal{M},s'}^{\max}[\diamondsuit T]$  for any target set  $T \subseteq S$ .

**PROOF.** Follows directly from [52, Lemma 1] (observe that the first claim is a special case of the second claim with  $T = \{s'\}$ ).

In other words, states in the same EC are equivalent for reachability and we can apply a quotienting construction w.r.t. to ECs. This idea has been exploited by the *MEC quotient* construction [61, 52, 73], a preprocessing step where first all MECs are identified and then "collapsed" into a representative state. However, this approach requires that the whole graph structure of the MDP is known. Constructing the whole graph of the system may be prohibitively expensive or even impossible, as, e.g., in our limited knowledge setting (see Definition 5.2). Hence, we propose a modification to the BRTDP algorithm, which detects and handles ECs "on-the-fly". The algorithm will repeatedly identify ECs and maintain a separate, simplified MDP, which is similar to a MEC quotient.

# 4.1 Collapsing End Components

As already explained, collapsing an EC can be viewed as replacing it with a single representative state, omitting the internal behaviour of the EC. In the following definition, we introduce the *collapsed MDP*, where end components are merged into representative states. Moreover, we again introduce the special states  $s_+$  and  $s_-$ , acting as a target and sink respectively, to avoid corner cases. Many statements in this section are similar to [61, Section 6.4] but adapted to our particular use case. Note that our definition of collapsed MDP in particular depends on the target set *T*.

**DEFINITION 4.3.** Let  $EC = \{(R_1, B_1), \dots, (R_n, B_n)\} \subseteq EC(\mathcal{M})$  be a (possibly empty) set of ECs in  $\mathcal{M}$  with  $R_i, B_i \neq \emptyset$  and pairwise disjoint. Define  $R_{EC} = \bigcup_i R_i$  and  $B_{EC} = \bigcup_i B_i$  the set of all states and actions in EC, respectively.

The *collapsed MDP* is defined as  $\mathcal{M}^c = (S^c, Act^c, Av^c, \Delta^c) = \text{collapse}(\mathcal{M}, \mathsf{EC}, \hat{s}, T)$ ,

- ---  $S^c = S \setminus R_{EC} \cup \{s_{(R_i,B_i)}\} \cup \{s_+, s_-\}$ , where  $s_{(R_i,B_i)} \notin S$  are new *representative* states,  $s_+$  is the new target state, and  $s_-$  is a new sink state,
- $Act^c = Act \setminus B_{EC} \cup \{rem_i\} \cup \{a_+, a_-\}$ , where  $rem_i \notin Act$  are new *remain* actions (one per state, as we assume actions to be uniquely associated with one state),
- $Av^c(s)$  is defined by
  - $-- Av^{c}(s) = Av(s) \text{ for } s \in S \setminus R_{\mathsf{EC}},^{\mathsf{8}}$
  - $-- Av^{c}(s_{(R_{i},B_{i})}) = \bigcup_{s \in R_{i}} Av(s) \setminus B_{i} \cup \{\operatorname{rem}_{i}\},$
  - $Av^{c}(s_{+}) = \{a_{+}\}, Av'(s_{-}) = \{a_{-}\}, \text{ and }$
- $\Delta^c$  is defined by (states is an auxiliary function defined below)
  - $\Delta^{c}(s^{c}, a^{c}, s'^{c}) = \sum_{s' \in \text{states}(s'^{c})} \Delta(\text{state}(a^{c}, \mathcal{M}), a^{c}, s') \text{ for } s^{c}, s'^{c} \in S^{c} \setminus \{s_{+}, s_{-}\} \text{ and } a^{c} \in Av^{c}(s^{c}) \cap B,$

$$\Delta^{c}(s_{(R_{i},B_{i})}, \operatorname{rem}_{i}) = \{s_{+} \mapsto 1\} \text{ if } T \cap R_{i} \neq \emptyset \text{ and } \{s_{-} \mapsto 1\} \text{ otherwise, and}$$
$$- \Delta^{c}(s_{+}, a_{+}, s_{+}) = 1, \Delta'(s_{-}, a_{-}, s_{-}) = 1,$$



**Figure 4.** Example of an MDP (left) and its collapsed version (right) with  $T = \{s_2\}$  and EC = {( $\{\hat{s}, s_1\}, \{a_0, a_1\}$ ), ( $\{s_2, s_3\}, \{a_2, a_3\}$ )}.

with the following auxiliary functions

- collapsed :  $S \to S^c$  maps states of  $\mathcal{M}$  to their corresponding state in the collapsed MDP, i.e. collapsed(s) =  $s_{(R_i,B_i)}$  if  $s \in R_i$  for some i and collapsed(s) = s otherwise,
- states :  $S^c \setminus \{s_+, s_-\} \to 2^S$  maps states in the collapsed MDP to the set of states they represent, i.e. states $(s^c) = R_i$  if  $s^c = s_{(R_i, B_i)}$  for some *i* and states $(s^c) = \{s^c\} \subseteq S$  otherwise,
- equiv :  $S \rightarrow 2^S$  maps states of  $\mathcal{M}$  to all states in their EC, i.e. equiv(s) =  $R_i$  if  $s \in R_i$  for some *i* and equiv(s) = {s} otherwise.

Note that equiv(s) = states(collapsed(s)). For ease of notation, we extend these auxiliary functions to sets of states in the obvious way, i.e.  $collapsed(R) = \{collapsed(s) \mid s \in R\}$ ,  $states(R^c) = \bigcup_{s^c \in R^c} states(s^c)$ , and  $equiv(R) = \bigcup_{s \in R} equiv(s)$ . Finally, if  $\hat{s} \in R_i$  for some *i*, we identify  $\hat{s}$  with  $s_{(R_i,B_i)}$  for ease of notation. This guarantees that we always have  $\hat{s} \in S^c$ .

See Figure 4 for an example of a collapsed MDP. Observe that given a set EC explicitly, the collapsed MDP can be computed on-the-fly, i.e. without constructing the original MDP completely. In particular, for a state *s* in the MDP  $\mathcal{M}$ , we can compute the corresponding state  $s^c = \text{collapsed}(s)$  as well as  $Av^c(s^c)$  and  $\Delta^c(s^c, a^c)$  for all actions  $a \in Av^c(s^c)$ , based on the given set EC.

Now, we prove some useful properties about the collapsed MDP. These properties are rather intuitive, however the corresponding proofs are surprisingly technical without revealing relevant insights. Thus, the proofs may be skipped. In essence, we prove that (i) there is a correspondence of paths between the original and the collapsed MDP, (ii) there is a correspondence of ECs between the two MDPs, and, most importantly, (iii) the reachability probability is equal on the two MDPs.

Fix a collapsed MDP of  $\mathcal{M}$  as  $\mathcal{M}^c = (S^c, Act^c, Av^c, \Delta^c) = \text{collapse}(\mathcal{M}, \text{EC}, \hat{s}, T)$  for the remainder of this section, where  $\text{EC} = \{(R_i, B_i)\}_{i=1}^n$  is any appropriate set of end components.

**LEMMA 4.4.** We have that collapsed(state(a, M)) = state(a,  $M^c$ ) for all  $a \in Act \cap Act^c$ .

**PROOF.** First, observe that  $Act \cap Act^c = Act^c \setminus \{a_+, a_-, rem_i\}$  by definition. The claim follows by a case distinction on  $s^c = \text{state}(a, \mathcal{M}^c)$ . If  $s^c \in S$ , then  $Av(s^c) = Av^c(s^c)$  and collapsed $(s^c) = s^c$ . If instead  $s^c = s_{(R_i,B_i)}$  for some  $(R_i, B_i) \in EC$ , we have that  $a \in \bigcup_{s \in R_i} Av(s) \setminus B_i$ . Thus, there exists a state  $s \in R_i$  such that  $s = \text{state}(a, \mathcal{M})$ . But then by definition collapsed $(s) = s^c$ .

The following two lemmas show how we can relate paths in the two MDPs with each other. See [61, Section 6.4.1] for an alternative view. Intuitively, the collapsed MDP also gives us a "quotient" on the set of paths. Essentially, a continuous sequence of state-action pairs belonging to the same EC from EC is "collapsed" to the corresponding representative. Vice-versa, any path in the collapsed MDP corresponds to a set of paths in the original MDP.

**LEMMA 4.5.** Let  $\varrho = s_1 a_1 \dots a_{n-1} s_n \in \text{FPaths}_{\mathcal{M}}$  be a finite path in the MDP  $\mathcal{M}$ . There exists a number  $m \leq n$  and indices  $i_1, \dots, i_m$  with  $1 \leq i_j < i_{j+1} \leq n$  such that

 $\varrho^{c} = \text{collapsed}(s_{i_{1}})a_{i_{1}} \dots a_{i_{m-1}}\text{collapsed}(s_{i_{m}}) \in \text{FPaths}_{\mathcal{M}^{c}}$ 

is a finite path in the collapsed MDP  $\mathcal{M}^c$  with collapsed $(s_1) = \text{collapsed}(s_{i_1})$  and collapsed $(s_n) = \text{collapsed}(s_{i_m})$ .

**PROOF.** We construct the path  $\varrho^c$  inductively. We start with  $i_1 = 1$  and  $s_1^c = \text{collapsed}(s_1)$ . Now, either all actions of  $\varrho$  are in  $B_{\text{EC}}$ , then by definition of ECs all states of  $\varrho$  are within the same EC and we are done. Otherwise, let a be the first action along the path  $\varrho$  such that  $a \in Act^c$  (i.e.  $a \notin B_{\text{EC}}$ ) and let its index equal j. Set  $i_2 = j$ ,  $a_1^c = a$  and  $s_2^c = \text{collapsed}(s_{i+1})$ . Then  $a \in Av(s_1^c)$ . Repeat the argument with the path  $\varrho'$  equal to the suffix of  $\varrho$  starting at j + 1.

**LEMMA 4.6.** Let  $\varrho^c = s_1^c a_1^c \dots a_{m-1}^c s_m^c \in \text{FPaths}_{\mathcal{M}^c}$  be a finite path in the collapsed MDP  $\mathcal{M}^c$  not containing the special states  $s_+$ ,  $s_-$ . There exists a finite path  $\varrho = s_1 a_1 \dots a_{n-1} s_n \in \text{FPaths}_{\mathcal{M}}$  in the MDP  $\mathcal{M}$  with  $n \ge m$  and indices  $i_1, \dots, i_m$  with  $1 \le i_j < i_{j+1} \le n$  and  $-s_k \in \text{states}(s_j^c)$  for all j and k with  $i_j \le k < i_{j+1}$  (defining  $i_{m+1} = n + 1$ ) and

- *if*  $s_j^c = s_{(R_i,B_i)}$  *then*  $a_k \in B_i$  *for all* j *and* k *with*  $i_j \leq k < i_{j+1} - 1$ .

**PROOF.** Similar to the above proof, we construct the path  $\varrho$  inductively. Distinguish two cases for  $s_1^c$ . If  $s_1^c \in S$ , set  $s_1 = s_1^c$  and  $a_1 = a_1^c$  and repeat the argument with the next step of  $\varrho^c$ . Otherwise, we have that  $s_1^c = s_{(R_i,B_i)}$  for some EC  $(R_i, B_i) \in$  EC. Since  $(R_i, B_i)$  is an EC in  $\mathcal{M}$ , there exists a finite path in FPaths $\mathcal{M}$  only using actions of  $B_i$  from any state in  $R_i$  to state  $(a_1^c, \mathcal{M})$ . This path corresponds to the first state-action pair in  $\varrho^c$ . By definition, there exists a state  $s' \in S$  such that  $s' \in \text{supp}(\Delta(\text{state}(a_1^c, \mathcal{M}), a_1^c))$  and collapsed $(s') = s_2^c$ . Thus, we can extend the above path by  $a_1^c s'$  and repeat the argument.

Based on the previous lemmas, we can establish a correspondence of end components between the original MDP and its (partly) collapsed version. In particular, for every EC in the original MDP there either exists a single state representing this EC or a new EC in the collapsed MDP. **LEMMA 4.7.** For any  $EC(R, B) \in EC(\mathcal{M})$  in the MDP  $\mathcal{M}$  we either have

- 1. an EC  $(R^c, B^c)$  in  $\mathcal{M}^c$ , where  $R^c = \text{collapsed}(R)$  and  $B^c = B \cap Act^c$ , or
- *2.* a state  $s_{(R',B')} \in S^c$  with  $R \subseteq R'$  and  $B \subseteq B'$ .

**PROOF.** Observe that Case 2 is trivial by definition, in particular this case is equivalent to  $B \subseteq B_i$  for some *i*. Moreover, Case 1 and Case 2 are mutually exclusive since by construction for any EC  $(R_i, B_i)$  the internal actions  $B_i$  are removed, thus there is no  $B \subseteq B_i$  such that  $(\{s_{(R_i, B_i)}\}, B)$  is an EC in  $\mathcal{M}^c$ .

Let thus (R, B) be an EC in the MDP  $\mathcal{M}$  with  $B \not\subseteq B_i$  for all *i*. We show that  $(R^c, B^c)$  with  $R^c = \text{collapsed}(R)$  and  $B^c = B \cap Act^c$  is an EC in  $\mathcal{M}^c$ .

First, we show by contradiction that  $B \nsubseteq B_{EC}$  [Fact I], i.e. *B* cannot comprise only internal actions of the ECs in EC. Recall that by assumption on EC the EC states  $R_i$  are disjoint and  $B_i$  are subsets of the actions enabled in the respective states of  $R_i$ . Since we assume not to be in Case 2, (R, B) is an EC with  $B \nsubseteq B_i$  for all *i*. Assume for contradiction that  $B \subseteq B_{EC} = \bigcup B_i$ . Then (R, B) necessarily has to contain states of at least two ECs from EC. Formally, there exist two states  $s, s' \in R$  with  $s \in R_i, s' \in R_j$ , and  $i \neq j$ . Since (R, B) is an EC, there exists a path from *s* to *s'* and vice versa, using only actions from *B*. As  $B \subseteq B_{EC}$ , these actions were available in the ECs before. Since *s* and *s'* are in two ECs with disjoint state sets and a path using only actions from *B* exists between them, there exists a state *s''* and action  $a \in B \subseteq B_{EC}$  with  $\sup(\Delta(s'', a)) \notin R_i$ . Since the  $a \in B_{EC}$ , we necessarily have  $a \in B_i$ , contradicting the assumption that  $(R_i, B_i)$  is an EC, proving [I].

Next, we prove that  $R^c = \bigcup_{a \in B^c} \text{state}(a, \mathcal{M}^c)$  [Fact II]. Observe that by assumption we have  $R = \bigcup_{a \in B} \text{state}(a, \mathcal{M})$ . By definition of  $B^c = B \cap Act^c$ , we thus have that  $\bigcup_{a^c \in B^c} \text{state}(a^c, \mathcal{M}) \subseteq R$ . Consequently

$$\bigcup_{a^c \in B^c} \text{collapsed}(\text{state}(a^c, \mathcal{M})) \subseteq \text{collapsed}(R) = R^c$$

Applying Lemma 4.4 yields

$$\bigcup_{a^c \in B^c} \text{collapsed}(\text{state}(a^c, \mathcal{M})) = \bigcup_{a^c \in B^c} \text{state}(a^c, \mathcal{M}^c),$$

thus  $\bigcup_{a^c \in B^c} \text{state}(a^c, \mathcal{M}^c) \subseteq R^c$ .

Now, assume for contradiction that there exists a state  $s^c \in R^c$  such that  $s^c \neq \text{state}(a^c, \mathcal{M}^c)$ for all  $a^c \in B^c$ . Due to the definition of  $\mathcal{M}^c$ , we either have  $s^c \in S$ ,  $s^c = s_{(R',B')}$  for some EC  $(R', B') \in \text{EC}$ , or  $s^c \in \{s_+, s_-\}$ . The third case immediately leads to a contradiction, since  $B^c \subseteq Act$ and thus  $a_+, a_- \notin B^c$ . In the first case, we have that  $s^c \notin R_i$  for any i, thus  $Av(s^c) = Av^c(s^c) \subseteq Act^c$ . Hence, any action a of this state contained in the EC (R, B) is still available in the collapsed MDP and thus also contained in the EC  $(R^c, B^c)$ . The second case implies, by definition of  $R^c = \text{collapsed}(R)$ , that there exists an EC  $(R_i, B_i) \in \text{EC}$  such that  $R_i \cap R \neq \emptyset$ . Recall that  $Av^c(s_{(R_i, B_i)}) = \bigcup_{s \in R_i} Av(s) \setminus B_i$ . The case assumption is thus equivalent to  $B^c \cap (\bigcup_{s \in R_i} Av(s) \setminus B_i) =$   $\emptyset$ . Inserting the definition of  $B^c$  and  $Act^c$  yields

$$B \cap (Act \setminus B_{\mathsf{EC}}) \cap (\bigcup_{s \in R_i} Av(s) \setminus B_i) = B \cap (\bigcup_{s \in R_i} Av(s) \setminus B_i) = \bigcup_{s \in R_i \cap R} Av(s) \cap B \setminus B_i = \emptyset.$$

This implies that  $Av(s) \cap B \subseteq B_i$  for all  $s \in R_i \cap R$ , i.e. all such states only have "internal" actions of the EC  $(R_i, B_i)$  available in (R, B). But this implies  $R \subseteq R_i$  and  $B \subseteq B_i$ , contradicting our assumptions. This concludes the proof of **[II]**.

Now, we prove that  $(R^c, B^c)$  is a proper EC in  $\mathcal{M}^c$ , i.e. that (i)  $R^c \neq \emptyset$ ,  $\emptyset \neq B^c \subseteq \bigcup_{s^c \in R^c} Av(s^c)$ , (ii) for all  $s^c \in R^c$ ,  $a \in B^c \cap Av^c(s^c)$  we have  $\operatorname{supp}(\Delta^c(s^c, a^c)) \subseteq R^c$ , and (iii) for all states  $s^c, s'^c \in R^c$ there exists a path from  $s^c$  to  $s'^c$  only using actions from  $B^c$ .

For (i), we have  $B^c \neq \emptyset$ , otherwise  $B^c = B \cap Act^c = \emptyset$  implies  $B \subseteq B_{EC}$ , contradicting [I]. [II] yields the second part of the first condition.

To prove (ii), assume a contradiction, i.e. let  $s^c \in R^c$ ,  $a \in B^c \cap Av^c(s^c)$  such that  $s'^c \in supp(\Delta^c(s^c, a^c)) \setminus R^c$ . Let  $s = state(a^c, \mathcal{M})$  (implying  $s^c = collapsed(s)$ ). Again, we proceed by a case distinction, this time on the successor  $s'^c$ . If  $s'^c \in S$ , we have that  $s'^c \in supp(\Delta(s, a^c))$ , since  $s \in R$  and  $a^c \in B$  and (R, B) is an EC. Further,  $\Delta^c(s^c, a^c, s'^c) = \Delta(s^c, a^c, s'^c)$ , thus  $s'^c \in supp(\Delta^c(s^c, a^c))$ , contradicting the assumption. If instead  $s'^c = s_{(R_i,B_i)}$ , then there exists a state  $s' \in supp(\Delta(s, a^c)) \cap R_i$  by definition of  $\Delta^c$ . But then  $s_{(R_i,B_i)} \in R^c$  by definition of  $R^c$ , contradiction.

Finally, to show (iii), we can directly apply Lemma 4.5 to obtain the required path as follows. Let  $s^c, s'^c \in R^c$  two states and pick two arbitrary  $s, s' \in R$  with collapsed $(s) = s^c$  and collapsed $(s') = s'^c$ . Since (R, B) is an EC, there exists a finite path  $\varrho$  from s to s', using only actions of B. By Lemma 4.5, we get a path  $\varrho^c$  from  $s^c$  to  $s'^c$  using only actions from  $B \cap Act^c = B^c$ , concluding the proof of Case 1.

As expected, the corresponding reverse statement holds true, too, i.e. every EC in the collapsed MDP yields a corresponding EC in the original MDP.

**LEMMA 4.8.** For all ECs  $(R^c, B^c)$  in  $\mathcal{M}^c$  with  $s_+, s_- \notin R^c$  we have that (R, B) with  $R = \text{states}(R^c)$ and  $B = B^c \cup \bigcup_{s_{(R,B_i)} \in R^c} B_i$  is an EC in  $\mathcal{M}$ .

**PROOF.** Fix an EC  $(R^c, B^c)$  in  $\mathcal{M}^c$  and set  $R = \text{states}(R^c)$  and  $B = B^c \cup \bigcup_{s_{(R_i, B_i)} \in R^c} B_i$ . We need to prove that (R, B) is an EC in  $\mathcal{M}$ . Clearly, R and B are non-empty. We show that  $R = \bigcup_{a \in B} \text{state}(a, \mathcal{M})$ . For any  $s \in R$ , there exists a  $s^c \in R^c$  such that  $s \in \text{states}(s^c)$  by definition of R. If  $s = s^c$  we have  $s \in R^c$  and there exists an action  $a^c \in B^c \subseteq B$  with  $\text{state}(a^c, \mathcal{M}) = s$ . Otherwise, there is an EC  $(R_i, B_i) \in \text{EC}$  with  $s \in R_i, s_{(R_i, B_i)} \in R^c$ , and, since  $(R_i, B_i)$  is in EC in  $\mathcal{M}$ , there is an action  $a \in B_i \subseteq B$  with  $\text{state}(a, \mathcal{M}) = s$ . Similarly, for any action  $a \in B$  we have that  $\text{state}(a, \mathcal{M}) \in R$  by analogous reasoning.

It remains to show that (i) for all  $s \in R$ ,  $a \in B \cap Av(s)$  we have  $supp(\Delta(s, a)) \subseteq R$ , and (ii) for all  $s, s' \in R$  there is a finite path from s to s' only using actions from B. For (i), we again assume contradiction, i.e. there are states  $s \in R$ ,  $s' \in S$  and an action  $a \in Av(s) \cap B$ such that  $s' \in \text{supp}(\Delta(s, a)) \setminus R$ . We again proceed by case distinctions, but now first on a. If  $a \in B^c$ , then  $\text{supp}(\Delta^c(\text{collapsed}(s), a)) \subseteq R^c$ , as  $(R^c, B^c)$  is an EC. By definition of  $\Delta^c$ , we have collapsed $(s') \in \text{supp}(\Delta^c(\text{collapsed}(s), a))$ . Together, this implies  $s' \in R$ , yielding a contradiction. If instead  $a \in B_i$  for some EC  $(R_i, B_i) \in \text{EC}$ , then  $s, s' \in R_i \subseteq R$ , also leading to a contradiction. Finally, to prove (ii), we can directly apply Lemma 4.6 to a path from collapsed(s) to collapsed(s')in  $(R^c, B^c)$ , yielding a path from s to s' in (R, B).

The previous statement implies that if we collapse a MEC of the original MDP, then there can be no EC in the collapsed MDP containing the MEC representative state.

**LEMMA 4.9.** Let  $\{(R'_i, B'_i)\}_{i=1}^m \subseteq EC \cap MEC(\mathcal{M})$  be some MECs of  $\mathcal{M}$  in EC. Then, we have that  $s_{(R'_i, B'_i)} \notin R^c$  for any EC  $(R^c, B^c)$  in  $\mathcal{M}^c$ .

**PROOF.** Assume there is such an EC  $(R^c, B^c)$  with  $s_{(R'_i, B'_i)} \in R^c$ . Lemma 4.8 yields an EC (R, B) with  $R'_i \subseteq R, B'_i \subsetneq B$ , contradiction to (R, B) being a MEC in  $\mathcal{M}$ .

The statement of Lemma 4.9 does not hold for any EC  $(R'_i, B'_i) \in$  EC, since there might be a larger EC containing  $s_{(R'_i, B'_i)}$ . For example, in Figure 4, the collapsed MDP has an EC containing representative states. However, if all MECs are collapsed, the resulting collapsed MDP indeed has no ECs except two trivial ones.

**COROLLARY 4.10.** Let  $\mathcal{M}^c = \text{collapse}(\mathcal{M}, \text{MEC}(\mathcal{M}), \hat{s}, T)$  be the collapsed MDP of  $\mathcal{M}$  with  $\text{EC} = \text{MEC}(\mathcal{M})$ . Then,  $\mathcal{M}^c$  satisfies Assumption 1.

**PROOF.** Follows directly from the above Lemma 4.9.

Finally, we also get that the reachability probabilities are preserved.

**LEMMA 4.11.** Let  $\mathcal{M}^c = (S^c, Act^c, Av^c, \Delta^c) = \text{collapse}(\mathcal{M}, \text{EC}, \hat{s}, T)$  be the collapsed MDP of  $\mathcal{M}$ , where  $\text{EC} = \{(R_i, B_i)\}_{i=1}^n$  is any appropriate set of end components. Then, for any state  $s \in S$  it holds that

$$\mathsf{Pr}_{\mathcal{M},s}^{\max}[\diamond T] = \mathsf{Pr}_{\mathcal{M}^{c},\mathsf{collapsed}(s)}^{\max}[\diamond \mathsf{collapsed}(T)] = \mathsf{Pr}_{\mathcal{M}^{c},\mathsf{collapsed}(s)}^{\max}[\diamond(\{s_{+}\} \cup (T \cap S^{c}))].$$

**PROOF.** First, observe that  $\Pr_{\mathcal{M}^c, S^c}^{\max}[\diamond\{s_+\}] = 1$  for any state  $s^c = s_{(R_i, B_i)}$  with  $R_i \cap T \neq \emptyset$  by definition. Moreover,  $T \cap S^c = T \setminus R_{EC}$ , i.e. all target states which are not part of an EC in EC. Every state  $s^c \in \text{collapsed}(T)$  is of one of these two kinds. Hence,  $\Pr_{\mathcal{M}^c, \text{collapsed}(s)}^{\max}[\diamond(\{s_+\} \cup (T \cap S^c))] = \Pr_{\mathcal{M}^c, \text{collapsed}(s)}^{\max}[\diamond\text{collapsed}(T)]$ , proving the second equality.

For the first equality, we argue how to transform the witness strategies, achieving the same overall reachability probability. Thus, let  $\pi \in \Pi_{\mathcal{M}}^{MD}$  be a (memoryless deterministic) strategy in  $\mathcal{M}$  maximizing the probability of reaching T. We define a strategy  $\pi^c$  on  $\mathcal{M}^c$  simulating  $\pi$  as

follows. Note that  $\pi^c$  does not have to be memoryless or deterministic. For all states  $s^c \in S$ , i.e.  $s^c$  is not a collapsed representative,  $\pi^c$  mimics  $\pi$ , i.e.  $\pi^c(s) = \pi(s)$ . For the other case, namely  $s^c = s_{(R_i,B_i)}$  for some EC  $(R_i, B_i) \in$  EC, recall that  $\pi^c$  is allowed to have memory. In particular, it can remember the action a leading to  $s^c$ . Clearly, for any such action a and other action  $a' \in Av^c(s^c)$  we can compute the probability of a' action being the first action not in  $B_i$  under  $\pi$ . Then,  $\pi^c$  simply selects a' in  $s^c$  after a with this probability. Moreover, we also need to compute the probability of remaining inside  $R_i$  forever, which corresponds to the probability of  $\pi^c$  choosing rem<sub>i</sub>. It is easy to see that  $\pi^c$  achieves the same reachability as  $\pi$ .

If we instead start with a strategy in the collapsed MDP  $\pi^c \in \Pi_{\mathcal{M}^c}^{\mathsf{MD}}$ , we construct the respective strategy  $\pi$  on  $\mathcal{M}$  as follows. Again, on states  $s \notin R_{\mathsf{EC}}$ , we simply replicate the choice of  $\pi^c$ . On states  $s_{(R_i,B_i)}$  the strategy  $\pi^c$  chooses a single action  $a^c \in Av^c(s_{(R_i,B_i)})$ , since it is deterministic. If that action is rem<sub>i</sub>,  $\pi$  simply picks any internal  $a \in B_i$  in each state  $R_i$ . Otherwise, there exists a strategy  $\pi'$  on  $R_i$  reaching state state  $(a, \mathcal{M})$  with probability 1. Thus,  $\pi$  mimics  $\pi'$  until that state is reached and then plays  $a^c$ , again achieving the same reachability.

## 4.2 The General BRTDP Algorithm

Now, we present our modification of Algorithm 2, using the idea of collapsing, to obtain the general approach as shown in Algorithm 3. On top of the previously presented ideas, the algorithm maintains a growing set of ECs and repeatedly collapses the input MDP.

The new auxiliary procedure UPDATEECs is supposed to identify ECs in  $\mathcal{M}$ . As with SAMPLEPAIRS, we only require some properties instead of giving a concrete implementation. Essentially, UPDATEECs should only grow its list of ECs and eventually identify all ECs which are repeatedly visited by SAMPLEPAIRS.

Assumption 4. Let  $EC_1 \subseteq EC(\mathcal{M})$  be an initial set of state-disjoint ECs,  $EC_{e+1} = UPDATEECs(\mathcal{M}, EC_e)$ the identified ECs, and  $\mathcal{M}_e^c = collapse(\mathcal{M}, EC_e, \hat{s}, T)$  the corresponding collapsed MDPs. Then, for any episode e and EC  $(R, B) \in EC_e$ , (R, B) is an EC of  $\mathcal{M}$  and there exists  $(R', B') \in EC_{e+1}$  with  $R \subseteq R'$  and  $B \subseteq B'$ .

This is, for example, easily satisfied by searching for ECs in the set of visited states in every step. However, an efficient implementation may want to choose the times when it actually searches heuristically.

Since there are only finitely many states, this assumption implies that eventually  $EC_e$ and thus  $\mathcal{M}_e^c$  stabilizes, i.e. there exists some episode  $\overline{e}$  such that for all  $e \geq \overline{e}$  we have that  $EC_e = EC_{e+1}$  and thus  $\mathcal{M}_e^c = \mathcal{M}_{e+1}^c$ . We call  $\overline{e}$  the *EC-stable episode*.

**Assumption 5.** Let  $EC_e$  and  $\mathcal{M}_e^c$  as in Assumption 4 and assume that assumption holds. Further, let  $\varrho_e \in FPaths_{\mathcal{M}_e^c}$  be an infinite series of sets of state-action pairs in  $\mathcal{M}_e^c$  and define  $S_{\infty}^c =$ 

```
Input: MDP \mathcal{M}, state \hat{s}, target set T, precision \varepsilon, initial bounds
                           Up_1 and Lo_1, and initial set of ECs EC_1.
           Output: \varepsilon-optimal values (l, u), i.e., \mathcal{V}(\hat{s}) \in [l, u] and 0 \le u - l < \varepsilon.
           e \leftarrow 1, \mathcal{M}_1^c \leftarrow \text{collapse}(\mathcal{M}, \text{EC}_1, \hat{s}, T)
 1:
           Up_1(s_+, a_+) \leftarrow 1, Lo_1(s_+, a_+) \leftarrow 1, Up_1(s_-, a_-) \leftarrow 0, Lo_1(s_-, a_-) = 0
 2:
           while Up_{e}(\hat{s}) - Lo_{e}(\hat{s}) \geq \varepsilon do
 3:
                    forall (R_i, B_i) \in EC_e do
                                                                                         > Initialize bounds of representative states
 4:
                            forall a \in Av(s_{(R_j,B_j)}) \setminus \{\text{rem}_j\} do
                                                                                                  > Copy bounds for existing actions
 5:
                                     Up_e(s_{(R_i,B_i)}, a) \leftarrow Up_e(state(a, \mathcal{M}), a)
 6:
                                     Lo_e(s_{(R_i,B_i)}, a) \leftarrow Lo_e(state(a, \mathcal{M}), a)
 7:
                            if R_i \cap T = \emptyset then
                                                                                                        > Set bounds for remain action
 8:
                                     Up_e(s_{(R_i,B_i)}, rem_i) \leftarrow 0, \ Lo_e(s_{(R_i,B_i)}, rem_i) \leftarrow 0
 9:
                            else
10:
                                     Up_e(s_{(R_i,B_i)}, rem_j) \leftarrow 1, Lo_e(s_{(R_i,B_i)}, rem_j) \leftarrow 1
11:
                    Up_{e+1} \leftarrow Up_e, Lo_{e+1} \leftarrow Lo_e
12:
                    \rho \leftarrow \text{SamplePairs}(\mathcal{M}_{e}^{c}, \hat{s}, \text{Up}_{e}, \text{Lo}_{e}, \varepsilon)
13:
                                                                                                   > Sample a path in collapsed MDP
                    forall (s, a) \in \rho do
                                                                                              > Update the upper and lower bounds
14:
                            Up_{e+1}(s, a) \leftarrow \Delta(s, a) \langle Up_e \rangle
15:
                            Lo_{e+1}(s, a) \leftarrow \Delta(s, a) \langle Lo_e \rangle
16:
                    EC_{e+1} \leftarrow UpdateECs(\mathcal{M}, EC_e)
                                                                                                                   > Search for new ECs
17.
                    \mathcal{M}_{e+1}^{c} \leftarrow \text{collapse}(\mathcal{M}, \text{EC}_{e+1}, \hat{s}, T)
                                                                                                          > Update the collapsed MDP
18:
                    e \leftarrow e + 1
19:
           return (Lo_e(\hat{s}), Up_e(\hat{s}))
20:
```

Algorithm 3. The BRTDP learning algorithm for general MDPs.

 $\bigcap_{k=1}^{\infty} \bigcup_{e=k}^{\infty} \{s \in S_{e}^{c} \mid s \in \varrho_{e}^{c}\} \text{ the set of states occurring infinitely often.} {}^{9} \text{ Then, there exists no EC} \\ (R^{c}, B^{c}) \text{ in } \mathcal{M}_{\underline{a}}^{c} \text{ with } R^{c} \subseteq S_{\infty}^{c} \text{ except } R^{c} = \{s_{+}\} \text{ or } R^{c} = \{s_{-}\}.$ 

# 4.3 **Proof of Correctness**

We now continue to prove correctness and termination of Algorithm 3. First, we argue that the algorithm indeed is well-defined, i.e. it never accesses undefined values.

**LEMMA 4.12.** Algorithm 3 is well-defined.

<sup>9</sup> As mentioned above, due to Assumption 4 we get a EC-stable episode  $\overline{e}$  and thus have  $S^c_{\infty} \subseteq S^c_{\overline{e}}$ , i.e. the set of infinitely often seen states are all states of  $\mathcal{M}^c_{\overline{e}}$ .

**PROOF.** We only need to show that the states introduced by the collapsing in Lines 1 and 18 are assigned bounds before being accessed. By definition of the collapsed MDP, we add a state for each EC together with an additional action, and the special states  $\{s_+, s_-\}$ . The initial collapse in Line 1 adds the special states together with their corresponding actions. Their values are initialised in the following line. Furthermore, the EC collapsing in Lines 1 and 18 adds a state  $s_{(R,B)}$  for any EC  $(R, B) \in EC_e$  and a corresponding rem action. Their values are initialised in Lines 4 and 11 and not accessed prior to that.

As in Assumption 2, we again assume that the initial inputs are correct.

Assumption 6. The given initial bounds  $Up_1$  and  $Lo_1$  are correct, i.e.  $Lo_1(s, a) \leq \mathcal{V}(s, a) \leq Up_1(s, a)$  for all  $s \in S$ ,  $a \in Av(s)$ . Furthermore, the given initial set of ECs is correct, i.e.  $EC_1 \subseteq EC(\mathcal{M})$  and pairwise disjoint.

**LEMMA 4.13.** Assume that Assumption 6 holds. Then, during any execution of Algorithm 3 we have for every episode e, all states  $s \in S_e$  and action  $a \in Av_e^c(s)$  that

$$Lo_e(s, a) \le Lo_{e+1}(s, a) \le \mathcal{V}(s, a) \le Up_{e+1}(s, a) \le Up_e(s, a).$$

**PROOF.** We prove that the initialization of values for newly added states is correct. The remaining proof then is completely analogous to the proof of Lemma 3.2.

Since  $s_+$  is the target in  $\mathcal{M}^c$ , setting  $\text{Lo}_1(s_+, a_+) = 1$  is correct. Analogously, we see that  $s_-$  has no outgoing action and thus cannot reach  $s_+$ , justifying  $\text{Up}_1(s_-, a_-) = 0$ .

The correctness of updates for the collapsed states follows from Lemma 4.11.

**LEMMA 4.14.** The result of Algorithm 3 is correct under Assumption 6, i.e. (i)  $0 \le u - l < \varepsilon$ , and (ii)  $\mathcal{V}(\hat{s}) \in [l, u]$ .

**PROOF.** As in Lemma 3.3, the claims follows from the algorithm and Lemma 4.13.

Finally, we can prove termination of our presented algorithm. The proof is very similar to the proof of Lemma 3.4 and we only need to incorporate the new assumptions about UPDATEECS.

**LEMMA 4.15.** Algorithm 3 terminates under Assumptions 3 to 6. It terminates almost surely if Assumption 3 is satisfied almost surely.

**PROOF.** We apply the same reasoning as in Lemma 3.4 until Assumption 1 is applied in the final part of the proof. Since we do not necessarily explore all of  $\mathcal{M}$ ,  $\mathcal{M}_{e}^{c}$  may still contain MECs. In the proof, Assumption 1 is used only to show that  $S_{\text{Diff}} \subseteq S_{\infty}$  does not contain MECs. Observe that any non-terminating execution eventually reaches an EC-stable episode  $\overline{e}$ , thus the collapsed MDP considered by the algorithm does not change. Now,  $S_{\infty}$  in the previous proof exactly corresponds to  $S_{\infty}^{c}$  of Assumption 5, which yields that again there is no EC in  $S_{\infty}^{c}$ . Thus, we can continue to apply the previous proof's reasoning.

Again, we get the overall soundness as a direct consequence.

**THEOREM 4.16.** Assume that (almost surely) Assumption 3, as well as Assumptions 4 to 6 hold. Then Algorithm 3 is correct and converges (almost surely).

### 4.4 Relation to Interval Iteration

We briefly outline how our BRTDP algorithm presented in Algorithm 3 generalizes both the original BRTDP algorithm of [33] and the interval iteration algorithm of [73]. To this end, we give a brief overview of interval iteration. The algorithm first identifies all MECs and constructs a quotient similar to the one we presented in Section 4.1. Then, each state is initialised with straightforward upper and lower bounds. These bounds then are iterated globally according to the Bellman operator. We can emulate this behaviour by directly yielding the set of all MECs in UPDATEECs and returning  $S^c \times Av^c$  on each call to SAMPLEPAIRS. All variants of [33] can be obtained by choosing the appropriate path sampling heuristics for SAMPLEPAIRS.

# 5. Limited Information – MDP without End Components

We adapt our approach to the setting of limited information, where we can access the system only as a "black box" and we are given some bounds on the shape of the system (see Section 2.3). Intuitively, since we are interested in an  $\varepsilon$ -precise solution, we can repeatedly sample the system to learn the transition probabilities with high confidence. By adapting our previous ideas, we can enhance this approach to only learn "interesting" transitions. Since we can never bound the transition probabilities with absolute certainty, we aim for a *probably approximately correct* algorithm, which gives an  $\varepsilon$ -optimal solution with probability at least  $1 - \delta$ .

**Relevance and Applicability** Before we go into the details, we discuss the purpose and motivation for the subsequent algorithms. As mentioned in the introduction, our primary aim is to provide a *possibility result*, showing that it is possible to obtain PAC bounds on the *maximal* value on *infinite horizon* reachability values in a *black box* setting, only using samples of *finite length* and only starting in the *initial state*, and all this for *general MDP* (with ECs) *even in a model-free setting* (see below for a brief comment on model-free). Due to this focus, the bounds that the presented approaches obtain are rather impractical and of mostly theoretical value. This can be alleviated in several ways. For one, tighter statistical methods could be used, see [116] for a recent discussion (we use the naïve Hoeffding's inequality to simplify proofs). Additionally, our approach is generic in the sense that it assumes the worst of the system. Specific knowledge about the model, e.g. (in-)dependence of states, could be incorporated to significantly improve practical scalability. Yet, these points are orthogonal to our aim of proving the possibility of (model-free) PAC, for which we provide a complete proof in the following.
Moreover, an additional aim of this work is to provide a re-usable framework for proofs in this direction. We believe that several statements in the proofs below might be useful for other endeavours of this kind, especially the auxiliary statements in Appendix A.

**REMARK 5.1.** Intuitively, the idea of "model-free" is that such approaches do not try to learn the concrete transition probabilities or the entire graph structure, but more "compressed" quantities such as state- or action-values. Indeed, our algorithm only stores a fixed number of values per state-action pair, not for each transition. In most literature, model-free is only loosely defined, as it is difficult to formalize precisely [129]. In [129, Definition 1], the authors try to capture model-free by requiring that the space complexity of an approach should be  $o(|S|^2|Act|)$  (in other words, less than the explicit graph representation of the MDP). At the same time, the space complexity naturally also depends on parameters such as  $\varepsilon$  and  $\delta$  (e.g. suppose that  $\varepsilon$  were of exponential size w.r.t. the entire system). As such, we are interested in the above complexity for *fixed* parameters. The estimates our algorithm obtains are based on repeated updates to action values. Later, in Lemma 5.3, we show that (for fixed parameters) the number of executed updates is bounded by |Act|, and thus one can prove that the updates only involves numbers that are of size |Act|. In any case, proving that our approach formally satisfies (one of the many) definition of model-free is not our main goal, but rather observing that it captures the "spirit" of model-free by not learning probabilities but rather values directly.

For a model-based approach to this problem, we direct the reader to [10, 116]. These approaches essentially obtain bounds on every single transition probability in the system and then solve the induced *interval MDP* to obtain bounds on the value.

## 5.1 Definition of Limited Information

We define the limited information setting.

**DEFINITION 5.2.** Let  $\mathcal{M} = (S, Act, Av, \Delta)$  be some MDP,  $\hat{s} \in S$  a starting state, and  $T \subseteq S$  a target set. An algorithm has *limited information* if it can access

- the starting state  $\hat{s}$ ,
- a target oracle for T, i.e. given a state s it can query whether  $s \in T$ ,
- an upper bound *A* of the number of actions,  $A \ge |Act|$ ,
- a lower bound q on the transition probabilities under any uniform strategy,  $0 < q \le p_{\min} = \min\{|Av(s)|^{-1} \cdot \Delta(s, a, s') \mid s \in S, a \in Av(s), s' \in \operatorname{supp}(\Delta(s, a))\},\$
- an oracle for the set of available actions *Av*, and
- a successor oracle succ, which given a state-action pair yields a successor state, sampled according to the underlying, hidden probability distribution  $\Delta$ .

To tackle this problem, we combine the BRTDP approach with *delayed Q-learning* (DQL) [129]. In essence, DQL temporarily accumulates sampled values for each state-action pair and

only attempts an update after a certain delay, i.e. after enough samples have been gathered for a particular pair. Intuitively, with a large enough delay, the average of the sampled values is close to the true average with high confidence. Moreover, the attempted update is only successful if the value is changed by at least some margin. If instead the update fails, another update is only allowed if any other value in the system has changed significantly. This way, we can bound the total number of attempted updates and thus control the overall probability of any "wrong" update occurring. We explain all these ideas in more detail later on.

#### 5.2 The No-EC DQL Algorithm

First, we again restrict ourselves to the case of no end components, as these pose an additional difficulty. Thus, we assume the MDP  $\mathcal{M}$  satisfies Assumption 1 and instead of a target state oracle, the algorithm is explicitly given the special states  $s_+$  and  $s_-$ . We present our DQL-based approach in Algorithm 4. While it is similar in spirit to Algorithm 2, we give a concrete instantiation of SAMPLEPAIRS, since this setting needs a lot of additional guarantees.

The algorithm contains several auxiliary variables. Most are values kept for each stateaction pair, and separate for both the upper and lower bound. We give a brief intuition for each variable, where  $\circ \in \{Up, Lo\}$  and (s, a) is a state-action pair in  $\mathcal{M}$ :

- t: The number of steps the algorithm took so far, increased by 1 after each iteration of the main loop, as already mentioned in the preliminaries.
- $s_t, a_t, s'_t$ : The state, action, and the sampled successor state in step t, respectively.
- $Up_t(s, a)$  and  $Lo_t(s, a)$ : The (estimated) upper and lower bounds for the state-action pair (s, a) at step t. Note that in contrast to the previous algorithm, the upper and lower bounds are updated at each step instead of each episode.
- learn<sup>o</sup><sub>t</sub>(*s*, *a*): A three-valued flag (yes, once, or no) indicating whether the algorithm currently tries to learn and update the o-bounds for (*s*, *a*). The meaning of once is explained in the following. We additionally use the DECREASE function for convenience, which is defined by yes  $\mapsto$  once, once  $\mapsto$  no, and no  $\mapsto$  no.
- $\operatorname{count}_{t}^{\circ}(s, a)$ : The number of times a value for (s, a) was experienced. When  $\operatorname{count}_{t}^{\circ}(s, a)$  is large enough, we can attempt an update with sufficient confidence.
- $\operatorname{acc}_{t}^{\circ}(s, a)$ : The accumulated sampled values of the last  $\operatorname{count}_{t}^{\circ}(s, a)$  visits to (s, a). We want  $\operatorname{acc}_{t}^{\circ}(s, a)/\operatorname{count}_{t}^{\circ}(s, a)$  to approximate the true  $\circ$ -bound.

Moreover, the algorithm contains the two constants  $\overline{\epsilon}$  and  $\overline{m}$ . We define their value (and the value of another constant, used for readability) as follows.

$$\overline{\varepsilon} = \frac{\varepsilon}{2} \cdot \frac{p_{\min}^{|S|}}{3|S|} \qquad \overline{\xi} = 2|Act| \left(1 + \frac{|Act|}{\overline{\varepsilon}}\right) \qquad \overline{m} = \left\lceil \frac{1}{2\overline{\varepsilon}^2} \ln\left(\frac{8}{\overline{\delta}}\overline{\xi}\right) \right\rceil$$

We call  $\overline{\epsilon}$  the *update step* (the smallest update increment considered significant by the algorithm),  $\overline{\xi}$  the *update count* (the maximal possible number of update attempts, mainly introduced for

Inputs as given in Definition 5.2 satisfying Assumption 1, Input: special states  $s_+, s_-$ , precision  $\varepsilon$ , and confidence  $\delta$ . **Output:** Values (l, u) which are  $\varepsilon$ -optimal, i.e.,  $\mathcal{V}(\hat{s}) \in [l, u]$  and  $0 \le u - l < \varepsilon$ , with probability at least  $1 - \delta$ .  $Up_1(\cdot, \cdot) \leftarrow 1$ ,  $Lo_1(\cdot, \cdot) \leftarrow 0$ ,  $Up_1(s_-, \cdot) \leftarrow 0$ ,  $Lo_1(s_+, \cdot) \leftarrow 1$ 1: for  $\circ \in \{Up, Lo\}$  do 2: learn<sup>°</sup><sub>1</sub> $(\cdot, \cdot) \leftarrow$  yes, acc<sup>°</sup><sub>1</sub> $(\cdot, \cdot) \leftarrow 0$ , count<sup>°</sup><sub>1</sub> $(\cdot, \cdot) \leftarrow 0$ 3:  $e \leftarrow 1, t \leftarrow 1$ 4: while  $Up_t(\hat{s}) - Lo_t(\hat{s}) \ge \varepsilon$  do 5: for  $s \in S$  do  $MaxA_e(s) \leftarrow arg max_{a \in Av(s)} Up_t(s, a)$ 6:  $s_t \leftarrow \hat{s}$ 7: while  $s_t \notin \{s_+, s_-\}$  do > Experience the current learning episode 8:  $a_t \leftarrow \text{sampled uniformly from } MaxA_e(s_t)$ 9: > Pick an action  $s'_t \leftarrow \text{succ}(s_t, a_t)$ > Query successor oracle 10: > Update bound estimates for  $\circ \in \{Up, Lo\}$  do 11: **if** learn<sup>o</sup><sub>t</sub>( $s_t, a_t$ )  $\neq$  no **then** 12:  $\operatorname{count}_{t+1}^{\circ}(s_t, a_t) \leftarrow \operatorname{count}_t^{\circ}(s_t, a_t) + 1$ 13:  $\operatorname{acc}_{t+1}^{\circ}(s_t, a_t) \leftarrow \operatorname{acc}_t^{\circ}(s_t, a_t) + \bigcirc_t(s'_t)$ 14: > Learn upper bounds if  $count_{t+1}^{Up}(s_t, a_t) = \overline{m}$  then > Attempt update of Up 15: if  $\operatorname{acc}_{t+1}^{Up}(s_t, a_t)/\overline{m} < Up_t(s_t, a_t) - 2\overline{\epsilon}$  then 16:  $Up_{t+1}(s_t, a_t) \leftarrow acc_{t+1}^{Up}(s_t, a_t) / \overline{m} + \overline{\varepsilon}$ > Successful update 17:  $learn_{t+1}^{Up}(\cdot, \cdot) \leftarrow yes$ > Re-enable learning for all actions 18: else 19: 
$$\begin{split} & \text{learn}_{t+1}^{\text{Up}}(s_t, a_t) \leftarrow \text{Decrease}(\text{learn}_t^{\text{Up}}(s_t, a_t)) \\ & \text{count}_{t+1}^{\text{Up}}(s_t, a_t) \leftarrow 0, \text{ acc}_{t+1}^{\text{Up}}(s_t, a_t) \leftarrow 0 \end{split}$$
> Failed update 20: 21: > Learn lower bounds if  $count_{t+1}^{Lo}(s_t, a_t) = \overline{m}$  then 22: > Attempt update of Lo if  $\operatorname{acc}_{t+1}^{\operatorname{Lo}}(s_t, a_t)/\overline{m} > \operatorname{Lo}_t(s_t, a_t) + 2\overline{\epsilon}$  then 23:  $Lo_{t+1}(s_t, a_t) \leftarrow acc_{t+1}^{Lo}(s_t, a_t)/\overline{m} - \overline{\epsilon}$ > Successful update 24:  $learn_{t+1}^{Lo}(\cdot, \cdot) \leftarrow yes$ > Re-enable learning for all actions 25: else 26:  $learn_{t+1}^{Lo}(s_t, a_t) \leftarrow Decrease(learn_t^{Lo}(s_t, a_t))$ > Failed update 27:  $\operatorname{count}_{t+1}^{\operatorname{Lo}}(s_t, a_t) \leftarrow 0$ ,  $\operatorname{acc}_{t+1}^{\operatorname{Lo}}(s_t, a_t) \leftarrow 0$ 28:  $s_{t+1} \leftarrow s'_t$ ,  $t \leftarrow t+1$ > Increase step counter 29:  $e \leftarrow e + 1$ 30: > Increase episode counter **return** (Lo<sub>t</sub>( $\hat{s}$ ), Up<sub>t</sub>( $\hat{s}$ )) 31:

Algorithm 4. The DQL learning algorithm for MDPs without ECs.



Figure 5. Example MDP to explain the choices and interpretations of some constants.

readability), and  $\overline{m}$  the *update delay* (the number of samples we want to obtain for a state-action pair before we attempt an update). These three constants are used throughout this and the following section. Note that bounds on these constants can be obtained from Definition 5.2 (recalling that |Act| is an upper bound on |S|). Within the proofs, an even smaller value for  $\overline{\varepsilon}$  or an even larger value for  $\overline{m}$  are also sufficient. We define the constants with "tight" values to aid readability and intuition.

These constants are closely related to the worst-case *mixing rate* (see e.g. [111, Chapter 5] for a detailed discussion) of the MDP, which intuitively indicates how fast information "propagates" through the system. For Markov chains, this is given by the difference between first and second eigenvalue of the transition matrix, which is also called *spectral gap*. This gap can be (quite conservatively) bounded by  $p_{\min}^{|S|}$ . This also gives a bound on the convergence rate of the *power iteration*, which in the context of Markov chains and MDP is closely related to value iteration. (See, for example, [118, Theorem 8.5.2], noting that  $p_{\min}^{|S|}$  is a lower bound for  $\eta$  with J = |S|.)

The concept of information propagation (and the tightness of the  $p_{\min}^{|S|}$  bound) is illustrated in Figure 5. In order to propagate any information about state  $s_n$  to the initial state  $\hat{s}$ , we need |S|steps. Moreover, after this many steps only a fraction  $p_{\min}^{|S|}$  of the information is propagated, so, intuitively, to "observe" a difference of  $\varepsilon$ , we need to perform  $\approx |S|p_{\min}^{-|S|}/\varepsilon$  steps. Thus, we need to visit a state-action pair often enough, i.e.  $\overline{m}$  times, before an update to ensure that relevant information has propagated already with high confidence. Dually, if a state-action pair was visited often enough and new information does not differ from the previous information by more than  $\overline{\varepsilon}$ , there likely is no new information to be propagated and we may assume that the values of this state-action pair have converged.

Inside the main loop, the algorithm repeats two steps to obtain a path. First, an action maximizing the upper bounds (at the beginning of the episode) is randomly picked. More precisely, we again consider the set  $MaxA_e(s) \coloneqq arg max_{a \in Av(s)} Up_{t_e}(s, a)$  and uniformly select an action thereof. To obtain the successor, we query the successor oracle with the given action to obtain the successor s'. In other words, in episode e the algorithm samples a path in the MDP using a memoryless strategy randomizing uniformly over  $MaxA_e(s)$  in each state. We call this strategy the sampling strategy  $\pi_e(s, a) \coloneqq |MaxA_e(s)|^{-1}$  if  $a \in MaxA_e(s)$  and 0 otherwise. We will later on introduce the upper bound maximizing strategy  $\pi_t$ , which selects among Up-optimal actions at the current step t. Note that if the algorithm follows this strategy  $\pi_t$  while sampling,

the samples would not be obtained from a memoryless strategy in general, since an update might happen while sampling and thus change the strategy. One might be tempted to solve this issue by first sampling a path until  $s_+$  or  $s_-$  is reached and then propagating the values. However this path might be of exponential size w.r.t. the number of states; this already occurs for the structurally simple example in Figure 5.

After sampling a tuple (s, a, s'), the algorithm learns from this "experience". It does so by learning upper and lower bounds separately, depending on the respective learn flags, which are explained later. In case one of the bounds should be learned (learn<sup>o</sup><sub>t</sub>(s, a)  $\neq$  no), the accumulator is updated with the newly observed values, i.e. the respective bound of the successor s'. Furthermore, if the algorithm has gathered enough information, i.e. this pair has been experienced  $\overline{m}$  times, an update of (s, a)'s estimate is attempted (if the respective learn is yes or once). By choosing  $\overline{m}$  large enough, the information we gathered about the bounds of (s, a) very likely is a faithful approximation of the true expected value over its successors. If the newly learned estimate, i.e. the average over the last  $\overline{m}$  experiences of (s, a), significantly differs from the current estimate stored in Up or Lo, the current estimates are updated conservatively. If instead this new estimate is close to the current estimate, the algorithm marks this state-action pair as (potentially) converged by "decreasing" its learn flag, as specified by DECREASE.

The learned bounds of a pair depend on the bounds of other state-action pairs. In particular, whenever any bound is changed, we may need to re-learn the values for all other state-action pairs. This is taken care of by globally resetting the learn flags to yes in Lines 18 and 25. We highlight that this is one of the main differences to [10], where samples are instead used to learn bounds on the transition probabilities while the actual values are propagated according to these estimates, trading memory for speed of convergence.

The need for the intermediate value once of learn arises from the asynchronicity of the updates. Suppose an update of some pair (s, a) succeeds and we reset all learn values to yes. However, for some other state-action pair (s', a') we are very close to an update, too. Then, the values which will be used for an attempted update of (s', a') were mostly learned before the update of (s, a). Now, if for example s is a successor of (s', a'), the values of (s', a') may be influenced significantly by the update of (s, a). Hence, we need to learn the value of (s', a') once more in order to be on the safe side. A different solution approach would be to simply reset all count and acc values after every successful update, however this would be much less efficient: If we again consider the above example, it might be the case that the values we gathered for (s', a') before the update of (s, a) already are sufficient for a successful update, discarding them would slow down convergence drastically.

In the algorithms of [129, 33], this problem instead is taken care of by remembering the last globally successful update. There, learn(s, a) is only set to no if the previous attempted update of (s, a) happened after the last successful update. This similarly implies that all values which

are considered in the current update attempt are "up to date". We decided for this alternative approach since we have to track less variables.

## 5.3 **Proof of Correctness**

We now prove that Algorithm 4 is probably approximately correct. We first prove correctness of the result by showing that the computed bounds are faithful upper and lower bounds in Lemma 5.6. However, we cannot guarantee that this is always the case due to statistical outliers. Thus we first obtain bounds on the probability of these outliers. Then, in order to prove termination with high probability, we argue that by our choice of constants the propagation of values is probably correct. This means that whenever we update the bounds of a state-action pair (*s*, *a*), the updated value is close to the true average under  $\Delta(s, a)$ . Finally, we show that with high probability an update will occur as long as the bounds are not  $\varepsilon$ -close.

**LEMMA 5.3.** The number of successful updates of Up and Lo is bounded by  $\frac{|Act|}{\overline{\epsilon}}$  each.

**PROOF.** Let  $a \in Act$  be some action and  $s = \text{state}(a, \mathcal{M})$  the associated state. The upper bound of (s, a) is initialised to 1 or 0, similar for the lower bound. Whenever  $Up_t(s, a)$  is updated in Line 17, its value is decreased by at least  $\overline{\epsilon}$ : We have that  $\operatorname{acc}_t^{Up}(s, a)/m < Up_t(s, a) - 2\overline{\epsilon}$ , hence  $\operatorname{acc}_t^{Up}(s, a)/m + \overline{\epsilon} < Up_t(s, a) - \overline{\epsilon}$ . Thus,  $Up_{t+1}(s, a) < Up_t(s, a) - \overline{\epsilon}$ . Analogously,  $\operatorname{Lo}_t(s, a)$  is always increased by at least  $\overline{\epsilon}$  whenever updated.

Moreover,  $\operatorname{acc}_{t}^{\operatorname{Up}}(s, a) \geq 0$  and  $\operatorname{acc}_{t}^{\operatorname{Lo}}(s, a) \leq \overline{m}$  by initialization and update of these values, hence we never set  $\operatorname{Up}_{t}(s, a)$  to a negative value and  $\operatorname{Lo}_{t}(s, a)$  is always smaller or equal to 1. Consequently, we change the value of  $\operatorname{Up}_{t}(s, a)$  and  $\operatorname{Lo}_{t}(s, a)$  at most  $\frac{1}{\overline{\varepsilon}}$  times and there are at most  $\frac{|Act|}{\overline{\varepsilon}}$  successful updates to the upper and lower bounds, respectively. Note that we do not necessarily have  $\operatorname{Up}_{t}(s, a) \leq \operatorname{Lo}_{t}(s, a)$  for all executions of the algorithm, hence there are at most  $\frac{|Act|}{\overline{\varepsilon}}$  updates for each of the bounds individually.

Observe that this implies that for every execution, eventually there will be no more successful updates of Up and the sampling strategy  $\pi_e$  does not change. This fact will be used in some of the subsequent proofs. Moreover, we can use the above result to show that similarly, the number of *attempted* updates is bounded.

**LEMMA 5.4.** The number of attempted updates of the upper bounds Up and lower bounds Lo is bounded by  $\overline{\xi} = 2|Act|(1 + \frac{|Act|}{\overline{s}})$ , respectively.

**PROOF.** Let  $(s, a) \in S \times Av$  be a state-action pair. Suppose an update of  $Up_t(s, a)$  is attempted at step t, i.e.  $a_t = a$ ,  $count_t(s, a) = \overline{m} - 1$ , and  $learn_t^{Up}(s, a) \neq no$ . Then, either the update is successful or  $learn_{t+1}^{Up}(s, a)$  is updated with DECREASE. The learn flag is only set to yes again if some other upper bound is successfully updated. Analogous reasoning applies to updates of the lower bounds.

By Lemma 5.3, there are at most  $\frac{|Act|}{\overline{\epsilon}}$  successful updates to either bounds in total. If an update of a particular state-action pair is attempted, it either succeeds or fails. In the latter case, at most one more update of this state-action pair will be attempted until an other update succeeds. Hence, for a particular state-action pair (*s*, *a*) we have in the worst case two attempted Up-updates after every successful Up-update (of *any* pair). Together, there are at most  $2 + 2\frac{|Act|}{\overline{\epsilon}}$  (two more attempts can occur after the last successful update). Since there are |Act| state-action pairs in total, the statement follows.

Assumption 7. Suppose an Up-update of the state-action pair (s, a) is attempted at step t. Let  $k_1 < k_2 < \ldots < k_{\overline{m}} = t$  be the steps of the  $\overline{m}$  most recent visits to (s, a). Then  $\frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \mathcal{V}(s'_{k_i}) \geq \mathcal{V}(s, a) - \overline{\epsilon}$ . Analogously, for an attempted Lo-update, we have  $\frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \mathcal{V}(s'_{k_i}) \leq \mathcal{V}(s, a) + \overline{\epsilon}$ .

**LEMMA 5.5.** The probability that Assumption 7 is violated during the execution of Algorithm 4 is bounded by  $\frac{\delta}{4}$ .

**PROOF.** We show that the claim for the upper bound is violated with probability at most  $\frac{\delta}{8}$ . The lower bound part follows analogously and the overall claim via union bound.

Let (s, a) and  $k_i$  as in Assumption 7, i.e. an Up-update of (s, a) is attempted at step  $k_m =$ t. First, observe that due to the Markov property, the successor state under (s, a) does not depend on the algorithm's execution. Hence, the states  $s'_{k_i}$ , i.e. the successor states after each visit of (s, a), are distributed i.i.d. according to the underlying probability distribution  $\Delta(s, a)$ . Define  $Y_i = \mathcal{V}(s'_{k_i})$ . Clearly,  $Y_i$  are i.i.d., since the actual value of a state  $\mathcal{V}(s)$  is independent of the algorithm's execution. Moreover,  $\mathbb{E}[Y_i] = \mathcal{V}(s, a)$ , since  $\mathcal{V}$  satisfies the fixed point conditions  $\mathcal{V}(s, a) = \Delta(s, a) \langle \mathcal{V} \rangle$ . Define the empirical average  $\underline{Y} = \frac{1}{m} \sum_{i=1}^{\overline{m}} Y_i$ . Observe that  $\mathbb{E}[\underline{Y}] = \frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \mathbb{E}[Y_i] = \mathcal{V}(s, a)$ . By the Hoeffding bound [85] we have that

$$\mathbb{P}_{\mathsf{A}}\left[\mathbb{E}\left[\underline{Y}\right] - \underline{Y} > \overline{\varepsilon}\right] \le e^{-2\overline{m\varepsilon}^2} = \frac{\delta}{8} \cdot \overline{\xi}^{-1}$$

By reordering, we obtain that  $\mathbb{P}_{A}[\mathcal{V}(s, a) - \overline{\varepsilon} > \frac{1}{m} \sum_{i=1}^{m} \mathcal{V}(s_{i})] \leq \frac{\delta}{8} \cdot \overline{\xi}^{-1}$  [Fact I]. To conclude the proof, we extend the above argument to all steps  $k_{1}$  satisfying the preconditions of the assumption. By Lemma 5.4, the number of attempted updates to Up and Lo is bounded by  $\overline{\xi}$ , respectively [Fact II]. Consequently, by employing the union bound, we see that

$$\mathbb{P}_{\mathsf{A}}\left[ \underbrace{}^{"}\frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \mathcal{V}(s_{k_{i}}) < \mathcal{V}(s, a) - \overline{\varepsilon} \text{ for some } k_{1} \right]$$

$$\leq \mathbb{P}_{\mathsf{A}}\left[ \bigcup_{k_{1}} \underbrace{}^{"}\frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \mathcal{V}(s_{k_{i}}) < \mathcal{V}(s, a) - \overline{\varepsilon} \text{ for } k_{1} \right]$$

$$\stackrel{[\mathsf{I}]}{\leq} \sum_{k_{1}} \underbrace{\frac{\delta}{8}}_{k_{1}} \cdot \overline{\xi}^{-1} \stackrel{[\mathsf{II}]}{\leq} \frac{\delta}{8}.$$

**LEMMA 5.6.** Assume that Assumption 7 holds. Then, during any execution of Algorithm 4 we have for every step t, all states  $s \in S_e$  and action  $a \in Av_e(s)$  that

$$\mathsf{Lo}_{\mathsf{t}}(s,a) \le \mathsf{Lo}_{\mathsf{t}+1}(s,a) \le \mathcal{V}(s,a) \le \mathsf{Up}_{\mathsf{t}+1}(s,a) \le \mathsf{Up}_{\mathsf{t}}(s,a).$$

**PROOF.** First, by definition of the algorithm we clearly have that Up can only decrease and Lo can only increase. It remains to show that  $Lo_t(s, a) \leq \mathcal{V}(s, a) \leq Up_t(s, a)$ . We proceed by induction on the step t. For t = 0, the statement clearly holds, since  $Up_1(s, a) = 1$  for all states except the special state  $s_-$ , which by assumption cannot reach the target  $s_+$ . Analogously, the statement holds for  $Lo_1(s, a)$ . Now, fix an arbitrary step t. We have that  $Up_{t'}(s, a) \geq \mathcal{V}(s, a)$  for all steps t'  $\leq$  t (IH). Assume that (s, a) is the state-action pair sampled at step t. If no successful update takes place there is nothing to prove, since the values of Up and Lo do not change. Otherwise, Assumption 7 is applicable and we get

$$\mathsf{Up}_{\mathsf{t+1}}(s,a) = \frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \mathsf{Up}_{k_i}(s_{k_i}) + \overline{\varepsilon} \stackrel{[\mathrm{IH}]}{\geq} \frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \mathscr{V}(s_{k_i}) + \overline{\varepsilon} \geq \mathscr{V}(s,a).$$

Analogously, we have  $Lo_{t+1}(s, a) \leq \mathcal{V}(s, a)$ .

This gives us correctness of the returned result with high confidence upon termination. It remains to show that the algorithm also terminates with high probability.

To this end, we introduce the upper bound maximizing strategy  $\pi_t$  which selects in each state *s* uniformly among all actions maximal with respect to the *current* upper bounds, i.e.  $Up_t(s, \cdot)$ . This allows us to reason about the current value at step t. Note that this strategy differs from the sampling strategy  $\pi_e$ , since  $\pi_t$  might change during an episode. However, once there are no updates to upper bounds, we have that  $\pi_e = \pi_t$ . We use this fact in the final convergence proof. Once the two strategies align, we can transfer properties proven with respect to  $\pi_t$  to the actual sampling behaviour of the algorithm.

Using this strategy, we define the set of converged state-action pairs.

**DEFINITION 5.7.** For every step t, define  $\mathcal{K}_t^{Up}$ ,  $\mathcal{K}_t^{Lo} \subseteq S \times Av$  by

$$\mathcal{K}_{t}^{\mathsf{Up}} \coloneqq \{(s, a) \mid \mathsf{Up}_{t}(s, a) - \Delta(s, a) \langle \pi_{t}[\mathsf{Up}_{t}] \rangle \leq 3\overline{\varepsilon} \} \text{ and}$$
$$\mathcal{K}_{t}^{\mathsf{Lo}} \coloneqq \{(s, a) \mid \Delta(s, a) \langle \pi_{t}[\mathsf{Lo}_{t}] \rangle - \mathsf{Lo}_{t}(s, a) \leq 3\overline{\varepsilon} \},$$

i.e. all state-action pairs whose Up- or Lo-value is close to the respective value of its successors under  $\pi_t$ . If  $(s, a) \in \mathcal{K}_t^{Up}$ , we say that (s, a) is Up-converged at step t, analogously  $(s, a) \in \mathcal{K}_t^{Lo}$  is called Lo-converged at step t.

The approach for the convergence proof is to show that (with high probability) (i) if an update of some bound fails, the current bound is consistent with its successors, i.e. the respective pair is converged, and (ii) we visit non-converged pairs only finitely often. Finally, we combine these two facts non-trivially to prove convergence.

**LEMMA 5.8.** We have for every step t and state s that

$$\pi_{t}[\mathsf{Up}_{t}](s) = \mathsf{Up}_{t}(s) \quad and \quad \pi_{t}[\mathsf{Lo}_{t}](s) \le \mathsf{Lo}_{t}(s).$$

Moreover, if  $(s, a) \notin \mathcal{K}_t^{Up}$ , then  $(s, a) \notin \mathcal{K}_{t'}^{Up}$  for all t' > t until an Up-update of (s, a) succeeds. If no more updates of upper bounds take place, the analogous statement holds for lower bounds, too.

**PROOF.** Since the strategy  $\pi_t$  maximizes the upper bound we have

$$\pi_{\mathsf{t}}[\mathsf{Up}_{\mathsf{t}}](s) = \sum_{a \in A\nu(s)} \pi_{\mathsf{t}}(s, a) \cdot \mathsf{Up}_{\mathsf{t}}(s, a) = \max_{a \in A\nu(s)} \mathsf{Up}_{\mathsf{t}}(s, a) = \mathsf{Up}_{\mathsf{t}}(s).$$

We also trivially have that  $\pi_t[Lo_t](s) \leq Lo_t(s)$ , as  $Lo_t(s)$  is the maximum over all actions.

For the second claim, recall that Up-values can only decrease. If  $(s, a) \notin \mathcal{K}_t^{Up}$ , we have  $Up_t(s, a) > 3\overline{\varepsilon} + \Delta(s, a)\langle \pi_t[Up_t] \rangle = 3\overline{\varepsilon} + \Delta(s, a)\langle Up_t \rangle$ . Since (i)  $Up_t(s, a) = Up_{t+1}(s, a)$  unless a successful Up-update of (s, a) occurs and (ii)  $Up_t(s) \ge Up_{t+1}(s)$  for all states *s*, we obtain the claim. The lower bound statement is proven analogously, noting that once upper bounds remain fixed the only way to change  $\mathcal{K}_t^{Lo}$  is a successful update of some lower bound.

**Assumption 8.** Suppose an update of the upper bound (lower bound) of the state-action pair (s, a) is attempted at step t. Let  $k_1 < k_2 < ... < k_{\overline{m}} = t$  be the steps of the  $\overline{m}$  most recent visits to (s, a). If (s, a) is not Up-converged (Lo-converged) at step  $k_1$ , the update at step t is successful.

Intuitively, this assumption says that whenever the bound for a state-action pair is significantly different from its successors and we visit that pair often enough, we obtain a significantly better estimate. We cannot guarantee this surely due to outliers, but we bound the probability of this assumption being violated using our choice of the delay  $\overline{m}$ .

**LEMMA 5.9.** The probability that Assumption 8 is violated during the execution of Algorithm 4 is bounded by  $\frac{\delta}{4}$ .

**PROOF.** As in Lemma 5.5, we prove that an attempted update of the upper bounds fails with probability at most  $\frac{\delta}{8}$ . The same bound then can be obtained for the lower bound variant with a mostly analogous proof. The overall result again follows using the union bound.

Let (s, a) and  $k_i$  as in Assumption 8, i.e.  $(s, a) \notin \mathcal{K}_{k_1}^{\cup p}$  and an update of the upper bound is attempted at step t **[Fact I]**. Define  $X_i = \pi_{k_1}[\bigcup p_{k_1}](s'_{k_i})$ . Note that all  $X_i$  are defined using  $\bigcup p_{k_1}$ and  $\pi_{k_1}$  (instead of  $\bigcup p_{k_i}$  and  $\pi_{k_i}$ ). Consequently, the  $X_i$  are i.i.d. and we can apply the Hoeffding bound to the empirical average  $\underline{X} = \frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} X_i$ . This yields that

$$\mathbb{P}_{\mathsf{A}}[\underline{X} - \mathbb{E}[\underline{X}] \geq \overline{\varepsilon}] \leq e^{-2\overline{m\varepsilon}^2} = \frac{\delta}{8} \cdot \overline{\xi}^{-1}.$$

Since the  $X_i$  are i.i.d., we have that  $\mathbb{E}[\underline{X}] = \mathbb{E}[X_i]$  for all  $1 \le i \le \overline{m}$ , in particular  $\mathbb{E}[\underline{X}] = \mathbb{E}[X_1]$ . Thus, the probability that  $\underline{X} - \mathbb{E}[X_1] \ge \overline{\varepsilon}$  is at most  $\frac{\delta}{8} \cdot \overline{\xi}^{-1}$  [Fact II]. For the lower bound proof, we analogously define  $X_i = \pi_{k_1}[\operatorname{Lo}_{k_1}](s'_{k_i})$  and prove that  $\mathbb{E}[X_1] - \underline{X} \ge \overline{\varepsilon}$  with the same probability. Now, we show that if  $\underline{X} - \mathbb{E}[X_1] < \overline{\varepsilon}$  the update at step t will be successful [Fact III]. Recall that an update is successful when the  $\overline{m}$  most recent samples significantly differ from the currently stored value, i.e. when the currently stored value  $Up_t(s, a)$  is significantly larger than the newly learned value. We have that (reasoning below)

$$Up_{t}(s, a) - \frac{1}{m} \sum_{i=1}^{\overline{m}} Up_{k_{i}}(s_{k_{i}}') \ge Up_{t}(s, a) - \frac{1}{m} \sum_{i=1}^{\overline{m}} Up_{k_{1}}(s_{k_{i}}')$$
(2)

$$= \mathsf{Up}_{\mathsf{t}}(s, a) - \frac{1}{m} \sum_{i=1}^{\overline{m}} \pi_{k_1} [\mathsf{Up}_{k_1}](s'_{k_i}) \tag{3}$$

$$> Up_t(s, a) - \mathbb{E}[X_1] - \overline{\varepsilon}$$
 (4)

$$= \mathsf{Up}_{k_1}(s, a) - \mathbb{E}[X_1] - \overline{\varepsilon}$$
(5)

$$= \mathsf{Up}_{k_1}(s, a) - \Delta(s, a) \langle \pi_{k_1}[\mathsf{Up}_{k_1}] \rangle - \overline{\varepsilon}$$
(6)

$$> 2\overline{\varepsilon}.$$
 (7)

Inequality (2) follows from the fact that Up-values can only decrease over time by definition of the algorithm. Equality (3) follows directly from Lemma 5.8. Inequality (4) follows from the above derivation. Equality (5) follows from the fact that  $Up_{k_i}(s, a) = Up_{k_1}(s, a)$  for all  $1 \le i \le \overline{m}$ : Since an update is attempted at step  $k_{\overline{m}} = t$ , there can be no update attempts in the previous  $\overline{m} - 1$  visits, consequently the value of  $Up_{k_i}(s, a)$  does not change between  $k_1$  and  $k_{\overline{m}}$ . Equality (6) follows directly from the definition of  $X_1$ . Finally, Inequality (7) follows from [I], i.e. that (s, a) is not Up-converged at step  $k_1$ , formally  $Up_{k_1}(s, a) - \Delta(s, a)\langle \pi_{k_1}[Up_{k_1}]\rangle > 3\overline{\epsilon}$ .

For the lower bound, we prove a similar result:

$$\begin{split} \frac{1}{m} \sum_{i=1}^{\overline{m}} \operatorname{Lo}_{k_i}(s'_{k_i}) - \operatorname{Lo}_{t}(s, a) &\geq \frac{1}{m} \sum_{i=1}^{\overline{m}} \operatorname{Lo}_{k_1}(s'_{k_i}) - \operatorname{Lo}_{t}(s, a) \\ &\geq \frac{1}{m} \sum_{i=1}^{\overline{m}} \pi_{k_1} [\operatorname{Lo}_{k_1}](s'_{k_i}) - \operatorname{Lo}_{t}(s, a) \\ &> \mathbb{E}[X_1] - \overline{\varepsilon} - \operatorname{Lo}_{t}(s, a) \\ &= \mathbb{E}[X_1] - \overline{\varepsilon} - \operatorname{Lo}_{k_1}(s, a) \\ &= \Delta(s, a) \langle \pi_{k_1}[\operatorname{Lo}_{k_1}] \rangle - \overline{\varepsilon} - \operatorname{Lo}_{k_1}(s, a) \\ &> 2\overline{\varepsilon}. \end{split}$$

The only major difference lies in the second inequality (corresponding to Equality (3)), where we instead use the fact that  $\pi_t[Lo_t](s) \le Lo_t(s)$ .

Finally, we again extend the argument to all steps  $k_1$  similar to Lemma 5.5, i.e. that by Lemma 5.4 the number of attempted updates is bounded by  $\overline{\xi}$  [Fact IV]. Together with the union bound, we thus obtain

 $\mathbb{P}_{A} ["Assumption 8 is violated for Up"]$   $= \mathbb{P}_{A} \left[ \bigcup_{k_{1}} "k_{1} \text{ satisfies condition [I], but the Up-update fails"} \right]$   $\leq \sum_{k_{1}} \mathbb{P}_{A} ["k_{1} \text{ satisfies condition [I], but the Up-update fails"}]$ 

$$\stackrel{[\operatorname{III}]}{\leq} \sum_{k_1} \mathbb{P}_{\mathsf{A}} \left[ \underbrace{\overset{``}{\underline{X}}}_{k_1} - \mathbb{E}[X_1] \ge \overline{\varepsilon} \text{ for } k_1 \underbrace{\overset{``}{\underline{z}}}_{k_1} \right]$$

$$\stackrel{[\operatorname{III}]}{\leq} \sum_{k_1} \underbrace{\overset{\delta}{\underline{\delta}}}_{k_1} \cdot \overline{\xi}^{-1} \stackrel{[\operatorname{IV}]}{\leq} \frac{\delta}{\underline{\delta}}.$$

**LEMMA 5.10.** Assume that Assumption 8 holds. If an attempted Up-update of (s, a) at step t fails and  $learn_{t+1}^{Up}(s, a) = no$ , then  $(s, a) \in \mathcal{K}_{t+1}^{Up}$ . If no more updates of upper bounds take place, the analogous statement holds for the lower bounds, too.

**PROOF.** We prove the statement for the upper bound, with the corresponding lower bound statement following analogously. Assume an unsuccessful Up-update of (s, a) occurs at step t and let  $k_1 < k_2 < \ldots < k_{\overline{m}} = t$  be the  $\overline{m}$  most recent visits to (s, a). We consider three cases:

- 1. If  $(s, a) \notin \mathcal{K}_{k_1}^{Up}$ , then by Assumption 8 the Up-update of (s, a) at step t will be successful and there is nothing to prove.
- 2. We have  $(s, a) \in \mathcal{K}_{k_1}^{\cup p}$  and there exists  $i \in \{2, ..., \overline{m}\}$  such that (s, a) is not Up-converged at step  $k_i$ . It follows that there must have been a successful update of some Up-value between steps  $k_1$  and  $k_{\overline{m}}$ , say step t'. By Line 18,  $\text{learn}_{t'+1}^{\cup p}(s, a)$  is set to yes and there is nothing to prove.
- 3. For the last case, we have that for all  $i \in \{1, ..., \overline{m}\}$  that (s, a) is Up-converged at step  $k_i$ , particularly  $(s, a) \in \mathcal{K}_{k_{\overline{m}}}^{Up} = \mathcal{K}_{t}^{Up}$ . As the attempt to update the Up-value of (s, a) at step t was unsuccessful, we have that  $\mathcal{K}_{t}^{Up} = \mathcal{K}_{t+1}^{Up}$ .

For the lower bound statement, observe that  $\mathcal{K}_t^{Lo}$  may be changed by a successful update of  $Up_t$ . Hence, the above reasoning can only be followed once upper bounds do not change.

**LEMMA 5.11.** Assume that Assumption 8 holds. Then, there are at most  $2\overline{m} \cdot \frac{|Act|}{\overline{\epsilon}}$  visits to state-action pairs which are not Up-converged. Moreover, once the upper bounds are not updated any more, there are at most  $2\overline{m} \cdot \frac{|Act|}{\overline{\epsilon}}$  visits to state-action pairs which are not Lo-converged.

**PROOF.** We show that whenever a state-action pair (s, a) is not Up-converged at step t, then in at most  $2\overline{m}$  more visits to (s, a) a successful Up-update will occur. Assume that (s, a) is visited at step t and it is not Up-converged, i.e.  $(s, a) \notin \mathcal{K}_t^{Up}$ . We distinguish two cases.

- 1.  $\operatorname{learn}_{t}^{\operatorname{Up}}(s, a) = \operatorname{no:}$  This implies that the last attempted Up-update of (s, a) was not successful. Let t' be the step of this attempt, t' < t. We have  $\operatorname{learn}_{t'+1}^{\operatorname{Up}}(s, a) = \operatorname{no.}$  By Lemma 5.10, we have that  $(s, a) \in \mathcal{K}_{t'+1}^{\operatorname{Up}}$ . Since we assumed  $(s, a) \notin \mathcal{K}_{t}^{\operatorname{Up}}$ , there was a successful update of some Up-value between t' and t, otherwise we would have  $\mathcal{K}_{t'+1}^{\operatorname{Up}} = \mathcal{K}_{t}^{\operatorname{Up}}$ . Consequently, we have  $\operatorname{learn}_{t+1}^{\operatorname{Up}}(s, a) = \operatorname{yes.}$  By Assumption 8 the next attempted Up-update of (s, a) will be successful. This attempt will occur after  $\overline{m}$  more visits to (s, a).
- 2. learn<sup>Up</sup><sub>t</sub>(s, a)  $\neq$  no: By construction of the algorithm, we have that in at most  $\overline{m} 1$  more visits to (s, a), an Up-update of (s, a) will be attempted. Suppose this attempt takes place at step t', t'  $\geq$  t and the most  $\overline{m}$  recent visits to (s, a) prior to t' happened at steps  $k_1 < k_2 < \ldots < k_{\overline{m}} = t'$ . Note that we do not necessarily have that t =  $k_1$  or t =  $k_{\overline{m}}$ , but

surely  $t \in \{k_1, ..., k_{\overline{m}}\}$ . If the Up-update at step t' succeeds, there is nothing to prove, hence assume that this update fails. There are two possibilities:

- a. If (s, a) is not Up-converged at step  $k_1$ , then by Assumption 8 the Up-update at step t' will be successful, contradicting the assumption.
- b. If instead (s, a) is Up-converged at step  $k_1$ , we have that  $\mathcal{K}_{k_1}^{Up} \neq \mathcal{K}_t^{Up}$ , since we assumed that  $(s, a) \notin \mathcal{K}_t^{Up}$ . Consequently, there was a successful Up-update of some other state-action pair at some step t" with  $k_1 < t^{"} \leq t$  and thus  $\operatorname{learn}_{t^{"+1}}^{Up}(s, a) =$  yes. Moreover, we necessarily have that no Up-update of (s, a) is attempted after t". Together, we have that  $\operatorname{learn}_{t'+1}^{Up}(s, a) =$  once even though the attempted Up-update at step t' fails. By Lemma 5.8, we have that  $(s, a) \notin \mathcal{K}_{t'+1}^{Up}$ , as  $(s, a) \notin \mathcal{K}_{t}^{Up}$  and no successful Up-update of (s, a) occurred between t and t'. By Assumption 8 the next attempt to update Up-value of (s, a) will succeed.

By Lemma 5.3, the number of successful Up-updates is bounded by  $\frac{|Act|}{\overline{\varepsilon}}$ , and by the previous arguments we have that if for some t the pair (s, a) is not Up-converged then in at most  $2\overline{m}$  more visits to (s, a), there will be a successful update to Up(s, a). Hence, there can be at most  $2\overline{m} \cdot \frac{|Act|}{\overline{\varepsilon}}$  steps t such that the current state-action pair is not Up-converged. Once no more Up-updates take place,  $\pi_t$  remains fixed and  $\mathcal{K}_t^{\text{Lo}}$  only changes due to successful updates of the lower bounds, yielding an analogous proof for Lo.

As a last auxiliary lemma, we show that whenever the probability of reaching a non-converged pair is low, we necessarily are close to the optimal value.

**LEMMA 5.12.** Assume that Assumption 7 holds and fix a step t. Then, for every state  $s \in S$  we have that

$$\begin{split} \mathsf{Up}_{\mathsf{t}}(s) &- 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} - \mathsf{Pr}_{\mathcal{M},s}^{\pi_{\mathsf{t}}} [\diamondsuit \overline{\mathcal{K}_{\mathsf{t}}^{\mathsf{Up}}}] \leq \\ & \mathsf{Pr}_{\mathcal{M},s}^{\pi_{\mathsf{t}}} [\diamondsuit \{s_{\mathsf{t}}\}] \leq \\ & \mathsf{Lo}_{\mathsf{t}}(s) + 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} + \mathsf{Pr}_{\mathcal{M},s}^{\pi_{\mathsf{t}}} [\diamondsuit \overline{\mathcal{K}_{\mathsf{t}}^{\mathsf{Lo}}}]. \end{split}$$

**PROOF.** The central idea of this proof is to apply Lemma A.5 twice, with  $X(s, a) = Up_t(s, a)$  and  $X(s, a) = Lo_t(s, a)$ , respectively.

For the first application, set  $\kappa_l = -1$ ,  $\kappa_u = 3\overline{\epsilon}$ , and  $\pi = \pi_t$ . Then,  $\mathcal{K} = \mathcal{K}_t^{Up}$  and

$$\mathsf{Pr}_{\mathcal{M}',s}^{\pi_{\mathsf{t}}}[\diamondsuit\{s_{+}\}] - \mathsf{Pr}_{\mathcal{M},s}^{\pi_{\mathsf{t}}}[\diamondsuit\overline{\mathcal{K}_{\mathsf{t}}^{\mathsf{Up}}}] \le \mathsf{Pr}_{\mathcal{M},s}^{\pi_{\mathsf{t}}}[\diamondsuit\{s_{+}\}]$$
(8)

since  $\mathcal{M}'$  and  $\mathcal{M}$  are equivalent on  $\mathcal{K}^{\text{Up}}_t.$  The lemma then yields that

$$\pi_{\mathsf{t}}[\mathsf{Up}_{\mathsf{t}}](s) - \mathsf{Pr}_{\mathcal{M}_{t}',s}^{\pi_{\mathsf{t}}}[\diamondsuit\{s_{+}\}] \le 3\overline{\varepsilon} \cdot |S|p_{\min}^{-|S|}.$$
(9)

Recall that  $\pi_t$  is a strategy randomizing uniformly over some of the available actions in each state, hence  $\delta_{\min}(\pi)$  is at least  $p_{\min}$ . For the second application, we dually set  $\kappa_l = -3\overline{\epsilon}$ ,  $\kappa_u = 1$ ,

and  $\pi = \pi_t$ . Again, we have  $\mathcal{K} = \mathcal{K}_t^{Lo}$  and

$$\mathsf{Pr}_{\mathcal{M},s}^{\pi_{\mathsf{t}}}[\diamondsuit\{s_{+}\}] \le \mathsf{Pr}_{\mathcal{M},s}^{\pi_{\mathsf{t}}}[\diamondsuit\{s_{+}\}] + \mathsf{Pr}_{\mathcal{M},s}^{\pi_{\mathsf{t}}}[\diamondsuit\overline{\mathcal{K}_{\mathsf{t}}^{\mathsf{Lo}}}].$$
(10)

The lemma gives us

$$\mathsf{Pr}_{\mathcal{M}'_t,s}^{\pi_t}[\diamondsuit\{s_+\}] - \pi_t[\mathsf{Lo}_t](s) \le 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|}.$$
(11)

Now, recall that  $\pi_t[Up_t](s) = Up_t(s)$  and  $\pi_t[Lo_t](s) \le Lo_t(s)$  [Fact I] due to Lemma 5.8. Together, we have

$$\begin{aligned} \mathsf{Up}_{\mathsf{t}}(s) - 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} \stackrel{[\mathbf{I}]}{=} \pi_{\mathsf{t}}[\mathsf{Up}_{\mathsf{t}}](s) - 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} \stackrel{(9)}{\leq} \mathsf{Pr}_{\mathcal{M}'_{t},s}^{\pi_{\mathsf{t}}}[\diamondsuit\{s_{+}\}], \\ \mathsf{Pr}_{\mathcal{M}',s}^{\pi_{\mathsf{t}}}[\diamondsuit\{s_{+}\}] - \mathsf{Pr}_{\mathcal{M},s}^{\pi_{\mathsf{t}}}[\diamondsuit\overline{\mathcal{K}}_{\mathsf{t}}^{\mathsf{Up}}] \stackrel{(8)}{\leq} \mathsf{Pr}_{\mathcal{M},s}^{\pi_{\mathsf{t}}}[\diamondsuit\{s_{+}\}] \stackrel{(10)}{\leq} \mathsf{Pr}_{\mathcal{M}',s}^{\pi_{\mathsf{t}}}[\diamondsuit\{s_{+}\}] + \mathsf{Pr}_{\mathcal{M},s}^{\pi_{\mathsf{t}}}[\diamondsuit\overline{\mathcal{K}}_{\mathsf{t}}^{\mathsf{Lo}}], \text{ and} \\ \mathsf{Pr}_{\mathcal{M}'_{t},s}^{\pi_{\mathsf{t}}}[\diamondsuit\{s_{+}\}] \stackrel{(11)}{\leq} 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} + \pi_{\mathsf{t}}[\mathsf{Lo}_{\mathsf{t}}](s) \stackrel{[\mathbf{I}]}{\leq} 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} + \mathsf{Lo}_{\mathsf{t}}(s). \end{aligned}$$

Combining all the above statements now yields the overall result.

**THEOREM 5.13.** Algorithm 4 terminates and yields a correct result with probability at least  $1 - \delta$  after at most  $O(\text{POLY}(|Act|, p_{\min}^{-|S|}, \varepsilon^{-1}, \ln \delta))$  steps.

**PROOF.** We only consider executions where Assumptions 7 and 8 hold. By Lemmas 5.5 and 5.9 together with the union bound, this happens with probability at least  $1 - \frac{\delta}{2}$ .

Now, observe that if the algorithm terminates at some step t, we have that  $Up_t(\hat{s}) - Lo_t(\hat{s}) < \varepsilon$  by definition. With Lemma 5.6, we get  $Lo_t(\hat{s}) \leq \mathcal{V}(\hat{s}) \leq Up_t(\hat{s})$ . Reordering yields the result.

We show by contradiction that the algorithm terminates for almost all considered executions. Thus, assume that the execution does not halt with non-zero probability. Since the MDP  $\mathcal{M}$  satisfies Assumption 1, almost all episodes eventually visit either  $s_+$  or  $s_-$  due to Lemma 2.8 and thus are of finite length. Thus, almost all executions for which the algorithm does not terminate comprise infinitely many episodes. We restrict our attention to only those executions.

Recall that due to Lemma 5.4, there are only finitely many attempted updates on almost all considered executions. Consequently, on these executions the algorithm eventually does not change Up, since no successful updates can occur from some step t onwards. This means that all following samples are obtained by sampling according to the strategy  $\pi_t$ . Note that both the time of convergence and the actual strategy  $\pi_t$  depends on the execution  $\mathfrak{a}$ . Thus, we need to employ Lemma A.7—the algorithm clearly qualifies as Markov process, since its evolution only depends on its current valuations. More precisely, it is not difficult to see that the whole execution of the algorithm (with fixed inputs) can be modelled as a (very unwieldy) countable Markov chain, showing that the considered properties are measurable. In particular, they are reachability objectives on this induced Markov chain.

Let us now consider the set of executions for which the upper bounds eventually converge and moreover  $\Pr_{\mathcal{M},\hat{s}}^{\pi_t}[\diamondsuit \overline{\mathcal{K}_t^{Up}}] \ge \rho > 0$  infinitely often. Assume that this set of executions has a non-zero measure. By Lemma A.7, on almost all of these executions  $\overline{\mathcal{K}_{t}^{Up}}$  is also reached infinitely often, contradicting Lemma 5.11. For the lower bounds, we can prove a completely analogous statement. Consequently,  $\Pr_{\mathcal{M},\hat{s}}^{\pi_{t}}[\diamond \overline{\mathcal{K}_{t}^{Up}}] \rightarrow 0$  and  $\Pr_{\mathcal{M},\hat{s}}^{\pi_{t}}[\diamond \overline{\mathcal{K}_{t}^{Lo}}] \rightarrow 0$  on almost all considered executions for  $t \rightarrow \infty$ .

Inserting the definition of  $\overline{\varepsilon}$ , we have for a sufficiently large step t that

$$\mathsf{Up}_{\mathsf{t}}(\hat{s}) - \frac{\varepsilon}{2} < \mathsf{Up}_{\mathsf{t}}(\hat{s}) - 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} - \mathsf{Pr}_{\mathcal{M},\hat{s}}^{\pi_{\mathsf{t}}}[\diamondsuit \overline{\mathcal{K}_{\mathsf{t}}^{\mathsf{Up}}}]$$

and dually

$$\mathsf{Lo}_{\mathsf{t}}(\hat{s}) + 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} + \mathsf{Pr}_{\mathcal{M},\hat{s}}^{\pi_{\mathsf{t}}}[\Diamond \overline{\mathcal{K}_{\mathsf{t}}^{\mathsf{Lo}}}] < \mathsf{Lo}_{\mathsf{t}}(\hat{s}) + \frac{\varepsilon}{2}$$

for all considered executions. Thus, by Lemma 5.12, we have

$$\mathsf{Up}_{\mathsf{t}}(\hat{s}) - \frac{\varepsilon}{2} < \mathsf{Pr}_{\mathcal{M},\hat{s}}^{\pi_{\mathsf{t}}}[\diamondsuit\{s_{+}\}] < \mathsf{Lo}_{\mathsf{t}}(\hat{s}) + \frac{\varepsilon}{2},$$

i.e.  $Up_t(\hat{s}) - Lo_t(\hat{s}) < \varepsilon$ , contradicting the assumption.

We have proven that the result is approximately correct with probability  $1 - \frac{\delta}{2}$ . Now, we additionally need to prove the step bound. To this end, we first bound the number of sampled paths and then bound the length of each path. Central to the following proof is Lemma 5.11, bounding the number of visits to non-converged state-action pairs. First, we treat the upper bounds. Observe that the probability of visiting a non-Up-converged state-action pair either is 0 or at least  $p_{\min}^{|S|}$  (due to Lemma A.1). Moreover, while this probability may fluctuate, once it reaches 0 it remains at 0, since then the sampling strategy does not change and all pairs reachable under this strategy are Up-converged. So, in the worst case, the probability of reaching such a pair is exactly  $p_{\min}^{|S|}$  until they are visited often enough. We model this process as a series of Bernoulli trials X<sub>i</sub>, equalling 1 if at least one Up-update happens while sampling the *i*-th path.<sup>10</sup> While the exact probabilities are not independent, they are always at least as large as the success probability  $p \coloneqq p_{\min}^{|S|}$  of these trials (or 0 if all reachable pairs are Upconverged). Hence, we approximate the number of trials we need to perform until we observe at least  $c := 2\overline{m} \cdot \frac{|Act|}{\overline{c}}$  successes with high probability—then, all upper bounds necessarily are converged by Lemma 5.11. Now, we are essentially dealing with a binomially distributed variable  $X_n = \sum_{i=1}^n X_i$  and want to find an *n* such that  $\mathbb{P}[X_n \ge c] \ge 1 - \frac{\delta}{4}$ . Since we are interested in the limit behaviour, we can apply the de Moivre–Laplace theorem, allowing us to replace this binomial distribution with an appropriate normal distribution. Thus, we obtain

$$\mathbb{P}[X_n \ge c] \approx 1 - \Phi\left(\frac{c - np}{\sqrt{np(1-p)}}\right),$$

<sup>10</sup> We deliberately use *i* instead of e to emphasize that  $X_i$  does not operate on the probability space of the algorithm  $(\mathfrak{A}, \mathcal{A}, \mathbb{P}_A)$ . Instead, they represent a crude under-approximation to allow for a feasible analysis.

and rearranging yields

$$n^{-\frac{1}{2}}(c-np) \approx \Phi^{-1}\left(\frac{\delta}{4}\right) \cdot \sqrt{p(1-p)}.$$

For readability, we set  $a \coloneqq \Phi^{-1}\left(\frac{\delta}{4}\right)$ . Solving for *n* gives us

$$n \approx \frac{c}{p} - \frac{a}{2p}\sqrt{(1-p)^2a^2 + 4c(1-p)} + \frac{(1-p)r^2}{2p}.$$

Inserting the definitions yields that  $n \in O(\text{POLY}(|Act|, p_{\min}^{-|S|}, \varepsilon^{-1}, \ln \delta))$ . This bounds the number of paths sampled by the algorithm. We furthermore prove that the length of all those paths is polynomial with high probability. To this end, we employ Lemma A.3. Recall that sampling of a path stops once we reach one of the two special states  $s_+$  and  $s_-$ . Due to Assumption 1, the probability of eventually reaching them is 1. Hence,  $\Pr_{\mathcal{M},\hat{s}}^{\pi_e}[\diamond^{\leq N}\{s_+, s_-\}] \geq 1 - \tau$ , where  $N \geq \ln(\frac{2}{\tau}) \cdot |S| p_{\min}^{-|S|}$  for any sampling strategy  $\pi_e$ . In other words, the probability of a sampled path being longer than N is at most  $\tau$ . Then, by the union bound, the probability of any of the npaths being longer than N is at most  $n \cdot \tau$ . By choosing  $\tau = \frac{\delta}{4n}$ , this happens with probability at most  $\frac{\delta}{4}$ . Then,  $\ln(\frac{2}{\tau}) = \ln(8n) - \ln(\delta)$ , i.e. the length of each path again is bounded by a polynomial in the input values. Together, we obtain the results, since polynomials are closed under multiplication.

**REMARK 5.14 (Relation to [129]).** Before we proceed to the general case, we briefly discuss how our proof structure relates to the one of **[129]** and how it can be used to derive a variant of their Theorem 1. Most of our proofs are quite analogous. For example, Assumption 8 is practically equivalent to their Assumption A1, similarly Lemmas 5.6 and 5.9 to 5.11 and the respective proofs correspond to their Lemma 1 to 4 (however, note the different bounds). Since we are dealing with unbounded reachability (assuming almost sure absorption by Assumption 1), the purpose of Lemma 5 corresponds to our Lemma A.5.

Major differences arise in the actual proof of [129, Theorem 1]. As we already pointed out, the Hoeffding bound is not applicable to variables indicating whether an update has occurred in a particular step due to the clear dependency. The related proof step aims to show that with high probability after a certain number of steps, the number of possible updates is exhausted (by virtue of Lemma 5.11) and then bounds the deviation from the true value based on this. We prove a similar statement via Lemma 5.12, connecting the probability of visiting a non-converged state-action pair to the convergence of the bounds. Note that the proof of Lemma 5.12 employs the auxiliary Lemma A.5.

## 6. Limited Information – General Case

As before, MECs pose an additional challenge, since they introduce superfluous upper fixed points. The key difference to the full information setting is that MECs cannot be directly

identified. Instead, we identify a set of state-action pairs as an end component if it occurs sufficiently often. By bounding the probability of falsely identifying such a set as an end component, we can replicate the previous proof structure.

## 6.1 Collapsing End Components with Limited Information

Before we present the complete algorithm, we first show how we identify end components in this section.

**DEFINITION 6.1.** Let  $\mathcal{M} = (S, Act, Av, \Delta)$  be an MDP,  $\rho \in \text{Paths}_{\mathcal{M}}$  and  $i, j \ge 0$ . We define the state-action pairs which appear at least *i* times on the path  $\rho$  during the first *j* steps as

$$Appear(\rho, i, j) = \{(s, a) \in S \times Av \mid |\{k \mid k \le j \land \rho^a(k) = a\}| \ge i\}.$$

We overload the definition of *Appear* to also accept finite paths of sufficient length. Moreover, we also define *Appear* for paths of Markov chains, which yields the states occurring more than *i* times.

For notational convenience, we identify the result of *Appear* with the corresponding state-action tuple (R, B) since we will use these results as candidates for end components. With appropriate *i* and *j*, *Appear* is an EC with high probability.

**LEMMA 6.2.** Let  $\mathcal{M} = (S, Act, Av, \Delta)$  be an MDP,  $\hat{s} \in S$  an initial state,  $T \subseteq S$  a set of target states, and  $\pi \in \Pi_{\mathcal{M}}^{\mathsf{MD}}$  a memoryless strategy on  $\mathcal{M}$  such that  $\mathsf{Pr}_{\mathcal{M},s}^{\pi}[\diamond \overline{T}] = 0$  for all  $s \in T$ , i.e. T is absorbing under  $\pi$ . Set  $S_{\pi} = \bigcup_{s \in S} \operatorname{supp}(\pi(s)), \kappa = |S_{\pi}| + 1$ , and pick  $i \geq \kappa$ . Then either  $\mathsf{Pr}_{\mathcal{M},\hat{s}}^{\pi}[\diamond^{\leq 2i^{3}}T] = 1$  or

$$\mathsf{Pr}_{\mathcal{M},\hat{s}}^{\pi}\Big[App_{i} \mid \overline{\diamond^{\leq 2i^{3}}T}\Big] \geq 1 - 2(1+i^{2}) \cdot e^{-(i-1)\frac{\delta_{\min}(\pi)^{\kappa}}{\kappa}} \cdot \delta_{\min}(\pi)^{-\kappa},$$

where  $App_i = \{ \rho \in \mathsf{Paths}_{\mathcal{M}} \mid Appear(\rho, i, 2i^3) \in \mathsf{EC}(\mathcal{M}) \}.$ 

Informally, this lemma shows that, when sampling according to a memoryless strategy, paths of sufficient length either end up in an already known set of ECs or frequently reappearing state-action pairs also form an EC with high probability.

**PROOF.** If  $\Pr_{\mathcal{M},\hat{s}}^{\pi}[\diamondsuit^{\leq 2i^{3}}T] = 1$ , there is nothing to prove, hence we assume the opposite, i.e. that  $\Pr_{\mathcal{M},\hat{s}}^{\pi}[\overline{\diamondsuit^{\leq 2i^{3}}T}] > 0$  [Fact I].

Given an MDP, a designated initial state  $\hat{s}$ , and a memoryless strategy, we can construct a finite state Markov chain which exactly captures the behaviour of the MDP under the given strategy. We define the Markov chain  $M_{\pi} = (\{\hat{s}\} \cup S_{\pi}, \delta_{\pi})$ , where  $\delta_{\pi}$  is defined as

$$\delta(\hat{s}, a) = \pi(\hat{s}, a) \text{ for } a \in \operatorname{supp}(\pi(\hat{s}))$$
  
$$\delta(a, a') = \Delta(\operatorname{state}(a, \mathcal{M}), a, \operatorname{state}(a', \mathcal{M})) \cdot \pi(\operatorname{state}(a', \mathcal{M}), a').$$

In other words,  $\delta(a, a')$  equals the probability of reaching some state s' after playing action a and then continuing with action a'. Recall that each action is tied to a unique state. As such, the paths in  $M_{\pi}$  exactly correspond to the paths in  $\mathcal{M}$  following  $\pi$ . Furthermore, it is easy to see that each BSCC of  $M_{\pi}$  corresponds to an end component in  $\mathcal{M}$ . Observe that, by definition,  $\kappa$  equals the number of states in  $M_{\pi}$  [Fact II] and  $\delta_{\min}(\pi)$  equals the smallest positive transition probability in  $M_{\pi}$  [Fact III]. For readability, we define  $c = \exp(-\delta_{\min}(\pi)^{\kappa}/\kappa)$ .

Let  $App_{i,\pi} \subseteq Paths_{M_{\pi}}$  be the event corresponding to  $App_i$  in the Markov chain  $M_{\pi}$ . Informally,  $App_{i,\pi}$  denotes the set of all (infinite) paths  $\rho$  which within  $2i^3$  steps (i) visit all states of some BSCC at least *i* times, and (ii) all other states at most i - 1 times, i.e. all paths such that  $Appear(\rho, i, 2i^3)$  is a BSCC of  $M_{\pi}$ . We now show that

$$\mathsf{Pr}_{\mathsf{M}_{\pi},\hat{s}}[App_{i,\pi} \mid \overline{\diamond^{\leq 2i^{3}}T}] \geq 1 - 2c^{i}i^{3} \cdot \delta_{\min}(\pi)^{-\kappa},$$

i.e. the probability of  $App_{i,\pi}$  given that T is not reached within  $2i^3$  steps is at least  $1 - 2c^i i^3 \cdot \delta_{\min}(\pi)^{-\kappa}$ . Since the paths of  $M_{\pi}$  exactly correspond to paths obtained in  $\mathcal{M}$  by following the strategy  $\pi$ , this proves the claim.

First, we show that [Fact IV]

$$\Pr_{M_{\pi},\hat{s}}[App_{i,\pi}] \ge 1 - 2(1 + i^2) \cdot c^{i-1}.$$

Let  $B = \bigcup_{R \in BSCC(M_{\pi})} R$  be the set of all states in BSCCs of  $M_{\pi}$ . We have that  $Pr_{M_{\pi},\hat{s}}[\diamond B] = 1$  by Lemma 2.7. We apply Lemma A.3 with N = i - 1 and  $\tau = 2c^{i-1}$ . By [II] and [III]

$$|S_{\pi}| \cdot \ln\left(\frac{2}{\tau}\right) \cdot \delta_{\min}(\pi)^{-|S_{\pi}|} = \kappa \cdot \ln\left(\exp\left((i-1) \cdot \frac{\delta_{\min}(\pi)^{\kappa}}{\kappa}\right)\right) \cdot \delta_{\min}(\pi)^{-\kappa} = i-1.$$

Thus  $\Pr_{M_{\pi},\hat{s}}[\diamondsuit^{\leq i-1}B] \geq 1 - 2c^{i-1}$ . In other words, an infinite path of  $M_{\pi}$  starting in  $\hat{s}$  does not visit a BSCC of  $M_{\pi}$  within i - 1 steps with probability at most  $2c^{i-1}$ .

Now, let  $R = \{s_1, \ldots, s_n\} \subseteq B$  be some BSCC of  $M_{\pi}$  and fix two states  $s_i, s_j \in R$ . Since R is an BSCC, we have  $\Pr_{M_{\pi}, s_i}[\diamondsuit \{s_j\}] = 1$ , and we can apply Lemma A.3 again to obtain that  $\Pr_{M_{\pi}, s_i}[\diamondsuit^{\leq i}\{s_j\}] \ge 1 - 2c^{i-1}$ . Consequently, the probability of visiting all states of R, one after another, with at most i - 1 steps between visiting the respective next state, is at least  $1 - n \cdot 2c^{i-1}$ . Repeating this argument, with probability at least  $1 - i \cdot n \cdot 2c^{i-1} \ge 1 - i \cdot \kappa \cdot 2c^{i-1}$ , this round trip is successful i times in a row and has a length of at most  $i \cdot n \cdot (i-1) \le i^2 \kappa \le i^3$ . Using the union bound again, we get that with probability at least  $1 - 2c^{i-1} - i\kappa \cdot 2c^{i-1} = 1 - 2c^{i-1}(1+i\kappa) \ge 1 - 2(1+i^2) \cdot c^{i-1}$  a path of length  $i^3$  ends up in a BSCC within i - 1 steps and then visits all states of the BSCC at least i times, proving [IV].

Let  $T_{\pi} = \{a \in S_{\pi} \mid \text{state}(a, \mathcal{M}) \in T\}$  the states of  $M_{\pi}$  corresponding to the given state set T. Recall that we assumed that  $\Pr_{\mathcal{M},s}^{\pi}[\diamond \overline{T}] = 0$  for  $s \in T$ , i.e.  $\Pr_{M,a}[\diamond \overline{T_{\pi}}] = 0$  for all  $a \in T_{\pi}$  (recall that the states of M are actions a of  $\mathcal{M}$ ). Consequently, each BSCC of  $M_{\pi}$  either is contained in  $T_{\pi}$  or disjoint from it: Assume that there exists a BSCC *R* with states  $a, a' \in R$  where  $a \in T_{\pi}$  and  $a' \notin T_{\pi}$ . Since *R* is a BSCC, we have  $\Pr_{M_{\pi},a}[\diamondsuit\{a'\}] = 1$ , contradicting  $\Pr_{M_{\pi},a}[\diamondsuit\overline{T_{\pi}}] = 0$ .

Due to **[I]**, there exists at least one BSCC which is disjoint from  $T_{\pi}$ —otherwise any run would eventually end up in  $T_{\pi}$ . Let *s* be some state in this BSCC. By construction, there exists a path of length at most  $\kappa$  from  $\hat{s}$  to *s* **[II]**, and thus the probability of reaching such a BSCC is bounded from below by  $\delta_{\min}(\pi)^{\kappa}$ , using **[III]**. Formally, we have **[Fact V]** 

$$\Pr_{\mathsf{M}_{\pi},\hat{s}}\left[\overline{\diamondsuit^{\leq 2i^{3}}T_{\pi}}\right] > \delta_{\min}(\pi)^{\kappa}$$

Finally, we obtain

$$\begin{aligned} \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ App_{i,\pi} \mid \overline{\diamond^{\leq 2i^{3}}T} \right] \stackrel{[I]}{=} & \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ App_{i,\pi} \cap \overline{\diamond^{\leq 2i^{3}}T} \right] / \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ \overline{\diamond^{\leq 2i^{3}}T} \right] \\ &= & \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ App_{i,\pi} \setminus \diamond^{\leq 2i^{3}}T \right] / \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ \overline{\diamond^{\leq 2i^{3}}T} \right] \\ &= & (\Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ App_{i,\pi} \right] - \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ App_{i,\pi} \cap \diamond^{\leq 2i^{3}}T \right] ) / \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ \overline{\diamond^{\leq 2i^{3}}T} \right] \\ &\geq & (\Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ App_{i,\pi} \right] - \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ \overline{\diamond^{\leq 2i^{3}}T} \right] ) / \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ \overline{\diamond^{\leq 2i^{3}}T} \right] \\ &\stackrel{[\mathsf{IV}]}{\geq} & (1 - 2c^{i-1}(1+i^{2}) - (1 - \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ \overline{\diamond^{\leq 2i^{3}}T} \right])) / \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ \overline{\diamond^{\leq 2i^{3}}T} \right] \\ &= & (\Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ \overline{\diamond^{\leq 2i^{3}}T} \right] - 2c^{i-1}(1+i^{2})) / \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ \overline{\diamond^{\leq 2i^{3}}T} \right] \\ &= & 1 - (2c^{i-1}(1+i^{2})) / \Pr_{\mathsf{M}_{\pi},\hat{s}} \left[ \overline{\diamond^{\leq 2i^{3}}T} \right] \\ &\stackrel{[\mathsf{V}]}{\geq} & 1 - 2(1+i^{2}) \cdot c^{i-1} \cdot \delta_{\min}(\pi)^{-\kappa}. \end{aligned}$$

#### 6.2 The General DQL Algorithm

We define the general DQL algorithm in Algorithm 5. Essentially, the algorithm works similar to the previous Algorithm 4. The main difference is that it further employs Lemma 6.2 to detect whether the current sample is stuck in a yet to be discovered EC. To this end, the algorithm introduces a small set of additional auxiliary variables, necessary to track representative states similar to the collapsed MDP of Section 4. In particular, collapsed<sub>e</sub> stores the representatives of each state. Since we might discover growing ECs, this representative might be part of another already discovered EC. Thus, we use rep<sub>e</sub> to resolve the current representative of a given state *s* by repeatedly applying collapsed<sub>e</sub> until a fixed point is reached. Practically, we would store rep<sub>e</sub> as a map, pointing each "original" state of the MDP to its current representative. We introduce the "layered" representation through collapsed<sub>e</sub> only as notational convenience. Additionally,  $Z_e$  contains all states which are part of a bottom EC without a target state. We choose the parameter i, controlling the length of each sample and when to check for an EC, such that

$$|Act| \cdot 2(1+i^2) \cdot e^{-(i-1)\frac{p_{\min}(\pi)^{|S|+1}}{|S|+1}} \cdot p_{\min}(\pi)^{-(|S|+1)} \le \frac{\delta}{4} \quad \text{and} \quad i \ge |Act|.$$
(12)

```
Inputs as given in Definition 5.2, precision \varepsilon, and
           Input:
                           confidence \delta.
           Output: Values (l, u) which are \varepsilon-optimal, i.e., \mathcal{V}(\hat{s}) \in [l, u] and
                             0 \le u - l < \varepsilon, with probability at least 1 - \delta.
           Initialize all variables as in Algorithm 4
 1:
           e \leftarrow 1, t \leftarrow 1
 2:
           for s \in S do collapsed<sub>e</sub>(s) \leftarrow s
 3:
           S_1 \leftarrow S, Av_1 \leftarrow Av, T_1 \leftarrow T, Z_1 \leftarrow \emptyset
 4:
           while Up_t(\hat{s}) - Lo_t(\hat{s}) \ge \varepsilon do
 5:
                    for s \in S_e do MaxA_e(s) \leftarrow arg max_{a \in Av_e(s)} Up_t(a)
 6:
                    s_t \leftarrow \hat{s}, t_e \leftarrow t
 7:
                    while s_t \notin T_e \cup Z_e and t - t_e < 2i^3 do
 8:
                            a_t \leftarrow \text{sampled uniformly from MaxA}_e(s_t)
                                                                                                                            > Pick an action
 9:
                            s''_t \leftarrow \operatorname{succ}(a_t)
                                                                                                                > Query successor oracle
10:
                            s'_t \leftarrow \operatorname{rep}_e(s''_t)
11:
                            Perform updates as in Algorithm 4
                                                                                                                          > Update Bounds
12:
                            s_{t+1} \leftarrow s'_t, t \leftarrow t+1
13:
                    if t - t_e \ge 2i^3 then
                                                                                                                               > Update ECs
14:
                            (\mathsf{R},\mathsf{B}) \leftarrow Appear(s_{\mathsf{t}_e}a_{\mathsf{t}_e}s_{\mathsf{t}_e+1}\dots a_{\mathsf{t}-1}s_{\mathsf{t}},\mathsf{i},\mathsf{2i}^3)
15:
                            C \leftarrow \bigcup_{s \in \mathbb{R}} Av_{e}(s) \setminus B
16:
                            if B \neq \emptyset then
17:
                                     if T_e \cap R \neq \emptyset then
18:
                                              T_{e+1} \leftarrow T_e \cup R
19:
                                              for a \in B do Lo_t(a) \leftarrow 1
20:
                                     else if C = \emptyset then
21:
                                              Z_{e+1} \leftarrow Z_e \cup R
22:
                                              for a \in B do Up_t(a) \leftarrow 0
23:
                                     else
24:
                                              S_{e+1} \leftarrow (S_e \setminus R) \cup \{s_{(R,B)}\}
25:
                                              Av_{e+1}(s_{(R,B)}) \leftarrow C
26:
                                              for s \in \mathbb{R} \cup \{s_{(\mathbb{R},\mathbb{B})}\} do collapsed<sub>e+1</sub>(s) \leftarrow s_{(\mathbb{R},\mathbb{B})}
27:
                                              if \hat{s} \in \mathbb{R} then \hat{s} \leftarrow s_{(\mathbb{R},\mathbb{B})}
28:
                    e \leftarrow e + 1
29:
            return (Lo_t(\hat{s}), Up_t(\hat{s}))
30:
```

Algorithm 5. The DQL learning algorithm for general MDPs.

This technical choice becomes more apparent in the proof of Lemma 6.13. Note that such an i always exists since the left side of the first inequality converges to 0 for  $i \rightarrow \infty$ . Moreover, we can find such an i using the values provided by the limited information setting as defined in Definition 5.2.

**REMARK 6.3.** In contrast to the previous sections, the domain of the bounds Up and Lo are actions instead of state-action pairs. This simplifies notation, since the algorithm frequently changes the state associated with an action.

**REMARK 6.4.** We implicitly assume that we can continue sampling with an action of our choice: When we collapse, for example, an EC (R, B) with states  $s, s' \in R$  into a single representative state, we might enter the EC in state s but then continue sampling with an action  $a \in Av(s')$ . This is not an essential restriction: Upon entering an already detected EC, we can simply pause the algorithm and randomly pick actions in B until we reach the state enabling the next action mandated by the algorithm.

# 6.3 **Proof of Correctness**

Now, to prove correctness of the algorithm, we again can reuse a lot of the previous reasoning. However, we need to invest significant effort in the treatment of end components. First of all, we again prove that the algorithm is well-defined.

**LEMMA 6.5.** During all episodes, we have that  $Av_e(s) \cap Av_e(s') = \emptyset$  for all states  $s, s' \in S_e$  with  $s \neq s'$ .

**PROOF.** The algorithm only modifies the set of available actions  $Av_e$  whenever a new representative state  $s_{(R,B)}$  is added. In this case, we have  $Av_{e+1}(s_{(R,B)}) \leftarrow C \subseteq \bigcup_{s \in R} Av_e(s)$  and all states of R are removed.

**LEMMA 6.6.** Algorithm 5 is well-defined.

**PROOF.** To prove this statement, we have to show that (i) no undefined values are accessed, (ii) all assignments are free of contradictions, and (iii) we require no more information than given by Definition 5.2.

For (i) and (ii), observe that when assigning the next episode's variables, we only use the variables of the current episode. Since we copy all unchanged variables, we only need to take care of the newly introduced arguments, i.e. the representative states  $s_{(R,B)}$ . Such a state is only added in Line 25. In the following lines, we define the state's actions Av, which is non-empty and disjoint from other states by Lemma 6.5. As no new actions are added, the action values in  $s_{(R,B)}$  still are defined. Observe that in Line 10 the successor oracle is only given states of the original MDP. Claim (iii) follows immediately.

Now, we show several statements related to the newly added handling of end components. Our goal is to show that the algorithm essentially samples from a collapsed MDP where the ECs identified by the algorithm are collapsed. Then, we replicate the proof ideas of the EC-free DQL algorithm on this collapsed MDP in order to again obtain the correctness.

## **LEMMA 6.7.** Algorithm 5 enters Line 15 at most |Act| times.

**PROOF.** First, observe that due to the pigeon-hole principle, *B* never is empty: By (12), our choice of i is larger than |Act|, thus a path of length at least i<sup>2</sup> contains at least one action i times. Consequently, whenever the algorithm enters Line 15, *B* is non-empty. Initially, the size of *B* is bounded by  $\sum_{s \in S_1} |Av_1(s)| = |Act|$ . We show that in any of the three cases, we remove at least one action which can never occur again as part of *B*. Consequently, after at most |Act| visits to Line 15, *B* would necessarily be empty, contradicting the above.

Whenever a state is added to either  $T_e$  or  $Z_e$ , this state and its actions will not be considered again—in particular, it will not occur as part of B. For the third case, we show that the number of available actions  $\sum_{s \in S_e} |Av_e(s)|$  is reduced whenever a new representative state is added. In that case, we have  $C \leftarrow \bigcup_{s \in R} Av_e(s) \setminus B$ ,  $S_{e+1} \leftarrow (S_e \setminus R) \cup \{s_{(R,B)}\}$ , and  $Av_{e+1}(s_{(R,B)}) \leftarrow C$ . By construction of the algorithm and definition of *Appear*, we have  $\emptyset \neq B \subseteq \bigcup_{s \in R} Av_e(s)$ . Using Lemma 6.5 we thus have  $|C| < |\bigcup_{s \in R} Av_e(s)|$ . Consequently,  $\sum_{s \in S_{e+1}} |Av_{e+1}(s)| < \sum_{s \in S_e} |Av_e(s)|$ .

## **LEMMA 6.8.** Algorithm 5 terminates or experiences an infinite number of episodes.

**PROOF.** Since the length of each episode is limited, i.e. the loop of Line 8 always terminates after a bounded number of steps, we only need to show that all other loops terminate. All for-loops iterate over (sub-)sets of states or actions, which are finite by assumption. The only remaining loop is the computation of rep<sub>e</sub> in Line 11, where the representative state is resolved. Observe that by construction of the algorithm, we either have that collapsed<sub>e</sub>(*s*) = *s* or collapsed<sub>e</sub>(*s*) =  $s_{(R,B)}$  with  $s \in R$ . Since we only modify collapsed when a new representative state is added, this happens only finitely often, due to Lemma 6.7.

**LEMMA 6.9.** If we add a representative state  $s_{(R,B)}$  in Line 25 after an episode e the bounds of any action  $a \in B$  are not changed after episode e.

**PROOF.** During each episode e, we only consider states in  $S_e$  and actions which are available in such states, as the call to rep<sub>e</sub> in Line 11 always yields an element of the current state set  $S_e$  due to Lemma 6.10. Since all states corresponding to actions in *B* are removed when adding a representative state  $s_{(R,B)}$  and these actions are not enabled in the newly added state, they do not appear again.

**LEMMA 6.10.** For any execution of the algorithm, we always have that  $rep_e(s) \in S_e$  for any state  $s \in S$ .

**PROOF.** We prove by induction: Initially, we have  $\operatorname{rep}_1(s) = \operatorname{collapsed}_1(s) = s$  for all  $s \in S_1$  by definition. Whenever we modify  $S_e$ , i.e. remove some states R and add a representative  $s_{(R,B)}$ , we set  $\operatorname{collapsed}_{e+1}(s) \leftarrow s_{(R,B)} \in S_{e+1}$  for all  $s \in R$ .

In order to properly reason about the paths sampled by the algorithm, we introduce a special MDP which corresponds to the current "view" of the given MDP.

**DEFINITION 6.11.** For any episode e, let the sampling MDP  $\mathcal{M}_{e} = (S_{e}, Act_{e}, Av_{e}, \Delta_{e})$ ,

$$\Delta_{\mathsf{e}}(s, a) = \{s \mapsto 1\} \text{ for } s \in S_{\mathsf{e}} \cap (T_{\mathsf{e}} \cup \mathsf{Z}_{\mathsf{e}}), a \in Av_{\mathsf{e}}(s), \text{ and} \\ \Delta_{\mathsf{e}}(s, a, s') = \sum_{\{s'' \in S | \mathsf{rep}_{\mathsf{e}}(s'') = s'\}} \Delta(\mathsf{state}(a, \mathcal{M}), a, s'') \text{ for other states } s, a \in Av_{\mathsf{e}}(s), s \in Av_{$$

and  $Act_{e} = \bigcup_{s \in S_{e}} Av_{e}(s)$ .

Note that the sampling MDP is well-defined due to Lemmas 6.5 and 6.10.

**LEMMA 6.12.** Fix an execution of the algorithm until some episode e and let  $\varrho$  be the finite path sampled by the algorithm during episode e. The probability of sampling this path equals the probability of obtaining this path on  $\mathcal{M}_{e}$  following the strategy  $\pi_{e}$  starting in state  $\hat{s}$ .

**PROOF.** We prove by induction over the path  $\varrho$ , using the Markov property. We show that for any finite prefix, the probability of selecting action a and then reaching state s' in the next step is equal in both the algorithm and the sampling MDP. Observe that we always have  $\hat{s} \in S_e$  due to Line 28 and the induction start is trivial.

For the induction step, suppose we are in a state *s*. By construction of the algorithm,  $s \notin T_e \cup Z_e$ . The algorithm now uniformly selects an action *a* from MaxA<sub>e</sub>(*s*), i.e. with probability  $|MaxA_e(s)|^{-1}$  for any such action. Then, a successor  $s'' \in S$  is sampled according to succ(*s*, *a*), i.e. with probability  $\Delta(s, a, s'')$ . The overall successor then equals  $s' = \operatorname{rep}_e(s'')$ . We have  $s' \in S_e$  by Lemma 6.10. Hence, a state  $s' \in S_e$  is sampled with probability  $\sum_{\{s'' \in S | \operatorname{rep}_e(s'') = s'\}} \Delta(s, a, s'')$ , just as in the MDP  $\mathcal{M}_e$  under strategy  $\pi_e$ .

Assumption 9. Whenever the algorithm reaches Line 15, (R, B) is an EC of  $\mathcal{M}_{e}$ .

**LEMMA 6.13.** The probability that Assumption 9 is violated during the execution of Algorithm 5 is bounded by  $\frac{\delta}{4}$ .

**PROOF.** We apply Lemma 6.2 with  $\mathcal{M} = \mathcal{M}_{e}$ ,  $T = T_{e} \cup Z_{e}$  and  $\pi = \pi_{e}$ . By construction of  $\mathcal{M}_{e}$  and the choice of T, we have that  $\pi_{e}$  trivially satisfies the condition of this lemma, since each state in T only has self-loops in  $\mathcal{M}_{e}$ . Clearly, we have that  $|S_{\pi}| \leq \sum_{s \in S_{e}} |Av(s)| \leq |Act|$ , since no actions are added during the execution of the algorithm. Consequently, we have that either  $\Pr_{\mathcal{M}_{e},\hat{s}}^{\pi_{e}}[\diamondsuit^{\leq 2i^{3}}(T_{e} \cup Z_{e})] = 1$  or

$$\Pr_{\mathcal{M}_{e},\hat{s}}^{\pi_{e}} \Big[ App_{i} \mid \overline{\diamond^{\leq 2i^{3}}(T_{e} \cup Z_{e})} \Big] \geq 1 - 2(1 + i^{2}) \cdot e^{-(i-1)\frac{p_{\min}(\pi)|S|+1}{|S|+1}} \cdot p_{\min}(\pi)^{-(|S|+1)}$$

where  $App_{i}$  are all paths  $\rho \in \mathsf{Paths}_{\mathcal{M}_{e}}$  such that  $Appear(\rho, i, 2i^{3})$  is an EC in  $\mathcal{M}_{e}$ .

Now, observe that the algorithm only enters Line 15 if after  $2i^3$  steps neither  $T_e$  nor  $Z_e$  is reached. By applying Lemma 6.12, we get that the probability of (R, B) being an EC given that Line 15 is entered exactly equals  $\Pr_{\mathcal{M}_e, \hat{s}}^{\pi_e}[App_i \mid \overline{\diamond^{\leq 2i^3}(T_e \cup Z_e)}]$ . Since Line 15 is entered at most |Act| times due to Lemma 6.7, the statement follows by inserting the definition of i from (12).

**LEMMA 6.14.** Assume that Assumption 9 holds and fix some episode e. Let  $s \in S_e$  some state of the MDP  $\mathcal{M}_e$  and  $s' \in S$  such that  $\operatorname{rep}_e(s') = s$  Then, s and s' have the same value:

$$\mathcal{V}_{\mathsf{e}}(s) = \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\max}[\diamond T_{\mathsf{e}}] = \mathsf{Pr}_{\mathcal{M},s'}^{\max}[\diamond T] = \mathcal{V}(s')$$

**PROOF.** We prove by induction over the episode number. Initially, we have that  $\mathcal{M}_1$  is quite similar to the original MDP  $\mathcal{M}$ . Recall that  $Z_1 = \emptyset$  and  $\operatorname{rep}_1(s) = s$  for all states. Hence, the only difference lies in the transition function of all states  $s \in T$ . These only have self-loops in  $\mathcal{M}_1$ , while in  $\mathcal{M}$  they may have arbitrary transitions. This is irrelevant for the value of the states, since it equals 1 in both cases.

Now fix an arbitrary episode e. We have that  $\mathcal{V}_{e}(s) = \mathcal{V}(s')$  (IH) for any two states *s*, *s'* as in the claim.  $\mathcal{M}_{e}$  is only modified when Line 15 is entered. Let (R, B) the identified set of states and actions. Due to Assumption 9, (R, B) is an EC of  $\mathcal{M}_{e}$ . To conclude, we distinguish the three cases in the algorithm:

- ---  $T_e \cap R \neq \emptyset$ : Since (R, B) is an EC, any state  $s \in R$  can reach  $T_e$  with probability one. Hence  $\mathcal{V}_{e+1}(s) = 1 = \mathcal{V}_e(s) = \mathcal{V}(s')$  [IH]. In particular, by adding all states of R to  $T_{e+1}$ , we do not change their value.
- ---  $C = \emptyset$ : Once in R, this EC cannot be left, i.e.  $\Pr_{\mathcal{M}_e, s}^{\max}[\Diamond \overline{R}] = 0$  for all  $s \in R$ . Consequently, we have that  $\mathcal{W}_e(s) = 0 = \mathcal{W}(s')$  [IH]. This value is unchanged by adding the states of R to  $Z_{e+1}$  and thus introducing a self-loop in  $\mathcal{M}_e$ .
- Add a representative state: By assumption, we have that  $rep_e(s') \in R$  and thus  $rep_{e+1}(s') = s_{(R,B)}$ . We need to prove that  $\mathcal{V}_{e+1}(s_{(R,B)}) = \mathcal{V}(s')$ . As (R, B) is an EC by assumption, each state in R has the same value by Lemma 4.2. The representative state  $s_{(R,B)}$  has this value by applying the same reasoning as in Lemma 4.11.

**LEMMA 6.15.** Assume that Assumption 9 holds and fix some episode e. For any  $EC(R, B) \in EC(\mathcal{M}_e)$  and  $e' \leq e$  there exists an  $EC(R', B') \in EC(\mathcal{M}_{e'})$  with  $B \subseteq B'$ .

**PROOF.** Note that we do not necessarily have that  $R \subseteq R'$ , since some states of the EC may have been replaced by a representative state.

We prove by induction on the episode e. Fix any such episode e and EC  $(R, B) \in EC(\mathcal{M}_{e+1})$ . We only modify the MDP  $\mathcal{M}_e$  when the algorithm enters Line 15, hence w.l.o.g. we assume that this happened in episode e. Let (R, B) be the set of states and actions identified in Line 15 during episode e. By Assumption 9, (R, B) is an EC of  $\mathcal{M}_e$ . As above, we distinguish the three cases in the algorithm:

- ---  $C = \emptyset$ : Analogously to the above, all actions in B are now a self-loop in  $\mathcal{M}_{e+1}$  and the same reasoning applies.
- −− Add a representative state: If  $s_{(R,B)} \notin R$ , we necessarily have that  $B \cap B = \emptyset$ . Hence, the EC (*R*, *B*) again already existed in  $\mathcal{M}_e$ , since none of its components was modified by this step. If instead  $s_{(R,B)} \in R$ , we have that  $(R \cup R, B \cup B)$  is an EC in  $\mathcal{M}_e$ , following the same reasoning as in Lemma 4.8.

**LEMMA 6.16.** Assume that Assumption 9 holds and fix some step t with corresponding episode e. Let  $(R, B) \in EC(\mathcal{M}_e)$  be any EC in  $\mathcal{M}_e$ . For any  $a \in B$  we have that (i) if state $(a, \mathcal{M}_e) \in Z_e$ , then  $Up_t(a) = 0$  and (ii)  $Up_t(a) = 1$  otherwise.

**PROOF.** Item (i) immediately follows from the definition of the algorithm and  $\mathcal{M}_e$ . When a state is added to  $Z_e$ , we set  $Up_t(a) = 0$  for all its actions. We prove Item (ii) by induction, showing that the statement holds for all ECs at each step t. Initially, we have  $Up_1(a) = 1$  for all actions by definition of the algorithm. For the induction step fix some step t. We have that  $Up_{t'}(a) = 1$  for all actions a in all ECs without zero-states for all  $t' \leq t$  (IH). Now, let e' be the episode of step t + 1 and fix any EC (R, B) in  $\mathcal{M}_{e'}$  with  $R \cap Z_e = \emptyset$ . By repeatedly applying Lemma 6.15, there exists an EC  $(R_{e'}, B_{e'}) \in EC(\mathcal{M}_{e'})$  with  $B \subseteq B_{e'}$  for all  $e' \leq e$ . Since we have no zero-states in the EC in step t + 1, none of the  $R_{e'}$  contain zero-states either, by construction of the algorithm and  $\mathcal{M}_e$ . Thus, the induction hypothesis [IH] is applicable and we have that  $Up_{t'}(a) = 1$  for any action  $a \in B_{e'}$  and  $t' \leq t$ . Hence, we necessarily have that  $Up_{t'}(s) = 1$  for all  $s \in R_{e'}$  and  $t' \leq t$  (also using Lemma 6.9). Whenever any action  $a \in B$  is selected at any step  $t' \leq t$  during episode  $e' \leq e$ , all of its successors are part of the EC  $(R_{e'}, B_{e'})$ , thus  $Up_{t'}(s) = 1$  for all successors by the above reasoning. Consequently, we always add a value of 1 to  $\operatorname{acc}_t^{Up}(a)$  and whenever an Up-update is attempted for action a at some step  $t' \leq t$ , we would set  $Up_{t'}(a) = 1$ .

**LEMMA 6.17.** Assume that Assumption 9 holds and fix some step t with corresponding episode e. Let t'  $\geq$  t with episode e'  $\geq$  e. We have for any state  $s \in S$  that  $Up_{t'}(rep_{e'}(s)) \leq Up_t(rep_e(s))$ and  $Lo_t(rep_e(s)) \leq Lo_{t'}(rep_{e'}(s))$ .

**PROOF.** The bounds of actions are modified by (i) the usual update, which only increases or decreases, respectively (ii) in Lines 20 and 23, where upper bounds are set to 0 and lower bounds set to 1, or (iii) when an EC is collapsed and thus the set of available actions is modified in Line 26. Cases (i) and (ii) preserve monotonicity of the state bound by definition. Case (iii) is proven separately for upper and lower bounds, with the proof of the lower bound being

significantly more involved. For the upper bounds, observe that  $Av_{e'}(s) \subseteq Av_{e}(s)$  by definition, i.e. we never add new actions to any state. Consequently, the maximum over the set of available actions does not increase. For the lower bounds, we have to show that while collapsing ECs and thus removing actions, we never remove all those which are optimal w.r.t. the lower bound, i.e. all actions  $a \in Av_{e}(s)$  with  $Lo_{t}(a) = Lo_{t}(s)$ .

We proceed by additionally proving an auxiliary statement by induction on the step t in parallel. In particular, we prove that for any step t with corresponding episode e (i) the statement of the lemma holds (IH1) and (ii)  $Lo_t(a) \leq \max_{s \in R, a' \in Av_e(s) \setminus B} Lo_t(a')$  for all actions  $a \in B$  (or 0 if no such actions a' exist) in all ECs  $(R, B) \in EC(\mathcal{M}_e)$  without a target state, i.e.  $R \cap T_e = \emptyset$ . (IH2).

Initially, we have  $Lo_1(a) = 0$  by definition of the algorithm and both statements trivially hold. For the induction step fix some time step t. We first treat the case when the lower bound of action an action a is successfully updated in step t and later on deal with the case of an EC being collapsed. Note that **[IH1]** trivially holds in this case, since the value of *a* is never decreased. We only need to show the second statement [IH2], thus assume that the updated action *a* is an internal action of some EC (R, B), i.e.  $a \in B$ . For readability, denote  $C = \bigcup_{s \in R} Av_e(s) \setminus B$  the set of outgoing actions of (R, B). If  $C = \emptyset$ , the statement follows directly: Since all lower bounds are initialised to zero, the EC does not contain any target states by assumption, and there are no outgoing actions, the algorithm never updates the lower bound of any action in B to a non-zero value. Thus, assume that  $C \neq \emptyset$ . By applying **[IH2]** to all states of the EC (R, B), we get that  $\max_{a' \in C} \text{Lo}_t(a') = \max_{s \in R} \text{Lo}_t(s)$  [Fact I]. Furthermore, let  $k_1 < \ldots < k_{\overline{m}} = t$  the steps of the most recent visits to *a* with corresponding episodes  $e_1 \leq \ldots \leq e_{\overline{m}} = e$  and sampled successors  $s'_{k_i}$ . Now, let  $R_i = \operatorname{rep}_{e_i}(\operatorname{states}_e(R))$  for  $1 \le i \le \overline{m}$  the set of states in episode  $e_i$  which eventually are collapsed to R. By applying the reasoning of Lemma 6.15 and 4.8, there exists a set of actions  $B_i$  with  $B \subseteq B_i$  such that  $(R_i, B_i)$  is an EC in  $\mathcal{M}_{e_i}$  and thus  $s'_{k_i} \in R_i$  [Fact II], since  $a \in B_i$ . By construction, we have that rep<sub>e</sub>( $R_i$ ) = R [Fact III]. Finally, we observe that the value of the outgoing actions does not decrease, hence the value we assign to a in step t satisfies

$$\begin{aligned} \mathsf{Lo}_{\mathsf{t}+1}(a) + \overline{\varepsilon} \stackrel{\text{def}}{=} \frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \mathsf{Lo}_{k_i}(s'_{k_i}) \\ & \stackrel{[\mathsf{III}]}{\leq} \frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \max_{s \in R_i} \mathsf{Lo}_{k_i}(s) \\ & \stackrel{[\mathsf{III1}]}{\leq} \frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \max_{s \in R_i} \mathsf{Lo}_{\mathsf{t}}(\mathsf{rep}_{\mathsf{e}}(s)) \\ & \stackrel{[\mathsf{IIII}]}{=} \frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \max_{s \in R_{\overline{m}}} \mathsf{Lo}_{\mathsf{t}}(s) \\ & = \max_{s \in R_{\overline{m}}} \mathsf{Lo}_{\mathsf{t}}(s) \\ & \stackrel{[\mathsf{III}]}{=} \max_{a' \in C_{\overline{m}}} \mathsf{Lo}_{\mathsf{t}}(a'). \end{aligned}$$

This concludes proof of the first part.

For the second part, i.e. when a set of states is collapsed by the algorithm, we have that the collapsed set (R, B) is an EC by Assumption 9 and *B* are only internal actions. If the collapsed EC contains target states, the statement trivially holds. Otherwise, we apply the result of the first part and get that the lower bound assigned to any action in *B* is less or equal to outgoing actions. Thus, removing the actions in *B* from the set of available actions does not reduce the value of the obtained representative state.

With basic properties about the sampling MDP in place, we can now mimic the previous idea of defining "converged" state-action pairs and, using those, show that the algorithm eventually converges with high probability.

**DEFINITION 6.18.** For every step t during episode e, define  $\mathcal{K}_t^{Up}$ ,  $\mathcal{K}_t^{Lo} \subseteq Act_e$  by

$$\mathcal{K}_{t}^{\mathsf{Up}} \coloneqq \{a \mid \mathsf{Up}_{t}(a) - \Delta_{\mathsf{e}}(\mathsf{state}(a, \mathcal{M}_{\mathsf{e}}), a) \langle \pi_{\mathsf{t}}[\mathsf{Up}_{t}] \rangle \leq 3\overline{\varepsilon}\} \text{ and}$$
$$\mathcal{K}_{t}^{\mathsf{Lo}} \coloneqq \{a \mid \Delta_{\mathsf{e}}(\mathsf{state}(a, \mathcal{M}_{\mathsf{e}}), a) \langle \pi_{\mathsf{t}}[\mathsf{Lo}_{\mathsf{t}}] \rangle - \mathsf{Lo}_{\mathsf{t}}(a) \leq 3\overline{\varepsilon}\}.$$

Again, an action *a* is Up-converged (Lo-converged) at step t if  $a \in \mathcal{K}_{t}^{Up}$  ( $a \in \mathcal{K}_{t}^{Lo}$ ).

Assumption 10. Suppose an Up-update of the action a is attempted at step t. Let  $k_1 < k_2 < \ldots < k_{\overline{m}} = t$  be the steps of the  $\overline{m}$  most recent visits to a, and  $e_1 \le e_2 \le \ldots \le e_{\overline{m}}$  the respective episodes. Then  $\frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \mathcal{W}_{e_i}(s'_{k_i}) \ge \mathcal{W}_{e_{\overline{m}}}(a) - \overline{\epsilon}$ . Analogously, for an attempted Lo-update, we have  $\frac{1}{\overline{m}} \sum_{i=1}^{\overline{m}} \mathcal{W}_{e_i}(s'_{k_i}) \le \mathcal{W}_{e_{\overline{m}}}(a) + \overline{\epsilon}$ .

**Assumption 11.** Suppose an update of the upper bound (lower bound) of the action *a* is attempted at step t. Let  $k_1 < k_2 < \ldots < k_{\overline{m}} = t$  be the steps of the  $\overline{m}$  most recent visits to *a*. If *a* is not Up-converged (Lo-converged) at step  $k_1$ , the update at step t is successful.

We replicate most of the statements from the previous DQL algorithm.

**LEMMA 6.19.** The following properties hold for Algorithm 5.

- 1. The number of successful updates of Up and Lo is bounded by  $\frac{|Act|}{\overline{s}}$  each.
- 2. The number of attempted updates of Up and Lo is bounded by  $\overline{\xi}$ .
- 3. Assume that Assumption 9 holds. Then, the probability that Assumption 10 is violated during the execution of Algorithm 5 is bounded by  $\frac{\delta}{4}$ .
- 4. Assume that Assumptions 9 and 10 hold. Then, we have  $Lo_t(a) \leq \mathcal{V}_e(a) \leq Up_t(a)$  for all episodes e, steps  $t \geq t_e$ , and actions  $a \in Act_e$ .
- 5. We have for every step t in episode e and state  $s \in S_e$  that

$$\pi_{t}[Up_{t}](s) = Up_{t}(s) \text{ and } \pi_{t}[Lo_{t}](s) \le Lo_{t}(s).$$

6. If  $a \notin \mathcal{K}_{t}^{Up}$ , then  $a \notin \mathcal{K}_{t'}^{Up}$  for all  $t' \ge t$  until an Up-update of action a succeeds or the upper bound is set to 0 in Line 23.

- 7. The probability that Assumption 11 is violated during the execution of Algorithm 4 is bounded by  $\frac{\delta}{4}$ .
- 8. Assume that Assumption 11 holds. If an attempted Up-update of action a at step t fails and  $learn_{t+1}^{Up}(a) = false$ , then  $a \in \mathcal{K}_{t+1}^{Up}$ . Once no more updates of Up succeed, the analogous statement holds true for the lower bounds.
- 9. Assume that Assumption 11 holds. Then, there are at most  $2\overline{m} \cdot \frac{|Act|}{\overline{\epsilon}}$  visits to state-action pairs which are not Up-converged. Once the upper bounds are not updated any more, there are at most  $2\overline{m} \cdot \frac{|Act|}{\overline{\epsilon}}$  visits to state-action pairs which are not Lo-converged.

**PROOF.** Items 1 and 2 follow directly as in Lemmas 5.3 and 5.4. The only additional observation is that the algorithm never adds new actions and that the changes to the bounds outside of Line 12 never reset the progress of an action's bounds.

Item 3 can be proven completely analogous to Lemma 5.5, since this proof only relies on the Markov property of the successor sampling. We need to adjust the definition of  $Y_i$  slightly to incorporate the modifications of the algorithm. Let thus  $s'_{k_i} \in S$  denote the states obtained by the successor oracle in Line 10. By Lemma 6.14 we have that  $\mathcal{V}_e(\operatorname{rep}_{e_i}(s'_{k_i})) = \mathcal{V}_e(s''_{k_i})$ , and thus  $Y_i = \mathcal{V}_e(\operatorname{rep}_{e_i}(s'_{k_i}))$  are i.i.d.

For Item 4, we first show that all newly introduced updates of Up and Lo are correct. Using Assumption 9, we prove the two special cases. The algorithm sets  $Up_t(a) \leftarrow 0$  if an EC (R, B) without outgoing transitions and no target state is identified. In this case, we clearly have that  $\mathcal{V}_e(a) = 0$  for all  $s \in R$ . Similarly, setting  $Lo_e(a) \leftarrow 1$  when any state in the EC (R, B) is an accepting state is correct, since clearly  $\mathcal{V}_e(a) = 1$  for all  $s \in R$ ,  $a \in Av_e \cap B$ . Due to Lemma 6.14, copying the respective bounds to the representative state  $s_{(R,B)}$  (which happens implicitly in Line 26) is correct, too. Now, the reasoning of Lemma 5.6 applies.

Items 5 and 6 can be proven as in Lemma 5.8.

Item 7 is proven analogous to Item 3, following the proof of Lemma 5.9. Again, this claim only depends on the sampled successors. We define  $X_i = \pi_{k_1}[Up_{k_1}](rep_{e_1}(s''_{k_i}))$ . Since we do not modify the underlying transition probabilities, from which  $s''_{k_i}$  is obtained, these  $X_i$  are i.i.d. again and we can apply the same reasoning. To conclude the proof as before, we need to employ Lemma 6.17. Note that since we only speak about the actual computed bounds Up and Lo, we do not need to employ Lemma 6.14.

Item 8 follows directly as in Lemma 5.10. Similarly, Item 9 follows as in Lemma 5.11, using Item 1 instead of Lemma 5.3.

In the proof of correctness for the no-EC DQL algorithm, we applied Lemma A.5 directly on the MDP to obtain bounds on the reachability of  $s_+$  based on the values of Up and Lo in Lemma 5.12. Now, we cannot apply this lemma directly on either  $\mathcal{M}$  or  $\mathcal{M}_e$  since both may contain ECs. Hence, we apply the lemma on an MDP derived from  $\mathcal{M}_e$  to obtain a similar result. Let us thus first define the set of all actions in "non-final" ECs as

$$E_{\mathsf{e}} = \bigcup_{\{(R,B)\in \mathsf{EC}(\mathcal{M}_{\mathsf{e}})|R\cap(T_{\mathsf{e}}\cup\mathsf{Z}_{\mathsf{e}})=\emptyset\}}B$$

**LEMMA 6.20.** Assume that Assumptions 9 and 10 hold and fix an episode e. Then, we have for every state  $s \in S_e$ 

$$\mathsf{Up}_{\mathsf{e}}(s) - 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} - \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\pi_{\mathsf{e}}} [\diamondsuit \overline{\mathcal{K}_{\mathsf{e}}^{\mathsf{Up}}}] - \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\pi_{\mathsf{e}}} [\diamondsuit E_{\mathsf{e}}] \le \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\pi_{\mathsf{e}}} [\diamondsuit T_{\mathsf{e}}].$$

**PROOF.** We first want to derive an MDP from  $\mathcal{M}_{e}$  without any ECs but still capturing its behaviour. For this, recall that there are two kinds of ECs in  $\mathcal{M}_{e}$ . Firstly, there are ECs which correspond to ECs in the original  $\mathcal{M}$ . Secondly, we get a self-loop EC for each identified target-or zero-state, i.e. states in  $T_{e}$  or  $Z_{e}$ . We define the derived MDP  $\mathcal{M}'_{e} = (S_{e} \cup \{s_{+}, s_{-}\}, Act_{e} \cup \{a_{+}, a_{-}\}, \Delta'_{e}, Av'_{e})$ , where

$$\begin{aligned} \Delta'_{\mathsf{e}}(s_{\circ}, a_{\circ}) &= \{s_{\circ} \mapsto 1\} & \text{for } \circ \in \{+, -\} \\ \Delta'_{\mathsf{e}}(s, a) &= \{s_{+} \mapsto 1\} & \text{for all } s \in T_{\mathsf{e}}, a \in Av_{\mathsf{e}}(s), \\ \Delta'_{\mathsf{e}}(s, a) &= \{s_{-} \mapsto 1\} & \text{for all } s \in \mathsf{Z}_{\mathsf{e}}, a \in Av_{\mathsf{e}}(s), \\ \Delta'_{\mathsf{e}}(s, a) &= \{s_{+} \mapsto 1\} & \text{for all } a \in E, s = \mathsf{state}(a, \mathcal{M}_{\mathsf{e}}), \\ \Delta'_{\mathsf{e}}(s, a) &= \Delta_{\mathsf{e}}(s, a) & \text{for all other } s \in S_{\mathsf{e}}, a \in Av_{\mathsf{e}}(s), \end{aligned}$$

and  $Av'_{e}(s) = Av_{e}(s)$  for  $s \in S_{e}$  and  $Av'_{e}(s_{\circ}) = \{a_{\circ}\}$  for  $\circ \in \{+, -\}$ . In essence,  $\mathcal{M}'_{e}$  equals  $\mathcal{M}_{e}$  except that we (i) added the special states  $s_{+}$  and  $s_{-}$ , (ii) all states in  $T_{e}$  and  $Z_{e}$  move to  $s_{+}$  and  $s_{-}$ , respectively, and (iii) all actions in ECs outside of  $T_{e}$  and  $Z_{e}$  move to  $s_{+}$ , in the spirit of Lemma 6.16.

Clearly,  $\mathcal{M}'_{e}$  has no ECs except the special states  $s_{+}$  and  $s_{-}$  and thus satisfies Assumption 1. Moreover, the probability of reaching  $s_{+}$  in  $\mathcal{M}'_{e}$  equals the probability of reaching  $T_{e} \cup E_{e}$  in  $\mathcal{M}_{e}$ by construction of  $\mathcal{M}'_{e}$  [Fact I].

Now, we extend  $\pi_e$  to select action  $a_\circ$  in the special state  $s_\circ$  to obtain  $\pi'_e$ . Furthermore, we set  $X(s, a) = Up_e(a)$  for all states  $s \in S_e$ ,  $a \in Av_e(s)$ ,  $X(s_+, a_+) = 1$ , and  $X(s_-, a_-) = 0$ . We apply Lemma A.5 with  $\mathcal{M} = \mathcal{M}'_e$ ,  $\pi = \pi'_e$ ,  $\kappa_l = -1$ , and  $\kappa_u = 3\overline{\epsilon}$ . As a result, for each state  $s \in S_e$  we have

$$\pi'_{\mathsf{e}}[X](s) - \mathsf{Pr}_{\mathcal{M}',s}^{\pi'_{\mathsf{e}}}[\diamondsuit\{s_{+}\}] \le 3\overline{\varepsilon} \cdot |S|p_{\min}^{-|S|},$$

where  $\mathcal{M}'$  is the MDP defined in the lemma. Observe that for  $s \in S_e$  [Fact II]

$$\pi'_{\mathsf{e}}[X](s) = \sum_{a \in Av'_{\mathsf{e}}(s)} \pi'_{\mathsf{e}}(s,a) \cdot X(s,a) = \sum_{a \in Av_{\mathsf{e}}(s)} \pi_{\mathsf{e}}(s,a) \cdot \mathsf{Up}_{\mathsf{e}}(a) = \pi_{\mathsf{e}}[\mathsf{Up}_{\mathsf{e}}](s).$$

To analyse how  $\mathcal{M}'$  and  $\mathcal{M}'_{e}$  are related, we first need to derive the structure of  $\mathcal{K}$  from the lemma. Thus, we now prove that  $\mathcal{K} = \mathcal{K}_{e}^{\cup p} \cup \{a_{+}, a_{-}\}$ . Recall that

$$\mathcal{K} = \{a \in Act_{\mathsf{e}} \cup \{a_+, a_-\} \mid X(s, a) - \Delta'_{\mathsf{e}}(s, a) \langle \pi'_{\mathsf{e}}[X] \rangle \le 3\overline{\varepsilon}\}$$

and

$$\Delta'_{\mathsf{e}}(s,a)\langle \pi'_{\mathsf{e}}[X]\rangle = \sum_{s'\in S_{\mathsf{e}}\cup\{s_{+},s_{-}\}}\Delta'_{\mathsf{e}}(s,a,s')\cdot \sum_{a'\in Av'_{\mathsf{e}}(s')}\pi(s',a')\cdot X(s',a')$$

Clearly,  $a_+$  and  $a_-$  satisfy the requirements due to their self-loop. Furthermore, we have  $\pi'_{e}[X](s_+) = 1$ ,  $\pi'_{e}[X](s_-) = 0$  [Fact III]. Now, let  $a \in Act_{e}$  and  $s \in S_{e}$  the corresponding state. By definition, we have  $X(s, a) = \bigcup_{e}(a)$ , hence we need to show that  $\Delta'_{e}(s, a)\langle \pi'_{e}[X] \rangle = \Delta_{e}(s, a)\langle \pi_{e}[\bigcup_{e}] \rangle$ . We proceed with a case distinction.

- ---  $s \in T_e \cup Z_e$ : By definition of the algorithm, we have  $Up_e(s) = 1$  or 0, respectively. The unique successor under any action  $a \in Av_e(s)$  in  $\mathcal{M}_e$  equals s by definition, thus  $\Delta_e(s, a)\langle \pi_e[Up_e] \rangle = Up_e(s)$ . In  $\mathcal{M}'_e$ , the unique successor equals  $s_+$  or  $s_-$ , respectively. Thus, with **[III]**, we have  $\pi'_e[X](s) = \pi_e[Up_e](s)$ . The claim follows.
- ---  $a \in E$ : Note that this case implies that  $s \notin T_e \cup Z_e$ . Due to Lemma 6.16, we have that  $Up_e(a) = 1$  for all such actions. Recall that  $\pi_e$  follows actions maximizing  $Up_e$ . Consequently,  $\pi_e[Up_e](s') = \pi'_e[X](s') = Up_e(s') = 1$  for all states s' inside an non-trivial EC of  $\mathcal{M}_e$ . Thus, we also have  $\Delta_e(s, a)\langle \pi_e[Up_e] \rangle = 1$ . From the definition of  $\mathcal{M}'_e$  and [III], we directly get  $\Delta'_e(s, a)\langle \pi'_e[X] \rangle = 1$ .
- −−  $s \notin T_e \cup Z_e$ ,  $a \notin E$ : By definition, we have  $\Delta_e(s, a) = \Delta'_e(s, a)$ . Together with [II] and [III], the statement follows.

Recall that  $\mathcal{M}'$  is defined as  $\mathcal{M}'_{e}$  except that  $\Delta'(s, a) = \{s_{+} \mapsto X(s, a), s_{-} \mapsto 1 - X(s, a)\}$  for all  $a \notin \mathcal{K}$ . Hence, as in Lemma 5.12, we get that for all states  $s \in S_{e}$ 

$$\mathsf{Pr}_{\mathcal{M}',s}^{\pi'_{\mathsf{e}}}[\diamondsuit\{s_{+}\}] - \mathsf{Pr}_{\mathcal{M}'_{\mathsf{e}},s}^{\pi'_{\mathsf{e}}}[\diamondsuit\overline{\mathcal{K}_{\mathsf{e}}^{\mathsf{Up}}}] \le \mathsf{Pr}_{\mathcal{M}'_{\mathsf{e}},s}^{\pi'_{\mathsf{e}}}[\diamondsuit\{s_{+}\}],$$

and thus with [I] we get [Fact IV]

$$\pi'_{\mathsf{e}}[X](s) - 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} - \mathsf{Pr}_{\mathcal{M}'_{\mathsf{e}},s}^{\pi'_{\mathsf{e}}}[\diamondsuit \overline{\mathcal{K}_{\mathsf{e}}^{\mathsf{Up}}}] \le \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\pi_{\mathsf{e}}}[\diamondsuit (T_{\mathsf{e}} \cup E_{\mathsf{e}})].$$

Further, we have  $\pi'_{e}[X](s) = \pi_{e}[Up_{e}](s) = Up_{e}(s)$  by Lemma 6.19, Item 5 [Fact V].

To conclude the proof, we show that  $\Pr_{\mathcal{M}'_{e},s}^{\pi'_{e}}[\diamond \overline{\mathcal{K}_{e}^{Up}}] \leq \Pr_{\mathcal{M}_{e},s}^{\pi_{e}}[\diamond \overline{\mathcal{K}_{e}^{Up}}]$  [Fact VI]. To this end, observe that (i) for each state  $s \in S_{e}$  and action  $a \in Av_{e}(s)$  we either have  $\Delta_{e}(s, a) = \Delta'_{e}(s, a)$  or  $\operatorname{supp}\Delta'_{\underline{e}}(s, a) \subseteq \{s_{+}, s_{-}\}$  and (ii) the added states  $s_{+}$  and  $s_{-}$  are absorbing. Thus, each run reaching  $\overline{\mathcal{K}_{e}^{Up}}$  in  $\mathcal{M}'_{e}$  has a corresponding, equally probable path in  $\mathcal{M}_{e}$ .

The overall claim follows from the above equations and a union bound.

$$\begin{split} \mathsf{Up}_{\mathsf{e}}(s) &- 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} - \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\pi_{\mathsf{e}}}[\diamondsuit \mathcal{K}_{\mathsf{e}}^{\mathsf{Up}}] \\ & \stackrel{[\mathbf{V}]}{=} \pi_{\mathsf{e}}'[X](s) - 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} - \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\pi_{\mathsf{e}}}[\diamondsuit \overline{\mathcal{K}_{\mathsf{e}}^{\mathsf{Up}}}] \\ & \stackrel{[\mathbf{VI}]}{\leq} \pi_{\mathsf{e}}'[X](s) - 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} - \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\pi_{\mathsf{e}}'}[\diamondsuit \overline{\mathcal{K}_{\mathsf{e}}^{\mathsf{Up}}}] \\ & \stackrel{[\mathbf{IV}]}{\leq} \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\pi_{\mathsf{e}}}[\diamondsuit (T_{\mathsf{e}} \cup E_{\mathsf{e}})]. \end{split}$$

**LEMMA 6.21.** Assume that Assumptions 9 and 10 hold and fix an episode e. Then, we have for every state  $s \in S_e$ 

$$\mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\pi_{\mathsf{e}}}[\diamond T_{\mathsf{e}}] \leq \mathsf{Lo}_{\mathsf{e}}(s) + 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} + \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\pi_{\mathsf{e}}}[\diamond \overline{\mathcal{K}_{\mathsf{e}}^{\mathsf{Lo}}}] + \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},s}^{\pi_{\mathsf{e}}}[\diamond E_{\mathsf{e}}].$$

**PROOF.** As in Lemma 6.20, we construct a second MDP without ECs, but slightly modify the transition function. In particular, let  $\mathcal{M}'_{e} = (S_{e} \cup \{s_{+}, s_{-}\}, Act_{e} \cup \{a_{+}, a_{-}\}, \Delta'_{e}, Av'_{e})$  be defined as before. However, for  $a \in E_{e}$  and  $s = \text{state}(a, \mathcal{M}_{e})$ , we define

$$\Delta'_{\mathsf{e}}(s, a) = \{s_{+} \mapsto \Delta_{\mathsf{e}}(s, a) \langle \pi_{\mathsf{e}}[\mathsf{Lo}_{\mathsf{e}}] \rangle, s_{-} \mapsto 1 - \Delta_{\mathsf{e}}(s, a) \langle \pi_{\mathsf{e}}[\mathsf{Lo}_{\mathsf{e}}] \rangle \}$$

Again,  $\mathcal{M}'_{e}$  has no ECs except in the two special states and thus Lemma A.5 is applicable. We set  $X(s, a) = Lo_{e}(a)$  for all states  $s \in S_{e}$ ,  $X(s_{+}, a_{+}) = 1$ , and  $X(s_{-}, a_{-}) = 0$ . As above, we have that  $\pi'_{e}[X](s) = \pi_{e}[Lo_{e}](s)$  for all  $s \in S_{e}$ . We apply the lemma with  $\mathcal{M} = \mathcal{M}'_{e}, \pi = \pi'_{e}, \kappa_{l} = -3\overline{\varepsilon}$ , and  $\kappa_{u} = 1$ . Thus, for each state  $s \in S_{e}$ 

$$\mathsf{Pr}_{\mathcal{M}',s}^{\pi'_{\mathsf{e}}}[\diamondsuit\{s_{+}\}] - \pi'_{\mathsf{e}}[X](s) \le 3\overline{\varepsilon} \cdot |S|p_{\min}^{-|S|},$$

where  $\mathcal{M}'$  is the MDP defined in the lemma. We again show that  $\mathcal{K} = \mathcal{K}_{e}^{Lo} \cup \{a_{+}, a_{-}\}$  by case distinction as follows:

- Trivially,  $a_+, a_- \in \mathcal{K}, \pi'_{e}[X](s_+) = 1$ , and  $\pi'_{e}[X](s_-) = 0$ .
- $s \in T_e \cup Z_e$ : The claims follow by an analogous argument. Recall that for these states we have  $Up_e(a) = Lo_e(a)$  for all  $a \in Av_e(s)$ .

—  $a \in E$ : Inserting the definitions, we get

$$\begin{aligned} \Delta_{\mathsf{e}}'(s,a)\langle \pi_{\mathsf{e}}'[X]\rangle &= \Delta_{\mathsf{e}}'(s,a,s_{+}) \cdot \pi_{\mathsf{e}}'[X](s_{+}) + \Delta_{\mathsf{e}}'(s,a,s_{-}) \cdot \pi_{\mathsf{e}}'[X](s_{-}) \\ &= \Delta_{\mathsf{e}}(s,a)\langle \pi_{\mathsf{e}}[\mathsf{Lo}_{\mathsf{e}}]\rangle \cdot 1 + (1 - \Delta_{\mathsf{e}}(s,a)\langle \pi_{\mathsf{e}}[\mathsf{Lo}_{\mathsf{e}}]\rangle) \cdot 0 \\ &= \Delta_{\mathsf{e}}(s,a)\langle \pi_{\mathsf{e}}[\mathsf{Lo}_{\mathsf{e}}]\rangle. \end{aligned}$$

—  $s \notin T_e \cup Z_e$ , *a* ∉ *E*: Follows analogously.

As in Lemma 5.12, we also get for all states  $s \in S_e$  that

$$\mathsf{Pr}_{\mathcal{M}'_{\mathsf{e}},s}^{\pi'_{\mathsf{e}}}[\diamondsuit\{s_{+}\}] \leq \mathsf{Pr}_{\mathcal{M}',s}^{\pi'_{\mathsf{e}}}[\diamondsuit\{s_{+}\}] + \mathsf{Pr}_{\mathcal{M}'_{\mathsf{e}},s}^{\pi'_{\mathsf{e}}}[\diamondsuit\overline{\mathcal{K}_{\mathsf{e}}^{\mathsf{Lo}}}].$$

Similar to the above proof, we have  $\pi'_{e}[X](s) = \pi_{e}[Lo_{e}](s) \leq Lo_{e}(s)$  by Lemma 6.19, Item 5. With completely analogous reasoning, we can show that  $\Pr_{\mathcal{M}'_{e},s}^{\pi'_{e}}[\diamondsuit \overline{\mathcal{K}_{e}^{Lo}}] \leq \Pr_{\mathcal{M}_{e},s}^{\pi_{e}}[\diamondsuit \overline{\mathcal{K}_{e}^{Lo}}]$ . Putting all equations together, we get that

$$\Pr_{\mathcal{M}'_{e},s}^{\pi'_{e}}[\diamondsuit\{s_{+}\}] \leq \operatorname{Lo}_{e}(s) + 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} + \Pr_{\mathcal{M}_{e},s}^{\pi_{e}}[\diamondsuit\overline{\mathcal{K}_{e}^{\operatorname{Lo}}}].$$

Now, it remains to show that  $\Pr_{\mathcal{M}_{e},s}^{\pi_{e}}[\diamond T_{e}] - \Pr_{\mathcal{M}_{e},s}^{\pi_{e}}[\diamond E_{e}] \leq \Pr_{\mathcal{M}'_{e},s}^{\pi'_{e}}[\diamond \{s_{+}\}]$ . This claim follows with the same reasoning as before, since we have that  $\Delta_{e}(s, a) = \Delta'_{e}(s, a)$  for  $a \notin E_{e}, s = \text{state}(a, \mathcal{M}_{e})$ .

Thus, every path in  $\mathcal{M}_{e}$  which does not visit *E* has a corresponding, equally probable path in  $\mathcal{M}'_{e}$ . The overall claim follows.

**THEOREM 6.22.** Algorithm 5 terminates and yields a correct result with probability at least  $1 - \delta$  after at most  $O(\text{POLY}(|Act|, p_{\min}^{-|S|}, \varepsilon^{-1}, \ln \delta))$  steps.

**PROOF.** This proof is largely analogous to the proof of Theorem 5.13, and we shorten some of its parts. Again, we only consider executions where Assumptions 9 to 11 hold. By Lemmas 6.13 and 6.19, Items 3 and 7 together with the union bound, this happens with probability at least  $1 - \delta$ . Correctness of the result upon termination follows from Lemma 6.19, Item 4.

We show by contradiction that the algorithm terminates for almost all considered executions. Thus, assume that the execution does not halt with non-zero probability. By Lemma 6.8, all of these executions experience an infinite number of episodes.

Due to Lemma 6.19, Item 2, there are only finitely many attempted updates on all considered executions and the algorithm eventually does not change Up, since no successful updates can occur from some step t onwards. Similarly, there are only finitely many EC collapses due to Lemma 6.7, and eventually the sampling MDP  $\mathcal{M}_e$  stabilizes. This means that all following samples are obtained by sampling according to the strategy  $\pi_t$  on the MDP  $\mathcal{M}_e$ . Again, we employ Lemma A.7 to continue the proof and we get  $\Pr_{\mathcal{M}_e,\hat{s}}^{\pi_t}[\diamond \overline{\mathcal{K}_t^{UP}}] = 0$  and  $\Pr_{\mathcal{M}_e,\hat{s}}^{\pi_t}[\diamond \overline{\mathcal{K}_t^{Lo}}] = 0$  on almost all considered executions. By an analogous argument, we can show that  $\Pr_{\mathcal{M}_e,\hat{s}}^{\pi_t}[\diamond E_e] = 0$ , since otherwise by Lemma 6.2 (with  $T = T_e \cup Z_e$ ) we have a non-zero probability of detecting a new EC, contradicting our assumption.

Thus, by applying Lemma 6.20

$$\mathsf{Pr}_{\mathcal{M}_{e},\hat{s}}^{\pi_{e}}[\Diamond T_{e}] \geq \mathsf{Up}_{e}(\hat{s}) - 3\overline{\varepsilon} \cdot |S|p_{\min}^{-|S|} - \mathsf{Pr}_{\mathcal{M}_{e},\hat{s}}^{\pi_{e}}[\Diamond \overline{\mathcal{K}_{e}^{\mathsf{Up}}}] - \mathsf{Pr}_{\mathcal{M}_{e},\hat{s}}^{\pi_{e}}[\Diamond E_{e}] > \mathsf{Up}_{e}(\hat{s}) - \frac{\varepsilon}{2}.$$

Dually, with Lemma 6.21 we get

$$\mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},\hat{s}}^{\pi_{\mathsf{e}}}[\Diamond T_{\mathsf{e}}] \leq \mathsf{Lo}_{\mathsf{e}}(\hat{s}) + 3\overline{\varepsilon} \cdot |S| p_{\min}^{-|S|} + \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},\hat{s}}^{\pi_{\mathsf{e}}}[\Diamond \overline{\mathcal{K}_{\mathsf{e}}^{\mathsf{Lo}}}] + \mathsf{Pr}_{\mathcal{M}_{\mathsf{e}},\hat{s}}^{\pi_{\mathsf{e}}}[\Diamond E_{\mathsf{e}}] < \mathsf{Lo}_{\mathsf{e}}(\hat{s}) + \frac{\varepsilon}{2}.$$

Together,  $Up_e(\hat{s}) - Lo_e(\hat{s}) < \varepsilon$ , contradicting the assumption.

For the step bound, we can mostly replicate the idea of the DQL variant without ECs. In particular, we can bound the number of paths by the same argument: The probability of reaching a non-Up-/non-Lo-converged action within |S| steps is at least  $p_{\min}^{|S|}$  (or 0). By Lemma 6.19, Item 9 we again get that the number of visits to such actions is bounded. Since  $i \ge |Act| \ge |S|$  and thus the sampling is not stopped early due to that condition, we again can bound the maximal number of paths by the same n. For the length of the paths, observe that they are bounded by  $2i^3$  by construction of the algorithm. From the definition of i in Equation (12), we see that this bound is polynomial, too, by considering the Taylor expansion of the exponential.

**REMARK 6.23.** To conclude, we briefly outline extensions to other objectives.

For safety, i.e. maximizing the probability of remaining inside a given set of states forever (or, equivalently, minimizing reachability of unsafe states), we only need to change the treatment of end components slightly. Assume w.l.o.g. that any unsafe state is collapsed into one sink state  $s_-$  (e.g. by testing for every encountered state whether it is safe and, if not, replace it by  $s_-$ ). Then, whenever we identify an end component, we know that this end component does not contain a sink state but rather only comprises safe states. However, this actually is exactly what we are looking for: a possibility of staying safe forever. Thus, we assign a value of 1 to all actions in such an EC. And indeed, by Lemma 2.8, we know that ECs are the *only* place that allow us to stay safe forever. Together, we can derive the desired result.

Extending to total reward has two major hurdles. Firstly, the total reward can be infinite, and we would first need to identify whether this is the case. To this end, we need to identify *all* end components in the system and check for each that it yields zero reward. Here, we would need to employ graph-based reasoning akin to [10], as we need to ensure that we have not missed any transition. Once this is established (or guaranteed due to domain knowledge), we can derive an upper bound on the total reward if we are given an upper bound on the reward that can be obtained in one step  $r_{\text{max}}$ . This bound is in the order  $O(p_{\min}^{-|S|} \cdot r_{\max})$ . Using this bound as initial value for the upper bound then would lead to a correct algorithm. (See also [115, Appendix B] and [51, Section 4] for related discussions.)

Finally, an extension to mean payoff (aka. long run average reward) or general  $\omega$ -regular objectives in a model-free setting seems to be rather unlikely. Both inherently are infinite horizon objectives, while sampling only ever gives us finite information. As such, we likely need to use graph-based reasoning to reach meaningful conclusions. In particular, for  $\omega$ -regular objectives, we would need to know at least the graph structure of identified end components to decide whether they are winning or not, and for mean payoff we even would need bounds on the transition probabilities. As a special case, models where each end component is guaranteed to only comprise a single state could be tractable.

## 7. Conclusion and Future Work

In this work, we improved and extended the ideas of [33], fixing several imprecisions and issues of the proofs. This results in a framework for verifying MDP, using learning algorithms. Building upon exiting methods, we thus provide novel techniques to analyse infinite-horizon reachability properties of arbitrary MDPs, yielding either exact bounds in the white-box scenario or probabilistically correct bounds in the black-box scenario. Moreover, we presented a generalization of the methods of [33], allowing for further, more sophisticated applications.

We deliberately omit an experimental evaluation. Since the inception of the presented idea, multiple tools have implemented variants and extensions thereof for several objectives and model classes. In particular, we want to point to the tool PET [113, 115], which implements

and evaluates the general complete information algorithm and presents a detailed evaluation. Moreover, as already mentioned, for DQL the associated constants are infeasible for practical application: Already for an MDP with 10 States, 20 actions and  $p_{\rm min} = 0.1$ , we obtain  $\overline{m} \approx 10^{26}$  for  $\varepsilon = 0.1$  and  $\delta = 0.01$ .

Given this framework, an interesting direction for future work would be to extend this approach with more sophisticated learning algorithms. Another, orthogonal direction is to explore whether our approach can be combined with symbolic methods.

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# A. Auxiliary Statements

In this chapter we provide some general statements about Markov chains and decision processes which are used in various proofs for the DQL algorithms.

## From Reachability to Step-bounded Reachability

In this section we prove several statements relating the infinite-horizon reachability with the reachability after a sufficiently large number of steps.

**LEMMA A.1.** For any Markov chain  $M = (S, \delta)$ , state *s*, and target set *T*, we have that either  $\Pr_{M,s}[\diamond T] = 0$  or  $\Pr_{M,s}[\diamond^{\leq |S|}T] \geq \delta_{\min}^{|S|}$ , where  $\delta_{\min}$  is the minimal transition probability, i.e.  $\delta_{\min} = \min\{\delta(s, s') \mid s \in S, s' \in \operatorname{supp} \delta(s)\}.$ 

**PROOF.** Fix the Markov chain M, state *s*, and target set *T* as in the lemma. In the first case there is nothing to prove, thus assume that  $\Pr_{M,s}[\diamond T] > 0$ . This means that there exists a finite path  $\varrho$  from *s* to some state in *T*. By the pigeon-hole principle, we can assume this path has length at most |S|. Clearly, the probability of any single transition on this path is at least  $\delta_{\min}$  and thus the overall probability of this path is at least  $\delta_{\min}^{|S|}$ .

**COROLLARY A.2.** For any MDP  $\mathcal{M} = (S, Act, Av, \Delta)$ , memoryless strategy  $\pi \in \Pi_{\mathcal{M}}^{\mathsf{MD}}$ , state *s*, and target set *T*, we have that either  $\mathsf{Pr}_{\mathcal{M},s}^{\pi}[\diamond T] = 0$  or  $\mathsf{Pr}_{\mathcal{M},s}^{\pi}[\diamond^{\leq |S|}T] \geq \delta_{\min}(\pi)^{|S|}$ , where  $\delta_{\min}(\pi) = \min\{\pi(s, a) \cdot \Delta(s, a, s') \mid s \in S, a \in Av(s), \pi(s, a) > 0, s' \in \operatorname{supp} \Delta(s, a, s')\}.$ 

**PROOF.** Follows directly from the above lemma by applying it to  $\mathcal{M}^{\pi}$ .

The following lemma shows that on a large enough horizon, step-bounded and unbounded reachability values coincide up to a small error, similar in spirit to [94, Lemma 2].

**LEMMA A.3.** Given a Markov chain  $M = (S, \delta)$ , a state  $s \in S$ , a constant  $\tau \in (0, 1]$ , and a target set T, for  $N \ge \ln(\frac{2}{\tau}) \cdot |S| \delta_{\min}^{-|S|}$  we have

$$\Pr_{\mathsf{M},s}[\Diamond T] - \Pr_{\mathsf{M},s}[\Diamond^{\leq N}T] \leq \tau.$$

**PROOF.** We can express  $\Pr_{M,s}[\diamond T]$  as a sum of  $\Pr_{M,s}[\diamond^{\leq N}T]$  and  $\Pr_{M,s}[\diamond^{>N}T]$ , where  $\diamond^{>N}T = \diamond T \setminus \diamond^{\leq N}T$  are all paths which reach the set T but only after at least N + 1 steps. Clearly,

$$\mathsf{Pr}_{\mathsf{M},s}[\diamondsuit T] - \mathsf{Pr}_{\mathsf{M},s}[\diamondsuit^{\le N}T] = \mathsf{Pr}_{\mathsf{M},s}[\diamondsuit^{>N}T]$$

By [34, Lemma 5.1] we have that  $\Pr_{M,s}[\diamondsuit^{>N}T] \le 2 \cdot c^N$ , where  $c = \exp(-|S|^{-1}\delta_{\min}^{|S|})$ .

$$2 \cdot c^{N} \leq \tau \quad \Leftrightarrow \quad N \cdot \ln c \geq \ln \frac{\tau}{2} \quad \Leftrightarrow \quad N \geq \ln \frac{\tau}{2} \cdot (\ln c)^{-1}$$
$$\Leftrightarrow \quad N \geq \ln \frac{\tau}{2} \cdot -|S|\delta_{\min}^{-|S|} \quad \Leftrightarrow \quad N \geq \ln \frac{2}{\tau} \cdot |S|\delta_{\min}^{-|S|} \qquad \blacksquare$$

### **Unique Solution of Bellman Equations**

Now, we prove that a particular class of Bellman equations has a unique solution by proving that the associated functor is a contraction.

**LEMMA A.4.** Let  $\mathcal{M}$  be an MDP,  $Av_? : S \to Act$  a function mapping a state s to a subset of its available actions  $Av_?(s) \subseteq Av(s)$ ,  $c : S \to \mathbb{R}$  a cost function, and  $\pi$  a memoryless strategy on  $\mathcal{M}$ . Define  $S_{=} = \{s \mid Av_?(s) = \emptyset\}$ .

If  $\Pr_{\mathcal{M},s}^{\pi}[\diamond S_{=}] > 0$  for all states  $s \in S$ , then the system of Bellman equations

$$f(s) = c(s) + \sum_{a \in Av_{?}(s)} \pi(s, a) \cdot \Delta(s, a) \langle f \rangle$$

has a unique solution f.

**PROOF.** Define the iteration operator *F* as

$$F(f)(s) = c(s) + \sum_{a \in Av_{?}(s)} \pi(s, a) \cdot \Delta(s, a) \langle f \rangle.$$

Trivially, a function  $f : S \to \mathbb{R}$  is a solution to the equation system if and only if it is a fixed point of *F*, i.e. F(f)(s) = f(s) for all states  $s \in S$ .

We show that  $F^{|S|}$ , i.e. F applied |S| times, is a contraction and thus has a unique fixed point, obtainable by iterating F. This means that there exists a contraction factor  $0 \le \gamma < 1$ such that for two arbitrary  $f, g : S \to \mathbb{R}$ , we have

$$\max_{s\in\mathcal{S}} \left| F^{|\mathcal{S}|}(f)(s) - F^{|\mathcal{S}|}(g)(s) \right| \le \gamma \cdot \max_{s\in\mathcal{S}} |f(s) - g(s)|.$$

$$\tag{13}$$

Let P(s, s', k) be the probability of reaching state s' starting from s in exactly k steps using the strategy  $\pi$  by using only actions from  $Av_2$ . Note that for  $s \in S_{=}$  this implies P(s, s', k) = 0 for any

 $s' \in S$  and any number k. For  $s \in S_? := S \setminus S_=$ , we have that

$$F^{|S|}(f)(s) = \sum_{s' \in S} \left( \sum_{i=0}^{|S|-1} P(s, s', i) \cdot c(s') \right) + \sum_{s' \in S_2} P(s, s', |S|) \cdot f(s')$$

Observe that the first term is independent of *f*, hence for  $s \in S_{?}$  we have

$$\begin{aligned} \left| F^{|S|}(f)(s) - F^{|S|}(g)(s) \right| \\ &= \left| \sum_{s' \in S_{?}} P(s, s', |S|) \cdot f(s') - \sum_{s' \in S_{?}} P(s, s', |S|) \cdot g(s') \right| \\ &\leq \sum_{s' \in S_{?}} P(s, s', |S|) \cdot |f(s') - g(s')| \\ &\leq \left( \sum_{s' \in S_{?}} P(s, s', |S|) \right) \cdot \max_{s' \in S} |f(s') - g(s')|. \end{aligned}$$

By assumption, we have that  $\Pr_{\mathcal{M},s}^{\pi}[\diamond S_{=}] > 0$ . This implies that  $\Pr_{\mathcal{M},s}^{\pi}[\diamond^{\leq |S|}S_{=}] \geq \delta_{\min}(\pi) > 0$ by Corollary A.2. For  $s \in S_{=}$ , observe that  $F^{|S|}(f)(s) = f(s) = c(s)$  and hence

$$\left|F^{|S|}(f)(s) - F^{|S|}(g)(s)\right| = |f(s) - g(s)| = |c(s) - c(s)| = 0.$$

Consequently,  $\gamma = \max_{s \in S_?} \sum_{s' \in S_?} P(s, s', |S|) \le \delta_{\min}(\pi) < 1$  satisfies Inequality (13) and we have that  $F^{|S|}$  is a contraction. By the Banach fixed point theorem we get that  $F^{|S|}$  has a unique fixed point and thus the equation system has a unique solution.

#### From Local to Global Error Bounds

The next lemma bounds the overall error of an approximation in an MDP given that the approximation is "close" locally. By definition

$$\Delta(s,a)\langle \pi[X]\rangle = \sum_{s'\in S} \Delta(s,a,s') \cdot \sum_{a'\in A\nu(s')} \pi(s',a') \cdot f(s',a').$$

Thus, the term  $X(s, a) - \Delta(s, a) \langle \pi[X] \rangle$  in the lemma essentially denotes the difference between the state-action value X(s, a) and the expected value obtained from X in the successors of (s, a)following  $\pi$ . Consequently,  $\mathcal{K}$  contains those state-action pairs for which the value under X is consistent with the value of its successors up to some error.

**LEMMA A.5.** Let  $\mathcal{M} = (S, Act, Av, \Delta)$  be an MDP satisfying Assumption 1,  $X : S \times Av \rightarrow [0, 1]$  a function assigning a value between 0 and 1 to each state-action pair,  $\pi$  a memoryless strategy on  $\mathcal{M}$ , and  $\kappa_l \leq \kappa_u$  two error bounds. Set

$$\mathcal{K} \coloneqq \{(s, a) \mid \kappa_l \leq X(s, a) - \Delta(s, a) \langle \pi[X] \rangle \leq \kappa_u \}.$$

Define a new MDP  $\mathcal{M}' = (S, Act, Av, \Delta')$  where

$$\Delta'(s, a) = \begin{cases} \Delta(s, a) & \text{if } (s, a) \in \mathcal{K}, \text{ and} \\ \{s_+ \mapsto X(s, a), s_- \mapsto 1 - X(s, a)\} & \text{otherwise.} \end{cases}$$

Then, for each state  $s \in S$  we have

$$\kappa_{l} \leq \frac{\delta_{\min}(\pi)^{|S|}}{|S|} \left( \pi[X](s) - \mathsf{Pr}_{\mathcal{M}',s}^{\pi}[\diamondsuit\{s_{+}\}] \right) \leq \kappa_{u},$$

where  $\delta_{\min}(\pi) = \min\{\pi(s, a) \cdot \Delta(s, a, s') \mid s \in S, a \in Av(s), \pi(s, a) > 0, s' \in \operatorname{supp}(\Delta(s, a))\}$  is the smallest transition probability in the Markov chain  $\mathcal{M}^{\pi}$ .

**PROOF.** Define  $v'(s) = \Pr_{\mathcal{M}',s}^{\pi}[\diamond\{s_+\}]$ . Furthermore, let  $\mathcal{K}(s) = \{a \in Av(s) \mid (s,a) \in \mathcal{K}\}$  and  $\neg \mathcal{K}(s) = \overline{\mathcal{K}(s)} \cap Av(s)$  the sets of all actions  $a \in Av(s)$  such that  $(s,a) \in \mathcal{K}$  and  $(s,a) \notin \mathcal{K}$ , respectively. Observe that v' is a solution to the following system of equations:

$$\begin{aligned} v'(s_{+}) &= 1\\ v'(s_{-}) &= 0\\ v'(s) &= \sum_{a \in \mathcal{K}(s)} \pi(s, a) \cdot \Delta(s, a) \langle v' \rangle + \sum_{a \in \neg \mathcal{K}(s)} \pi(s, a) \cdot X(s, a) \end{aligned}$$

We apply Lemma A.4 to show that v' is the unique solution. Let  $\varepsilon(s_+) = 1$ ,  $\varepsilon(s_-) = 0$ , and  $\varepsilon(s) = \sum_{a \in \neg \mathcal{K}(s)} \pi(s, a) \cdot X(s, a)$  for all other  $s \in S$ . Further, set  $Av_?(s_+) = Av_?(s_-) = \emptyset$  and  $Av_?(s) = \mathcal{K}(s)$  for all other  $s \in S$ . Then,  $\{s_+, s_-\} \subseteq S_=$ . The MDP  $\mathcal{M}'$  also satisfies Assumption 1, since no new ECs are introduced, and thus  $\Pr_{\mathcal{M},s}^{\pi}[\diamondsuit S_=] = 1 > 0$  for all  $s \in S$  by Lemma 2.8. Consequently, Lemma A.4 is applicable and v' is the unique solution of the above equations.

 $\pi[X]$  satisfies a similar set of equations:

$$\pi[X](s_{+}) = 1$$
  

$$\pi[X](s_{-}) = 0$$
  

$$\pi[X](s) = \sum_{a \in Av(s)} \pi(s, a) \cdot X(s, a)$$
  

$$= \sum_{a \in \mathcal{K}(s)} \pi(s, a) \cdot X(s, a) + \sum_{a \in \neg \mathcal{K}(s)} \pi(s, a) \cdot X(s, a)$$
  

$$= \kappa(s) + \sum_{a \in \mathcal{K}(s)} \pi(s, a) \cdot \Delta(s, a) \langle \pi[X] \rangle + \sum_{a \in \neg \mathcal{K}(s)} \pi(s, a) \cdot X(s, a)$$

where  $\kappa(s) = \sum_{a \in \mathcal{K}(s)} \pi(s, a) \cdot (X(s, a) - \Delta(s, a) \langle \pi[X] \rangle)$  is bounded by  $\kappa_l \leq \kappa(s) \leq \kappa_u$ . Again, by Lemma A.4, these equations then have a unique fixed point, setting  $\varepsilon(s) = \kappa(s) + \sum_{a \in \neg \mathcal{K}(s)} \pi(s, a) \cdot X(s, a)$ .

Now, we prove a bound for the difference between X and v' using the above characterizations. Observe that the above equation systems only differ structurally by the error term  $\kappa(s)$ . Let thus  $f(s) = \pi[X](s) - \nu'(s)$ . This f is a fixed point of the following equation system:

$$f(s_{+}) = f(s_{-}) = 0$$
  
$$f(s) = \kappa(s) + \sum_{a \in \mathcal{K}(s)} \pi(s, a) \cdot \Delta(s, a) \langle f \rangle$$

Clearly, f again is unique by Lemma A.4.

Given a state *s*, the probability to reach the terminal states  $s_+$  and  $s_-$  in |S| steps following strategy  $\pi$  is bounded from below by  $\delta_{\min}(\pi)^{|S|}$  due to Corollary A.2. Consequently, the probabil-

ity of not reaching these states in |S| steps is bounded from above by  $1 - \delta_{\min}(\pi)^{|S|} < 1$ . Hence, we can bound the difference between  $\pi[X]$  and  $\nu'$  by

$$\kappa(s) \cdot \sum_{n=0}^{\infty} |S| \left(1 - \delta_{\min}(\pi)^{|S|}\right)^n = \kappa(s) \cdot |S| \delta_{\min}(\pi)^{-|S|}.$$

#### **Bounding Reachability on Similar MDP**

In this lemma, we show that MDP which are sufficiently "similar" also have similar reachability values. In particular, we are concerned with MDP that agree on a subset of states. For another notion of similarity (same transition structure but different transition probabilities) see [44].

**LEMMA A.6.** Let  $\mathcal{M} = (S, Act, Av, \Delta)$  be an MDP,  $T \subseteq S$  a set of target states,  $\mathcal{K} \subseteq S \times Av$  a set of state-action pairs, and  $\mathcal{M}' = (S', Act', Av', \Delta')$  an arbitrary MDP with  $\mathcal{K} \subseteq S' \times Av'$  that coincides with  $\mathcal{M}$  on  $\mathcal{K}$  and T, i.e. (i) Av(s) = Av'(s) for all  $s \in \mathcal{K}$ , (ii)  $\Delta(s, a) = \Delta'(s, a)$  for all  $(s, a) \in \mathcal{K}$ , and (iii)  $T \subseteq S'$ . Moreover, let  $\pi$  be a strategy in  $\mathcal{M}$ ,  $s \in S \cap S'$  an arbitrary state in both MDP, and  $N \in \mathbb{N}$  a natural number. Then,

$$\mathsf{Pr}_{\mathcal{M},s}^{\pi}[\diamondsuit^{\leq N}T] \geq \mathsf{Pr}_{\mathcal{M}',s}^{\pi'}[\diamondsuit^{\leq N}T] - \mathsf{Pr}_{\mathcal{M},s}^{\pi}[\diamondsuit^{\leq N}\overline{\mathcal{K}}],$$

where  $\pi'$  is an arbitrary strategy equal to  $\pi$  on all finite paths over  $\mathcal{K}$ , i.e.  $\pi(\varrho) = \pi'(\varrho)$  for all  $\varrho \in \mathcal{K}^* \times S \cap \text{FPaths}_{\mathcal{M}}$ .

**PROOF.** For a finite path  $\varrho = s_1 a_1 \dots a_{n-1} s_n \in \text{FPaths}_{\mathcal{M}}$ , let  $\Pr_{\mathcal{M},s}^{\pi}[\varrho]$  denote the probability of path  $\varrho$  occurring when following strategy  $\pi$  from state s. Let  $\mathcal{K}_N$  denote the (finite) set of all finite paths  $\varrho$  of length N starting in s such that all state-action pairs  $(s_i, a_i)$  in  $\varrho$  are in  $\mathcal{K}$ . Similarly, let  $\neg \mathcal{K}_N$  denote the set of all such paths containing at least one state-action pair not in  $\mathcal{K}$ . Let  $\mathcal{R}(\varrho)$  be a function which returns 1 if some target state of T is in path  $\varrho$  and 0 otherwise. Then, we have the following:

$$\Pr_{\mathcal{M}',s}^{\pi'}[\diamondsuit^{\leq N}T] - \Pr_{\mathcal{M},s}^{\pi}[\diamondsuit^{\leq N}T]$$

$$\sum \left(\Pr_{\mathcal{M}',s}^{\pi'}[\varrho] \cdot \mathcal{R}(\varrho) - \Pr_{\mathcal{M},s}^{\pi}[\varrho] \cdot \mathcal{R}(\varrho)\right) +$$
(14)

$$= \frac{\sum_{\varrho \in \mathcal{K}_{N}} (\mathsf{Pr}_{\mathcal{M}',s}^{\pi'}[\varrho] \cdot \mathcal{R}(\varrho) - \mathsf{Pr}_{\mathcal{M},s}^{\pi}[\varrho] \cdot \mathcal{R}(\varrho))}{\sum_{\varrho \in \neg \mathcal{K}_{N}} (\mathsf{Pr}_{\mathcal{M}',s}^{\pi'}[\varrho] \cdot \mathcal{R}(\varrho) - \mathsf{Pr}_{\mathcal{M},s}^{\pi}[\varrho] \cdot \mathcal{R}(\varrho))}$$
(15)

$$= \sum_{\varrho \in \neg \mathcal{K}_{N}} \left( \mathsf{Pr}_{\mathcal{M}',s}^{\pi'}[\varrho] \cdot \mathcal{R}(\varrho) - \mathsf{Pr}_{\mathcal{M},s}^{\pi}[\varrho] \cdot \mathcal{R}(\varrho) \right)$$
(16)

$$\leq \sum_{\varrho \in \neg \mathcal{K}_{N}} \Pr_{\mathcal{M}',s}^{\pi'}[\varrho] \cdot \mathcal{R}(\varrho)$$
(17)

$$\leq \sum_{\varrho \in \neg \mathcal{K}_N} \mathsf{Pr}_{\mathcal{M}',s}^{\pi'}[\varrho] \tag{18}$$

$$= \mathsf{Pr}^{\pi}_{\mathcal{M},s}[\diamondsuit^{\leq N}\overline{\mathcal{K}}] \tag{19}$$

In Equation (15), we simply split the set of all paths of length N into  $\mathcal{K}_N$  and  $\neg \mathcal{K}_N$ . For Equations (16) and (19), note that  $\Pr_{\mathcal{M}',s}^{\pi'}$  and  $\Pr_{\mathcal{M},s}^{\pi}$  agree on  $\mathcal{K}_N$  by choice of  $\mathcal{M}'$  and  $\pi'$ .

# **Repeating Events in Markov Processes**

Finally, we prove a general statement of Markov processes. The statement itself seems to be quite obvious, yet surprisingly tricky to prove. In essence, we want to show the following. Suppose that we are given a Markov process  $X_t$  on some probability space  $\Omega$  together with a sequence of events  $A_t$ . Moreover, assume that for a significant set of atoms  $\omega \in \Omega$  there is an infinite set of times T such that the *conditional* probability of  $A_t$  occurring is at least  $\varepsilon > 0$ , i.e.  $\mathbb{P}[X_t \in A_t \mid X_{t-1}(\omega)] > \varepsilon$ . Then, the set of atoms for which infinitely many  $A_t$  actually occur is also significant. The subtle difficulty of this statement arises from the fact that (i) conditional probabilities are considered, and (ii) the set T depends on the particular atom  $\omega$ .

**LEMMA A.7.** Fix some probability space  $(\Omega, \mathcal{F}, \mathbb{P})$  and a measure space (S, S). Let  $X_t : \Omega \to S$ be a Markov process on  $\Omega$  and  $A_t \in S$  measurable events in S. Assume that the set  $\Omega' = \{\omega \in \Omega \mid \exists T. |T| = \infty \land \forall t \in T. \mathbb{P}[X_t \in A_t \mid X_{t-1}](\omega) > \varepsilon\}$  has positive measure, i.e.  $\mathbb{P}[\Omega'] > 0$ , and that  $\Omega'_t = \{\omega \in \Omega \mid \mathbb{P}[X_t \in A_t \mid X_{t-1}](\omega) > \varepsilon\}$  is measurable for all  $t \in \mathbb{N}$ . Then,  $\mathbb{P}[\{\omega \in \Omega \mid \exists T. |T| = \infty \land \forall t \in T. X_t(\omega) \in A_t\}] = \mathbb{P}[\Omega']$ .

**PROOF.** Let  $\omega \in \Omega'$ . By assumption, for each such  $\omega$ , there exists an infinite set of time-points  $\operatorname{Tries}(\omega) = \{t_1, t_2, \cdots\}$  with  $1 \leq t_1 < t_2 < \cdots$  where  $\mathbb{P}[X_t \in A_t \mid X_{t-1}](\omega) > \varepsilon$ . We call such an event a *try* of  $\omega$ . Denote  $\operatorname{Try}_i(\omega) = t_i$  or  $\infty$  if no such  $t_i$  exists, e.g. for  $\omega \notin \Omega'$ . Informally,  $\operatorname{Try}_i$  is the time of the *i*-th try of some outcome  $\omega$ .  $\operatorname{Try}_i$  is measurable by assumption, since its pre-images can be constructed using  $\Omega'_t$ . Moreover, let  $\operatorname{Succs}(\omega) = \{s_1, s_2, \cdots\} \subseteq \operatorname{Tries}(\omega)$  be the times where  $X_{s_j}(\omega) \in A_{s_j}$ , called *j*-th success(ful try). Note that  $\operatorname{Succs}(\omega)$  possibly is finite or even empty for some outcomes  $\omega$ , even for  $\omega \in \Omega'$ , since infinitely many tries may fail. Now, let  $\operatorname{Succ}_j(\omega) = s_j \in \operatorname{Succs}(\omega)$  the time of the *j*-th success or  $\infty$  if no such  $s_j$  exists, i.e.  $j > |\operatorname{Succs}(\omega)|$ . Succ<sub>j</sub> is measurable since  $\operatorname{Try}_i, X_t$  and  $A_t$  are measurable. To succinctly capture corner-cases, we further define  $\operatorname{Succ}_j(\omega) = 0$ . The successes  $\operatorname{Succs}(\omega)$  naturally partition the set  $\operatorname{Tries}(\omega)$  into  $\operatorname{TriesJ}_j(\omega) = \{t \in \operatorname{Tries}(\omega) \mid \operatorname{Succ}_j(\omega) < t \leq \operatorname{Succ}_{j+1}(\omega)\}$ . We use  $\operatorname{TryJ}_{i,j}(\omega)$  to refer to the *i*-th element of  $\operatorname{TriesJ}_j(\omega)$ , or  $\infty$  if no such element exists.  $\operatorname{TryJ}_{i,j}$  is measurable due to  $\operatorname{Succ}_j$  being measurable. Informally,  $\operatorname{TryJ}_{i,j}(\omega)$  denotes the time of the *i*-th try since the *j*-th success.

We show that after a sufficient number of tries, there is a success with high probability. Repeating this argument inductively, we then show that there are infinitely many successes for almost all outcomes  $\omega$  in  $\Omega'$ .

Let thus  $\text{TryAtTJ}_{i,j}^{t}$  denote the set of runs which at time *t* have succeeded *j* times and since the *j*-th success experienced *i*-th tries, where this *i*-th try happens exactly at time *t*. Formally,

$$\mathsf{TryAtTJ}_{i,j}^t \coloneqq \{\omega \in \Omega' \mid \mathsf{TryJ}_{i,j}(\omega) = t\}.$$

Note that this definition implicitly includes the condition  $\text{Succ}_{j}(\omega) \leq t < \text{Succ}_{j+1}(\omega)$  by definition of  $\text{TryJ}_{i,j}$ . Thus,  $\text{TryAtTJ}_{i,j}^{t}$  are disjoint for fixed *i* and *j*.

We furthermore define  $\text{TriesJ}_{i,j} = \bigcup_{t=1}^{\infty} \text{TryAtTJ}_{i,j}^{t} = \{\omega \in \Omega' \mid \text{TryJ}_{i,j}(\omega) < \infty\}$  as the set of outcomes which after their *j*-th success experienced at least  $i - 1^{11}$  unsuccessful tries. We have  $\text{TriesJ}_{i,j} = \text{TriesJ}_{i+1,j} \cup \text{TriesJ}_{1,j+1}$ , since the *i*-th try either fails and the i + 1-th try is experienced later (since  $\text{TriesJ}_{i,j} \subseteq \Omega'$ , implying infinitely many tries) or the try succeeds. Observe that  $\text{TriesJ}_{i+1,j}$  and  $\text{TriesJ}_{1,j+1}$  are not disjoint, since, for example, the runs succeeding at the i + 1-th try also are an element of  $\text{TriesJ}_{1,j+1}$ . On the contrary, we show that  $\mathbb{P}[\text{TriesJ}_{i,j} \setminus \text{TriesJ}_{1,j+1}] = 0$ , i.e. almost all runs in  $\text{TriesJ}_{i,j}$  will eventually succeed again.

To this end, we argue that for any fixed j we have that  $\lim_{i\to\infty} \mathbb{P}[\text{TriesJ}_{i,j}] = 0$ . Fix some jand i with  $\mathbb{P}[\text{TriesJ}_{i,j}] > 0$  (otherwise there is nothing to prove, since  $\text{TriesJ}_{i,j}$  is monotonically decreasing in i). Let  $\text{TryTimesJ}_{i,j} = \{t \mid \mathbb{P}[\text{TryAtTJ}_{i,j}^t] > 0\}$  which is non-empty by the previous condition. Clearly,  $\mathbb{P}[\text{TriesJ}_{i,j}] = \sum_{t=1}^{\infty} \mathbb{P}[\text{TryAtTJ}_{i,j}^t] = \sum_{t\in\text{TryTimesJ}_{i,j}} \mathbb{P}[\text{TryAtTJ}_{i,j}^t]$ , as  $\text{TryAtTJ}_{i,j}^t$  are disjoint. Observe that  $\text{TryAtTJ}_{i,j}^t$  is the intersection of several conditions on  $X_{t'}$  for t' < t and requiring that  $\mathbb{P}[X_t \in A_t \mid X_{t-1}] > \varepsilon$ . Hence, by the Markov property

$$\mathbb{P}[X_t \notin A_t \mid \mathsf{TryAtTJ}_{i,j}^t] = 1 - \mathbb{P}[X_t \in A_t \mid \mathsf{TryAtTJ}_{i,j}^t] = 1 - \mathbb{P}[X_t \in A_t \mid X_{t-1}] < 1 - \varepsilon.$$

Intuitively, this means that the probability of a try at time t succeeding does not depend on the number of previous tries and successes. Thus, for all  $t \in \text{TryTimesJ}_{i,j}$ , we have  $\mathbb{P}[X_t \notin A_t \cap \text{TryAtTJ}_{i,j}^t] < (1 - \varepsilon) \cdot \mathbb{P}[\text{TryAtTJ}_{i,j}^t]$ . Observe that  $\bigcup_{t=1}^{\infty} (X_t \notin A_t \cap \text{TryAtTJ}_{i,j}^t) = \text{TriesJ}_{i+1,j}$  since the intersection implies that the *i*-th try at time t was unsuccessful. Together,

$$\mathbb{P}[\mathsf{TriesJ}_{i+1,j}] = \mathbb{P}[\bigcup_{t=1}^{\infty} X_t \notin A_t \cap \mathsf{TryAtTJ}_{i,j}^t] = \sum_{t=1}^{\infty} \mathbb{P}[X_t \notin A_t \cap \mathsf{TryAtTJ}_{i,j}^t] \\ = \sum_{t \in \mathsf{TryTimesJ}_{i,j}} \mathbb{P}[X_t \notin A_t \cap \mathsf{TryAtTJ}_{i,j}^t] \\ < \sum_{t=1}^{\infty} (1-\varepsilon) \cdot \mathbb{P}[\mathsf{TryAtTJ}_{i,j}^t] = (1-\varepsilon) \cdot \mathbb{P}[\bigcup_{t=1}^{\infty} \mathsf{TryAtTJ}_{i,j}^t] \\ = (1-\varepsilon) \cdot \mathbb{P}[\mathsf{TriesJ}_{i,j}].$$

Consequently,  $\lim_{i\to\infty} \mathbb{P}[\text{TriesJ}_{i,j}] = 0$  for any fixed *j*.

As argued before, we have  $\text{TriesJ}_{i,j} = \text{TriesJ}_{i+1,j} \cup \text{TriesJ}_{1,j+1}$ . Iterating this equation yields  $\text{TriesJ}_{i,j} = \text{TriesJ}_{i+k,j} \cup \text{TriesJ}_{1,j+1}$  for any  $k \ge 1$  and consequently  $\text{TriesJ}_{1,j} = \bigcap_{i=1}^{\infty} \text{TriesJ}_{i,j} \cup \text{TriesJ}_{1,j+1}$ . Informally, this equation can be read as "all outcomes which succeed at least j times either try infinitely often or succeed at least j+1 times." Let  $\text{TriesJ}_{\infty,j} = \bigcap_{i=1}^{\infty} \text{TriesJ}_{i,j} = \{\omega \in \Omega' \mid \text{Succ}_j(\omega) < \omega = \text{Succ}_{j+1}(\omega)\}$ . Clearly,  $\text{TriesJ}_{\infty,j} \cap \text{TriesJ}_{1,j+1} = \emptyset$ , thus we have  $\mathbb{P}[\text{TriesJ}_{1,j+1} \setminus \text{TriesJ}_{1,j}] = \mathbb{P}[\text{TriesJ}_{\infty,j}]$ . Additionally, we have  $\mathbb{P}[\text{TriesJ}_{\infty,j}] = \inf_{i \in \mathbb{N}} \mathbb{P}[\text{TriesJ}_{i,j}] = 0$  by the above reasoning. Hence  $\mathbb{P}[\text{TriesJ}_{1,j+1} \setminus \text{TriesJ}_{1,j}] = 0$ . This implies that almost all runs in  $\Omega'$  succeed infinitely often, concluding the proof.

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# TheoretiCS

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<sup>11</sup> TryJ<sub>*i*,*j*</sub>( $\omega$ ) = *t* does not exclude that the try at time t is successful.