Finding Safe Zones of Markov Decision Processes Policies

Lee Cohen[*] **Yishay Mansour**[†] **Michal Moshkovitz**[‡]

Abstract

Given a policy, we define a SAFEZONE as a subset of states, such that most of the policy's trajectories are confined to this subset. The quality of the SAFEZONE is parameterized by the number of states and the escape probability, i.e., the probability that a random trajectory will leave the subset. SAFEZONES are especially interesting when they have a small number of states and low escape probability.

We study the complexity of finding optimal SAFEZONES, and show that in general, the problem is computationally hard. For this reason, we concentrate on computing approximate SAFEZONES. Our main result is a bi-criteria approximation algorithm which gives a factor of almost 2 approximation for both the escape probability and SAFEZONE size, using a polynomial size sample complexity. We conclude the paper with an empirical demonstration of our algorithm.

1 Introduction

Most research in reinforcement learning (RL) deals with the problem of learning an optimal policy for some Markov decision process (MDP). One notable exception for that is Safe RL, that focuses on finding the best policy that meets safety requirements. Typically, these problems are handled by adjusting the objective to include safety requirements and then optimizing over it, or incorporating additional safety constraints to the exploration stage. Anomaly Detection is the problem of identifying patterns in data that do not correspond to what is expected, i.e., anomalies. Anomaly Detection addresses a variety of applications: cyber-security, fraud detection, failure detection, etc. (see Chandola et al. (2009) for survey).

In this paper, we introduce the SAFEZONE problem, a general approach for safe RL and anomaly detection that concentrates on a given policy rather than finding a policy that follows some predefined safety specifications and emphasizes entire trajectories in order to detect anomalies.

Consider a policy for a finite horizon MDP. The policy induces a Markov Chain (MC) on the MDP. Given a subset of states, we define the *escape probability* to be the probability that a random trajectory has at least one state outside this subset (hence the trajectory *escapes* it). A SAFEZONE is a subset of states whose quality is measured by its' size and escape probability (ideally, both are small). If a SAFEZONE has low escape probability, we consider it *safe*.

Trivial SAFEZONE solutions are the entire set of states (which has minimal escape probability of 0 on the account of maximal size), and the empty set (which has minimal size but has maximal escape probability of 1). We are interested to find SAFEZONE with a good tradeoff: namely a relatively small set size with small escape probability. More precisely, given a bound over the escape probability, $\rho > 0$, the goal of the learner is, using trajectory sampling, to find the smallest SAFEZONE with escape probability at most ρ. We address unknown environment, by which we

[*]Tel Aviv University. Email: leecohencs@gmail.com.
[†]Tel Aviv University and Google Research. Email: mansour.yishay@gmail.com.
[‡]Tel Aviv University. Email: moshkovitz5@mail.tau.ac.il.

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mean no prior knowledge on the transition function or the policy used. The learner can only access random trajectories generated by the induced MC. For many applications, if there exists such a small SAFEZONE it is useful to find it.

Consider for example automatic robotic arm that assembles products. If something unusual happened during the assembly of a product, it might result in a malfunctioning product. In that case, the operator should be notified (anomaly detection). On the other hand, we would not like to call the operator too often. If we find a SAFEZONE, we can make sure that we notify the operator only in the rare events the production process (trajectory) escapes it. Furthermore, if the SAFEZONE is small, the manufacturer can potentially test the SAFEZONE states and verify their compliance, ensuring that the majority of products are well constructed for a significantly lower testing budget.

Another useful application is infrastructure design for autonomous vehicles. Even though a lot of the progress in the field of autonomous driving is credited to sensors installed on Autonomous Vehicles, relying solely on the vehicles' sensors has its limitations (e.g., Yang et al. (2020)). For example, in extreme weather, if a vehicle unintentionally deviates from the current lane, the sensors' data might not trigger a response in time. Vehicular-to-Infrastructure (V2I) is a type of communication network between vehicles and road infrastructures that are designed to fill the need for an extra layer of security. In particular, the 'V2I Deployment Coalition' is an initiative by U.S. Department of Transportation with the vision of "An integrated national infrastructure that provides the country a connected, safe and secure transportation system taking full advantage of the progress being made in the Connected and Autonomous Vehicle arenas."[4] Road Side units (RSUs) are the sensors installed along roads that together with on-board units (on vehicles) span the V2I communication. As the resources for RSUs distribution are limited, and their enhanced safety abilities are key for autonomous vehicle adaptation, SAFEZONE can help distributing RSUs in a way that covers popular commutes efficiently. Namely, given data commutes in populated areas, governments can install RSUs in the SAFEZONE which will accommodate popular commutes, from starting point to destination.

We remark that finding a SAFEZONE alone does not suffice for safety; Rather, a nearly optimal SAFEZONE is a behavioral description that can be used for safety applications, such as safer self driving cars. As another example, efficient testing (of states within the SAFEZONE) that "captures" most of the products' assembly process would improve safety.

Other motivations include imitation learning with compact policy representation. Namely, design a smaller state policy that preforms well for most cases but might be undefined on some states. In this case, trajectories that reach undefined states have zero reward, and such trajectories are captured by the escape probability. One natural application for that is creating a 'lite' version for a given software such as Microsoft's Windows Lite.

Our work can also be viewed through the lens of explainable RL, where the goal is to explain a specific policy. SAFEZONE is a new post-hoc explanation of the summarization type (Alharin et al., 2020). Going back to the V2I example, a goverment could provide a convincing explanation to its community for the chosen design.

Our results include approximation algorithms for the SAFEZONE problem, which we show is NP-hard, even when the model is given and the horizon is small ($H = 2$). We are interested in a good tradeoff between the escape probability of the SAFEZONE and its size. Our algorithms are evaluated based on two criteria: their approximation factors (w.r.t. the escape probability bound and the optimal set size for this bound), and their trajectory sample complexity bounds (e.g., Even-Dar et al. (2002)).

Our results are the following:

1. Introducing the SAFEZONE problem (Section 2), and some of its applications.
2. We explore naive approaches, namely greedy algorithms that select SAFEZONES based on state distributions and trajectory sampling. In addition, we show cases in which their solutions are far from optimal, either in terms of high escape probability or significantly larger set size (see Section 3).
3. We design FINDING SAFEZONE, an efficient approximation algorithm with provable guarantees. The algorithm returns a SAFEZONE which is slightly more than twice in terms of both the size and the escape probability compared to the optimal (see Section 4).

[4]https://transportationops.org/V2I/V2I-overview

4. We prove that finding a SAFEZONE is NP-hard, even for horizon $H = 2$ and known environment setting (i.e., when the induced Markov chain is given) in Section 6.
5. We conclude the paper with an empirical demonstration in Appendix A.

For brevity, some algorithms and (full) proofs are relegated to the appendix.

Trajectory escaping. The SAFEZONE problem deals escaping trajectories. In particular, given a SAFEZONE, a trajectory escapes it, no matter if only one of its states is outside the SAFEZONE or all of them. A related, yet very different problem, is that of minimizing a subset size, such that the expected number of states outside the set is minimized. This related problem, while significantly easier (as it is solved by returning the most visited states), does not apply to the applications we described earlier. In Section 3, we show that the solution for the SAFEZONE does not necessarily overlaps with the most visited states. Furthermore, simply returning states which appeared in trajectory samples could result in a set size far from optimal.

1.1 Related Work

MDPs have been studied extensively in the context of decision making in particular by the Reinforcement Learning (RL) community (see Puterman (1994) for a broad background on MDPs, and Sutton & Barto (2018) for background on reinforcement learning).

Safe RL. A related line of research is safe RL, where the learner's goal is to find the best policy that satisfies safety guarantees. The two main methodologies to handle such problems are: (1) altering the objective to include the safety requirement and optimizing over it, and (2) adding safety constraints to the exploration part. See Pfrommer et al. (2021); Emam et al. (2021); Xu et al. (2021); Hendrycks et al. (2021); HasanzadeZonuzy et al. (2021) for recent works and García & Fernández (2015); Amodei et al. (2016) for surveys. In our work, the goal is not to find the optimal policy, but instead given a policy, finding its SAFEZONE. Moreover, the SAFEZONE problem is not characterized by specific requirements, and beyond the MDP, the solution could very much depend on the given policy.

Imitation Learning. In imitation learning, the learner observes a policy behaviour and wants to imitate it (see Hussein et al. (2017) for survey). Similar to imitation learning, we are given access to samples of a given policy. In contrast, rather than imitating the policy we find the policy's SAFEZONE, which is an important property of the policy.

Approximate MDP equivalence. Another related research line is that of finding an (almost) equivalent minimal model for a given MDP, where the goal is that the optimal policy on the (almost) equivalent model induces an (approximately) optimal policy in the original MDP, e.g., Givan et al. (2003); Even-Dar & Mansour (2003). This line of works and ours differ in that we do not try to modify the MDP (e.g., cluster similar states), but rather to find a SAFEZONE, a property which is defined for the existing MDP and a specific policy.

Explainability. In explainability, the goal is to provide a post-hoc explanation to a specific given model Molnar (2019), e.g., using decision trees Blanc et al. (2021); Moshkovitz et al. (2021), influential examples Koh & Liang (2017), or a local approximation explanations Li et al. (2020). We focus on explainability for reinforcement learning, and specifically we suggest a new summarization explanation through our SAFEZONE, Amir & Amir (2018).

MC with traps. A decision problem that might seem related to ours is that of MC with traps (den Hollander et al. (1995)): Given an input of a MC (with possibly infinite state space), a starting state, and states trapping (absorbing) probabilities, the goal is to decide whether or not a (possibly infinite) random walk would reach an absorbing state with probability 1, or not. In Appendix G, we explain why this problem is inherently different than SAFEZONE.

2 The Safe Zone Problem

We model the problem using a Markov model with finite horizon $H > 1$. Formally, there is a Markov chain (MC) $\langle \mathcal{S}, P, s_0 \rangle$ where $\mathcal{S}$ is the set of states, $s_0 \in \mathcal{S}$ is the initial state and $P : \mathcal{S} \times \mathcal{S} \to [0, 1]$ is the transition function that maps a pair of states into probability by $P(s, s') = \Pr[s_{t+1} = s' | s_t = s]$. We assume the transition function P is induced by a policy $\pi : \mathcal{S} \to \text{Simplex}^{\mathcal{A}}$ on an MDP $\langle \mathcal{S}, s_0, P', \mathcal{A} \rangle$ with transition function $P' : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \to [0, 1]$ such that $P(s, s') =$

Table 1: Upper bounds for safety and size. * Only for layered MDPs.

ALGORITHM	SAFE	SET SIZE	SAMPLE COMPLEXITY
GREEDY BY THRESHOLD	2ρ	$k^* H/\rho$	–
SIMULATION	2ρ	$O(k^* H \ln k^*)$	$poly(k^*, \frac{1}{\rho})$
GREEDY AT EACH STEP*	ρH	k^*	–
FINDING SAFEZONE	$2\rho + 2\epsilon$	$(2+\delta)k^*$	$poly(k^*, H, \frac{1}{\epsilon}, \frac{1}{\delta})$

$\sum_{a \in \mathcal{A}} P'(s,a,s') \cdot \pi(a|s)$ for all $s, s' \in \mathcal{S}$ (though any MC can be generated this way, thus our theoretical guarantees apply for general MCs).

A *trajectory* $\tau = (s_0, \ldots, s_H)$ starts in the initial state s_0 and followed by a sequence of H states generated by P, i.e., $\Pr[s_{i+1} = s' | s_i = s] = P(s, s')$ for all $i \in [H]$, where $[H] := \{1, \ldots, H\}$. We abuse the notation and regard a trajectory τ both as a sequence and a set.

Given a subset of states $F \subseteq \mathcal{S}$, a trajectory τ *escapes* F if it contains at least one state $s \in \tau$ such that $s \notin F$, i.e., $\tau \nsubseteq F$. We refer to the probability that a random trajectory escapes F as *escape probability* and denote it by $\Delta(F) = \Pr_\tau[\tau \nsubseteq F]$. We call F a $\rho-$*safe* (w.r.t. the model $\langle \mathcal{S}, s_0, P \rangle$) if its escape probability, $\Delta(F)$, is at most ρ. Formally,

Definition 2.1. *A set $F \subseteq \mathcal{S}$ is $\rho-$safe if*

$$\Delta(F) := \Pr_\tau[\tau \nsubseteq F] \leq \rho,$$

where τ is a random trajectory.

A set $F \subseteq \mathcal{S}$ is called $(\rho, k)-$SAFEZONE if F is $\rho-$safe and $|F| \leq k$. Given a safety parameter $\rho \in (0,1)$, we denote the smallest size $\rho-$safe set by $k^*(\rho)$:

$$k^*(\rho) = \min_{F \subseteq \mathcal{S} \text{ is } \rho-\text{safe}} |F|.$$

Whenever the discussed parameter ρ is clear from the context we use k^* instead of $k^*(\rho)$. We remark that there might be multiple different $(\rho, k)-$SAFEZONE sets.

The learner knows the set of states, $\mathcal{S}$, the initial state, s_0, and the horizon H but has no knowledge regarding the transition function P or the minimal size of the $\rho-$safe set, k^*. Instead, the learner receives information about the model from sampling trajectories from the distribution induced by π.

Given $\rho > 0$, the ultimate goal of the learner would have been to find a $(\rho, k^*(\rho))-$SAFEZONE. However, as we show in Section 6, finding a $(\rho, k^*(\rho))-$SAFEZONE is NP-hard, even when the transition function P is known. This is why we loosen the objective to find a bi-criteria approximation $(\rho', k')-$SAFEZONE . (Bi-criteria approximations are widely studied in approximation and online algorithms Vazirani (2001); Williamson & Shmoys (2011).) In our setting, given ρ the objective is to find a set F which is $(\rho', k')-$SAFEZONE with minimal size $k' \geq k^*$ and minimal escape probability $\rho' \geq \rho$. In addition, we are interested in minimizing the sample complexity.

Notice that the learner can efficiently verify, with high probability, whether a set F is approximately $\rho-$safe or not. The following proposition formalize this and follows directly from Lemma C.2.

Proposition 2.2. *There exists an efficient algorithm such that for every set $F \subseteq \mathcal{S}$ and parameters $\epsilon, \lambda > 0$, the algorithm samples $O(\frac{1}{\epsilon^2} \ln \frac{1}{\lambda})$ random trajectories and returns $\widehat{\Delta}(F)$, such that with probability at most λ we have $|\Delta(F) - \widehat{\Delta}(F)| \geq \epsilon$.*

Summary of Contributions. We summarize the results of all the algorithms that appear in the paper in Table 1. The bounds of GREEDY BY THRESHOLD and GREEDY AT EACH STEP requires the Markov Chain model as input, and a pre-processing step that takes $O(|S|^2 H)$ time. Additionally, the bounds for first three algorithms (the naive approaches) requires an additional knowledge of $k^*(\rho)$. Beyond the upper bounds, we provide instances that show that the upper bounds are tight up to a constant for each of the first three algorithms (the naive approaches). The following theorem is an informal statement of our main theorem, Theorem 4.2.

Theorem 2.3. *For every $\rho, \epsilon, \delta > 0$, with probability ≥ 0.99 there exists an algorithm that returns a set which is* $(2\rho + 2\epsilon, (2+\delta)k^*) - \text{SAFEZONE}$.

The running time of the algorithm is also bounded by $poly(k^*, H, \frac{1}{\delta}, \frac{1}{\epsilon})$. We empirically evaluate the suggested algorithms on a grid-world instance (where the goal is to reach an absorbing state), showing that FINDING SAFEZONE outperforms the naive approaches. Moreover, we show that different policies have qualitatively different SAFEZONES. Finally, an informal statement of Theorem 6.2.

Theorem 2.4. SAFEZONE *is NP-hard.*

3 Gentle Start

This section explains and analyzes various naive algorithms to the SAFEZONE problem. We show that even if the transition function is known in advance, these naive algorithms result in outputs that are far from optimal. To describe the algorithms, we define for each state s the probability to appear in a random trajectory and denote it by $p(s) = \Pr_\tau[s \in \tau] \in [0, 1]$. Note that $\sum_{s \in \mathcal{S}} p(s)$ is a number between 1 and H (e.g., $p(s_0) = 1$), and can be estimated efficiently using dynamic programming if the environment and policy are known and sampling otherwise. To be precise, some of the algorithms assume the probabilities $\{p(s)\}_{s \in \mathcal{S}}$ are received as input.

Greedy by Threshold Algorithm. The algorithm gets, in addition to ρ, the distribution p and a parameter $\beta > 0$ as input. It returns a set F that contains all states s with probability at least β, i.e., $p(s) \geq \beta$. We formalize this idea as Algorithm 3 in Appendix B. For $\beta = \frac{\rho}{k^*}$, the output of the algorithm is $\left(2\rho, \frac{k^* H}{\rho}\right) - \text{SAFEZONE}$. More generally, we prove the following lemma.

Lemma 3.1. *For any $\rho, \beta \in (0,1)$, the* GREEDY BY THRESHOLD ALGORITHM *returns a set that is* $(\rho + k^*\beta, \frac{H}{\beta}) - \text{SAFEZONE}$. *In particular, for $\beta = \frac{\rho}{k^*}$, this set is* $\left(2\rho, \frac{k^* H}{\rho}\right) - \text{SAFEZONE}$.

While it is clear why there are instances for which the safety is tight, Lemma B.1 in Appendix B shows that the set size is tight as well.

Simulation Algorithm. The algorithm samples $O(\frac{\ln k^*}{\beta})$ random trajectories and returns a set F with all the states in theses trajectories. It is formalized in Appendix B as Algorithm 4.

Lemma 3.2. *Fix $\rho, \beta \in (0, 1)$. With probability at least 0.99,* SIMULATION *Algorithm returns a set that is* $\left(\rho + k^*\beta, O(k^* + \frac{\rho H \ln k^*}{\beta})\right) - \text{SAFEZONE}$. *In particular, for $\beta = \frac{\rho}{k^*}$, this set is* $(2\rho, O(k^* H \ln k^*)) - \text{SAFEZONE}$.

While this algorithm achieves a low escape probability, only 2ρ, in Lemma B.2 in the appendix we prove that the size of F is tight up to a constant, i.e., an MDP instance where $|F| = \Omega(k^* H \ln k^*)$.

So far, the presented algorithms were approximately safe (i.e., low escape probability), but might return large subsets. Without further assumptions, the following algorithm provides a $(\rho H, Hk^*) - \text{SAFEZONE}$. However, when considering MDPs with a special structure it provides an optimal sized SAFEZONE , at the price of large escape probability.

Greedy at Each Step Algorithm. For the analysis of the next algorithm we assume the MDP is *layered*, i.e., there are no states that appear in more than a single time step and denote $\mathcal{S} = \bigcup_{i=1}^{H} \mathcal{S}_i$. I.e., the transitions $P(s, s')$ are nonzero only for $s' \in \mathcal{S}_{i+1}$ and $s \in \mathcal{S}_i$. The GREEDY AT EACH STEP ALGORITHM takes at each time step i the minimal number of states such that the sum of their probabilities is at least $1 - \rho$. It is formalized in Appendix B as Algorithm 5.

Lemma 3.3. *For any $\rho \in (0, 1)$, if the MDP is layered,* GREEDY AT EACH STEP ALGORITHM *returns a set that is* $(\rho H, k^*) - \text{SAFEZONE}$.

In Lemma B.3 we have a lower bound on the escape probability, which asymptotically matches.

Weaknesses of the naive algorithms. We showed algorithms that identify SAFEZONE with either escape probability much greater than ρ or with size much greater than k^*. This holds even when providing extra information (such as the transition function and/or the optimal size of the $\rho-$safe set, i.e., k^*). Moreover, we showed tight lower bounds for these algorithms.

4 Algorithm for Detecting Safe Zones

In this section we suggest a new algorithm that builds upon and improves the added trajectory selection of the SIMULATION Algorithm. One reason for why SIMULATION returns a large set is that it treats every sampled trajectory identically, regardless of how many states are being added.

More precisely, fix any $(\rho, k^*)-$SAFEZONE set, F^*, and consider a trajectory τ that escapes it, i.e., $\tau \nsubseteq F^*$. If τ was sampled, its states are added to the constructed set F, which might increase the size of F by up to H states that are not in F^*, without significantly improving the safety.

In contrast, when selecting which trajectory to add to F, we would consider the number of states it adds to the current set. For the sake of readability, we refer to any state which is not in the current set F as *new*, and denote by $new_F(\tau)$ the number of new states in τ w.r.t. F, i.e.,

$$new_F(\tau) := |\tau \setminus F|.$$

Note that for every $F \subseteq \mathcal{S}$, we have that $\Pr_\tau[new_F(\tau) \neq 0] = \Delta(F)$.

The new algorithm does not sample each trajectory uniformly at random, but sample from a new distribution, which will be denoted by Q_F. While favoring trajectories with higher probabilities, which we already get by the sampling process, another key idea would guide this new distribution: To prefer trajectories that *gradually* increase the size of F. To implement this idea, we will ensure that the probability of adding a trajectory τ to F should be *inversely proportional* to $new_F(\tau)$.

Formally, the support of Q_F is the trajectories with new states, i.e., $X = \{\tau | new_F(\tau) \neq 0\}$. For every $\tau \in X$, $Q_F(\tau) \propto \frac{\Pr[\tau]}{new_F(\tau)}$, where $\Pr[\tau]$ is the probability of trajectory τ under the Markov Chain with dynamics P. Note that the new distribution depends on the current set F, and changes as we modify it. Intuitively, adding trajectories to F according to Q_F instead of adding trajectories sampled directly from the dynamics (as we do in SIMULATION) would increase the expected ratio between the added safety and the number of new states we add to F, thus improving the set size guarantee of the output set. We elaborate on this in Section 4.2.

Our main algorithm is FINDING SAFEZONE, Algorithm 1. The algorithm receives, in addition to the safety parameter ρ, parameters $\epsilon, \lambda \in (0, 1)$, and maintains a set F that is initiated to $\{s_0\}$. On a high level, to implement the idea of adding trajectories to F according to Q_F, we use *rejection sampling*. Namely, in each iteration of the while–loop we first sample a trajectory τ and if $new_F(\tau) \neq 0$, we *accept* it with probability $1/new_F(\tau)$. If the trajectory is accepted, it is added to F. More precisely, if $new_F(\tau) \neq 0$, we sample a Bernoulli random variable, $accept \sim Br(1/new_F(\tau))$. If $accept = 1$, we add τ to F. This process of adding trajectories to F generates the desired distribution, Q_F.

Whenever a trajectory is added to F, we estimate the escape probability $\Delta(F)$ (w.r.t. the updated set, F). The algorithm stops adding states to F and returns it as output when it becomes "safe enough". To be precise, let $\widehat{\Delta}(F)$ denote the result of the escape probability estimation (by sampling trajectories as suggested in Proposition 2.2). If $\widehat{\Delta}(F) \leq 2\rho + \epsilon$, it means that F is $(2\rho + 2\epsilon)-$safe with probability $\geq 1 - \lambda_j > 1 - \lambda$, in which case the algorithm terminates and returns F as output. To implement the estimation $\widehat{\Delta}(F)$, the algorithm calls *EstSafety* Subroutine. The subroutine samples $N_j = \Theta(\frac{1}{\epsilon^2} \ln \frac{2}{\lambda_j})$ trajectories, and returns the fraction of trajectories that escaped F.

For cases in which the transition function P is known to the learner, we provide an alternative implementation for *EstSafety* which computes the exact probability $\Delta(F)$ (see Appendix F).

4.1 Algorithm Analysis

We define the event

$$\mathcal{E} = \{\forall i \; |\widehat{\Delta}(F_{i-1}) - \Delta(F_{i-1})| \leq \epsilon\},$$

which states that all our *EstSafety* Subroutine estimations are accurate. We show that $\mathcal{E}$ holds with high probability using Hoeffding's inequality. In most of the analysis we condition on $\mathcal{E}$ to hold.

The following theorem is the central component in the proof of the main theorem that follows it.

Theorem 4.1. *Given $\rho, \epsilon, \lambda \in (0, 1)$,* FINDING SAFEZONE *Algorithm returns a subset $F \subseteq \mathcal{S}$ such that:*

1. *The escape probability is bounded from above by $\Delta(F) \leq 2\rho + 2\epsilon$, with probability $1 - \lambda$.*

2. *The expected size of F given $\mathcal{E}$ is bounded by $\mathbb{E}[|F| \mid \mathcal{E}] \leq 2k^*$.*
3. *The sample complexity of the algorithm is bounded by $O\left(\frac{k^*}{\lambda\epsilon^2}\ln\frac{k^*}{\lambda} + \frac{Hk^*}{\rho\lambda}\right)$, and the running time is bounded by $O\left(\frac{Hk^*}{\lambda\epsilon^2}\ln\frac{k^*}{\lambda} + \frac{H^2k^*}{\rho\lambda}\right)$, with probability $1-\lambda$.*

To obtain the main theorem, we run FINDING SAFEZONE Algorithm several times and return the smallest output set, F, see the next section for more details.

Theorem 4.2. *(main theorem) Given $\epsilon, \rho, \delta > 0$, if we run* FINDING SAFEZONE *for $\Theta(\frac{1}{\delta})$ times and return the smallest output set, $F \subseteq \mathcal{S}$, then with probability ≥ 0.99*

1. *The escape probability is bounded by $\Delta(F) \leq 2\rho + 2\epsilon$.*
2. *The size of F is bounded from above by $|F| \leq (2+\delta)k^*$.*
3. *The total sample complexity and running time are bounded by $O(\frac{k^*}{\delta^2\epsilon^2}\ln\frac{k^*}{\delta} + \frac{Hk^*}{\rho\delta^2})$, and $O(\frac{Hk^*}{\delta^2\epsilon^2}\ln\frac{k^*}{\delta} + \frac{H^2k^*}{\rho\delta^2})$, respectively.*

Algorithm 1 FINDING SAFEZONE

```
Input: ρ ∈ (0,1)
Parameters: ϵ, λ ∈ (0,1)
F ← {s_0}, j ← 1, Δ̂(F) ← 1
while Δ̂(F) > 2ρ + ϵ do
  τ ← sample a random trajectory
  Compute new_F(τ)
  if new_F(τ) ≠ 0 then
    sample accept ~ Br(1/new_F(τ))
    if accept = 1 then
      F ← F ∪ τ
      λ_j ← 3λ / (2(jπ)^2), j ← j + 1
      Δ̂(F) ← EstSafety(ϵ, λ_j, F)
    end if
  end if
end while
return F
```

Algorithm 2 *EstSafety* Subroutine

```
Input: subset F
Parameters: ϵ, λ_j ∈ (0,1)
Δ̂(F) ← 0
𝒯 ← sample N_j = (1/(2ϵ^2)) ln(2/λ_j) trajectories
for τ ∈ 𝒯 do
  if τ ⊈ F then
    Δ̂(F) ← Δ̂(F) + 1/N_j
  end if
end for
return Δ̂(F)
```

4.2 Proof Technique

Escape probability set size bounds. To ease the presentation of the proof, we assume that $\widehat{\Delta}(F) = \Delta(F)$. This case is interesting by its own, since if the policy and transition function are known, we can compute $\Delta(F)$ efficiently using dynamic programming (see Appendix F). As a result, event $\mathcal{E}$ always holds. In addition, it is clear that the termination of the algorithm implies that $\widehat{\Delta}(F) = \Delta(F) \leq 2\rho$, thus F is $(2\rho + 2\epsilon)-$safe. The main challenge is bounding the size of F.

A few notations before we start. Let F^* denote a minimal $\rho-$safe set (of size k^*). Consider iteration i inside the while–loop. The random variable G_i is the number of states in F^* that are added to F in iteration i and B_i is the number of states added to F in iteration i that are not in F^* (G stands for *good* and B for *bad*). Notice that both G_i and B_i depend on the current set F. Notice that the size of the output set is exactly $\sum_i B_i + G_i$ and that $\sum_i G_i \leq k^*$.

The main idea of the proof technique is to show that by adding trajectories according to the new distribution Q_F, we ensure that, in expectation, there are at least as much good states that are added to F as bad states. Suppose the trajectory τ was chosen to be added to F^* by the algorithm. If $\tau \subseteq F^*$, then G_i is equal to $new_F(\tau)$ and $B_i = 0$. If $\tau \not\subseteq F^*$, then $B_i \leq new_F(\tau)$. Summarizing these observations, we have the following bounds

$$G_i \geq new_F(\tau) \cdot \mathbb{I}[\tau \subseteq F^*] \text{ and } B_i \leq new_F(\tau) \cdot \mathbb{I}[\tau \not\subseteq F^*],$$

where $\mathbb{I}[\cdot]$ is the indicator function.

Moreover, a direct consequence of the probability in which τ is added to F is that for any set of trajectories T it holds that

$$\begin{aligned}&\mathbb{E}_{\tau\sim Q_F}[new_F(\tau)\cdot\mathbb{I}[\tau\in T]]=\sum_{\tau\in T}Q_F(\tau)new_F(\tau)\\&=\frac{1}{Z}\sum_{\tau\in T,new_F(\tau)\neq 0}\left(\frac{\Pr[\tau]}{new_F(\tau)}\right)new_F(\tau)=\frac{1}{Z}\Pr_{\tau}[\tau\in T\wedge new_F(\tau)\neq 0],\end{aligned}\tag{1}$$

where Z is the normalization factor of Q_F.

To bound the size of F, we want to show that the algorithm does not add too many states outside of F^*. We therefore bound $\mathbb{E}[B_i]/\mathbb{E}[G_i]$, where the expectations are over the trajectory τ that is added to F according to Q_F. Applying Equation (1) twice, once with $T=\{\tau\mid\tau\subseteq F^*\}$ and once with $T=\{\tau\mid\tau\not\subseteq F^*\}$, we bound the ratio between B_i and G_i by

$$\frac{\mathbb{E}[B_i]}{\mathbb{E}[G_i]}\leq\frac{\Pr_\tau[\tau\not\subseteq F^*\wedge new_F(\tau)\neq 0]}{\Pr_\tau[\tau\subseteq F^*\wedge new_F(\tau)\neq 0]}.\tag{2}$$

We know that $\Pr_\tau[\tau\not\subseteq F^*]$ is always smaller than ρ, so the numerator is $\leq\rho$. A lower bound for the denominator is

$$\Pr_\tau[new_F(\tau)\neq 0]-\Pr_\tau[\tau\not\subseteq F^*].\tag{3}$$

Whenever the algorithm is inside the main loop, the safety is at least $\Pr_\tau[new_F(\tau)\neq 0]=\Delta(F)>2\rho$. Thus (3) is lower bounded by ρ, and overall (2) is less or equal to 1, which implies that

$$\mathbb{E}[B_i]\leq\mathbb{E}[G_i].\tag{4}$$

This completes the proof because we know that the algorithm does not add too many states outside of F^*. More precisely,

$$\mathbb{E}[|F|]=\mathbb{E}\left[\sum_i B_i+G_i\right]\leq\mathbb{E}\left[2\sum_i G_i\right]\leq 2k^*.$$

Sample complexity. To discuss the sample complexity, we drop the assumption that the MC is known to a learner, and uses *EstSafety* Subroutine to approximate $\Delta(F)$. The number of calls to *EstSafety* is bounded by the size of the output set, F. Hence, this part of the sample complexity is bounded by $|F|\cdot N_{|F|}$ and we show that is $O(\frac{k^*}{\epsilon^2}\log k^*)$. Another source of sampling is trajectories sampled for purposes of potentially adding them to F. Observe that at any iteration the set F has escape probability of at least 2ρ, and each trajectory that escapes F is accepted with probability at least $1/H$. This implies a lower bound for the probability that a random trajectory is accepted is $2\rho/H$. This gives an upper bound of $\frac{2|F|\rho}{H}$ for the expected sample complexity.

Amplification. Theorem 4.1 shows that if $\mathcal{E}$ holds, then the set size, $|F|$, is bounded *in expectation* by $2k^*$. As $\Pr[\mathcal{E}]\geq 1-\lambda$ implies, from Markov's inequality, that the size $(2+\delta)k^*$ with small probability of about $\delta+\lambda=O(\delta)$. If we want to make sure that the actual size is at most $(2+\delta)k^*$ with high probability, we can repeat the process about $\Theta\left(\frac{1}{\delta}\right)$ times and take the smallest size set.

For full proofs we refer to Appendix C.

5 Discussion and Open Problems

In this paper, we have introduced the SAFEZONE problem. We have shown the it is NP-hard even when the model is known, and designed a nearly $(2\rho,2k^*)$ approximation algorithm for the case where the model and policy are unknown to the algorithm. Beyond improving the approximation factors (or showing that it cannot be done unless $P=NP$), a natural direction for future work is the following. Given $\rho>0$ and an MDP (known or unknown to the learner), find a policy with a small $\rho-$safe set, with nearly optimal value. In fact, an efficient solution for this could pave the way to improve compactness of the policy representation. An interesting observation that comes up from the empirical demonstration is that different policies result in different sizes of SAFEZONES, and that the optimal policy does not necessarily has the smallest SAFEZONE.

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References

Alharin, A., Doan, T.-N., & Sartipi, M. (2020). Reinforcement learning interpretation methods: A survey. *IEEE Access*, *8*, 171058–171077.

Amir, D., & Amir, O. (2018). Highlights: Summarizing agent behavior to people. In *Proceedings of the 17th International Conference on Autonomous Agents and MultiAgent Systems*, (pp. 1168–1176).

Amodei, D., Olah, C., Steinhardt, J., Christiano, P. F., Schulman, J., & Mané, D. (2016). Concrete problems in AI safety. *CoRR*, *abs/1606.06565*.
URL `http://arxiv.org/abs/1606.06565`

Blanc, G., Lange, J., & Tan, L.-Y. (2021). Provably efficient, succinct, and precise explanations. *Advances in Neural Information Processing Systems*, *34*.

Brandes, U., Holm, E., & Karrenbauer, A. (2016). Cliques in regular graphs and the core-periphery problem in social networks. In *International Conference on Combinatorial Optimization and Applications*, (pp. 175–186). Springer.

Chandola, V., Banerjee, A., & Kumar, V. (2009). Anomaly detection: A survey. *ACM Comput. Surv.*.

den Hollander, F., Menshikov, M., & Volkov, S. (1995). *Two problems about random walk in a random field of traps*. Citeseer.

Emam, Y., Glotfelter, P., Kira, Z., & Egerstedt, M. (2021). Safe model-based reinforcement learning using robust control barrier functions. *CoRR*.

Even-Dar, E., Mannor, S., & Mansour, Y. (2002). PAC bounds for multi-armed bandit and markov decision processes. In J. Kivinen, & R. H. Sloan (Eds.) *Computational Learning Theory, 15th Annual Conference on Computational Learning Theory, COLT 2002, Sydney, Australia, July 8-10, 2002, Proceedings*.

Even-Dar, E., & Mansour, Y. (2003). Approximate equivalence of markov decision processes. In B. Schölkopf, & M. K. Warmuth (Eds.) *Computational Learning Theory and Kernel Machines, 16th Annual Conference on Computational Learning Theory and 7th Kernel Workshop, COLT/Kernel 2003, Washington, DC, USA, August 24-27, 2003, Proceedings*.

García, J., & Fernández, F. (2015). A comprehensive survey on safe reinforcement learning. *J. Mach. Learn. Res.*, *16*, 1437–1480.

Givan, R., Dean, T., & Greig, M. (2003). Equivalence notions and model minimization in markov decision processes. *Artificial Intelligence*.

HasanzadeZonuzy, A., Bura, A., Kalathil, D. M., & Shakkottai, S. (2021). Learning with safety constraints: Sample complexity of reinforcement learning for constrained mdps. In *AAAI*.

Hendrycks, D., Carlini, N., Schulman, J., & Steinhardt, J. (2021). Unsolved problems in ML safety. *CoRR*.

Hussein, A., Gaber, M. M., Elyan, E., & Jayne, C. (2017). Imitation learning: A survey of learning methods. *ACM Comput. Surv.*.

Koh, P. W., & Liang, P. (2017). Understanding black-box predictions via influence functions. In *International Conference on Machine Learning*, (pp. 1885–1894). PMLR.

Li, J., Nagarajan, V., Plumb, G., & Talwalkar, A. (2020). A learning theoretic perspective on local explainability. *arXiv preprint arXiv:2011.01205*.

Molnar, C. (2019). *Interpretable Machine Learning*.

Moshkovitz, M., Yang, Y.-Y., & Chaudhuri, K. (2021). Connecting interpretability and robustness in decision trees through separation. *arXiv preprint arXiv:2102.07048*.

Pfrommer, S., Gautam, T., Zhou, A., & Sojoudi, S. (2021). Safe reinforcement learning with chance-constrained model predictive control. *CoRR*.

Puterman, M. L. (1994). Markov decision processes: Discrete stochastic dynamic programming. In *Wiley Series in Probability and Statistics*.

Sutton, R. S., & Barto, A. G. (2018). *Reinforcement Learning: An Introduction*. Cambridge, MA, USA: A Bradford Book.

Vazirani, V. V. (2001). *Approximation Algorithms*. Berlin, Heidelberg: Springer-Verlag.

Williamson, D. P., & Shmoys, D. B. (2011). *The Design of Approximation Algorithms*. Cambridge University Press.

Xu, W., Xu, K., Bastani, H., & Bastani, O. (2021). Safely bridging offline and online reinforcement learning. *CoRR*.

Yang, J., Chen, T., Payne, B., Guo, P., Zhang, Y., & Guo, J. (2020). Generating routes for autonomous driving in vehicle-to-infrastructure communications. *Digital Communications and Networks*.

6 Hardness

In this section we show that SAFEZONE is NP-hard to solve, and this is why approximation is necessarily. Moreover, SAFEZONE is hard even if the MC and optimal $\rho-$safe size, k^* is known. Our starting point is the NP-hardness of regular cliques. The REGULARCLIQUE(G, k_c) problem gets as an input (i) a regular graph G with n nodes where each node has degree d, and (ii) an integer k_c. It returns whether G contains a clique of size k_c. Whenever G and k_c are clear from the context we simply write REGULARCLIQUE. The following fact follows, e.g., from Brandes et al. (2016).

Fact 6.1. REGULARCLIQUE *is NP-hard.*

Markov chain (random walk). Fix a graph $G = (V, E)$ and a starting vertex $v_0 \in V$. The graph induces a Markov Chain (random walk) in the following way. The states of the process correspond to the vertices V in the graph G. The transition function is defined as $P(v|u) = \frac{1}{d} \cdot \mathbb{1}_{(u,v)\in E}$, where d is the degree any node. The process starts from node v_0 and then proceeds according to the transition function P for H steps.

Reduction. To prove the hardness of SAFEZONE , we show how to solve REGULARCLIQUE given a solver to SAFEZONE. For each vertex $v \in V$, run an algorithm for SAFEZONE with horizon $H = 2$, $k = k_c$, and $\rho = 1 - \left(\frac{k_c-1}{d}\right)^2$, and v as the starting state. If there is at least one run of the algorithm that returns YES, then the final answer is YES. Otherwise, the answer is NO. Note that this reduction is efficient.

Theorem 6.2. *For every graph $G = (V, E)$ and an integer k_c there exists a clique of size k_c in G $\iff$ SAFEZONE$(M(G), k_c, \rho)$ answers YES.*

Given an environment, a policy and SAFEZONE , one could compute exactly how much safe it is (see Appendix F for details), from which we deduce our next corollary.

Corollary 6.3. SAFEZONE *is NP-complete.*

Note that for $H = 1$, the GREEDY AT EACH STEP Algorithm is optimal.

A Empirical Demonstration

Each of the naive approaches in Section 3, has a specific instance that the naive approach is guaranteed (w.h.p.) to return a solution which is far from optimal, as we show in Appendix B. The purpose of this section is to demonstrate, using a simple standard setup that, FINDING SAFEZONE outperforms the both GREEDY BY THRESHOLD and SIMULATION (in accordance with our theory) [5]. Additional figures and a visual comparison of two policies' different SAFEZONES can be found in Appendix E.

The MDP. We focus on a simple $N \times N$ grid problem, for some parameter N. The agent starts off at mid-left state, $(0, \lfloor \frac{N}{2} \rfloor)$ and wishes to reach the (absorbing) goal state at $(N-1, \lfloor \frac{N}{2} \rfloor)$ with minimal number of steps. At each step it can take one of four actions: {'up', 'down', 'right', 'left'} by 1 grid square. With probability 0.9, the intended action is preformed and with probability 0.1 there is a drift down. The agent stops either way after $H = 300$ steps.

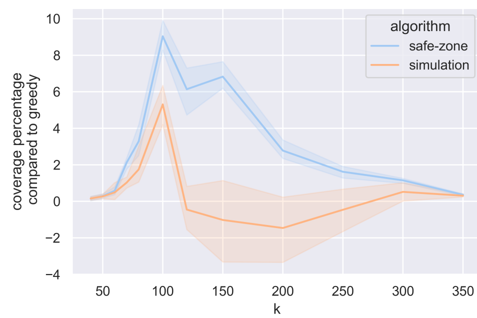


Figure 1: Empirical results regarding Coverage (safety) differences between the algorithms FINDING SAFEZONES (safe-zone) and SIMULATION and GREEDY BY THRESHOLD. The coverage of GREEDY BY THRESHOLD for $k \leq 100$ is negligible (not more than 1%). For $k = 150, 200, 250, 300$, GREEDY BY THRESHOLD obtains $30\%, 63\%, 83\%, 94\%$ coverage, respectively, and for $k = 350$ all algorithms obtain 100% coverage.

FINDING SAFEZONE vs. naive approaches

To compare the FINDING SAFEZONE Algorithm to the naive approaches, we focus on the policy that first goes to the right and when it reaches the rightmost column, it goes up (see Figure 6(a) and Figure 5(c) in Appendix E for depictions of the number of total visits at each state using the described policy, respectively). We take $N = 30$ and 2000 episodes (i.e., the coverage (safety) of each algorithm is estimated for 2000 random trajectories). [6] Appendix A depicts the trajectories coverage of each algorithm minus the coverage of the GREEDY BY THRESHOLD algorithm. A figure with the absolute values can be found in Appendix E (Figure 5(b)). We see that the new algorithm exhibits better performance compared to its competitors. Moreover, taking less than 30% of the states ($k = 250$ out of 900 states) is enough to get a coverage of more 80% the trajectories. In Appendix E.2, we show a second policy which is slightly less optimal than this one the in terms of the expected number of steps to reach to the goal state. The two policies have a very different SAFEZONES and we can clearly see that the second policy requires less states to achieve the same level of safety.

B Proofs of Section 3

B.1 Greedy by Threshold Algorithm

A naive approach to the SAFEZONE problem is to return all states $s \in \mathcal{S}$ with probability $p(s) \geq \beta$, for some parameter $\beta > 0$, see Algorithm 3.

Algorithm 3 Greedy by Threshold

Parameter: $\beta > 0, \{p(s)\}_{s \in \mathcal{S}}$
return $\{s \in \mathcal{S} : p(s) \geq \beta\}$

[5]As the MDP in this setup is not layered, we do not test GREEDY BY EACH STEP algorithm.

[6]To illustrate the algorithms performance, we have changed the stopping condition in their implementations from the desired safety level to desired set size, deciding randomly between different states of the trajectory in case the set side exceeds k. For GREEDY BY THRESHOLD, we gradually decrease the threshold β until the set contains the desired amount of states.

Lemma 3.1. *For any $\rho, \beta \in (0,1)$, the* Greedy by Threshold Algorithm *returns a set that is* $(\rho + k^*\beta, \frac{H}{\beta}) -$ SafeZone. *In particular, for $\beta = \frac{\rho}{k^*}$, this set is* $\left(2\rho, \frac{k^* H}{\rho}\right) -$ SafeZone.

Proof. There are at most $\frac{H}{\beta}$ states with probability $p(s) \geq \beta$. Thus $|F| \leq \frac{H}{\beta}$.

Denote by F^* the optimal $(\rho, k^*) -$ SafeZone set. By law of total probability,

$$\Pr_{\tau}[\tau \not\subseteq F] \leq \Pr_{\tau}[\tau \not\subseteq F^*] + \Pr_{\tau}[\tau \subseteq F^* \setminus F].$$

Looking at the R.H.S of the inequality, the left term is smaller than ρ by the definition of SafeZone. The right term is equal to the probability to reach a state in F^* that its probability is smaller than β, i.e., a state in $F^* \setminus F$.

Using union bound, this can be bounded by $k^*\beta$. □

Lemma B.1. *For every $\rho \in (0, 1/2), H \in \mathbb{N}$, there exists an MDP and a minimal integer k such that the MDP has a $(\rho, k)-$*SafeZone *, but for $\beta = \rho/k$* Greedy by Threshold *Algorithm returns F with escape probability $\leq 2\rho$ and of size $|F| = \Omega(H/\beta)$.*

Proof. Fix $\rho \in (0,1)$. For ease of the presentation we will assume that $\frac{1-\rho}{\beta}$ is an integer (if not, it should be rounded to the nearest integer). Define A to contain $\frac{1-\rho}{\beta} \cdot H$ states, B to contain $k-1$ states, and $\mathcal{S} = \{s_0\} \cup A \cup B$. Consider the following MDP with states $\mathcal{S}$ and starting state s_0. The transition function is defined as follows:

- For every $i \in A$, $\Pr[s^A_{1,i}|s_0] = \beta$ and for every $j \in [H-1]$, $\Pr[s^A_{j+1,i}|s^A_{j,i}] = 1$.
- For $s \in B$, $\Pr[s|s_0] = \frac{1-\rho}{k-1}$
- For $s \in B$, $\Pr[s|s] = 1$

The MDP is illustrated in Figure 2. Clearly, $\{s_0\} \cup B$ is a $(\rho, k)-$SafeZone . In addition, Greedy by Threshold Algorithm returns the set of all states, as for every state $s \in A$ we have that $p(s) = \beta$, $p(s_0) = 1 > \rho \geq \beta$, and for every $s \in B$ we have that $p(s) = \frac{1-\rho}{k-1} > \frac{\rho}{k} = \beta$. Thus the size of the returned set is $\mathcal{S}$, which is of size $\Omega(H/\beta)$, which completes the proof. □

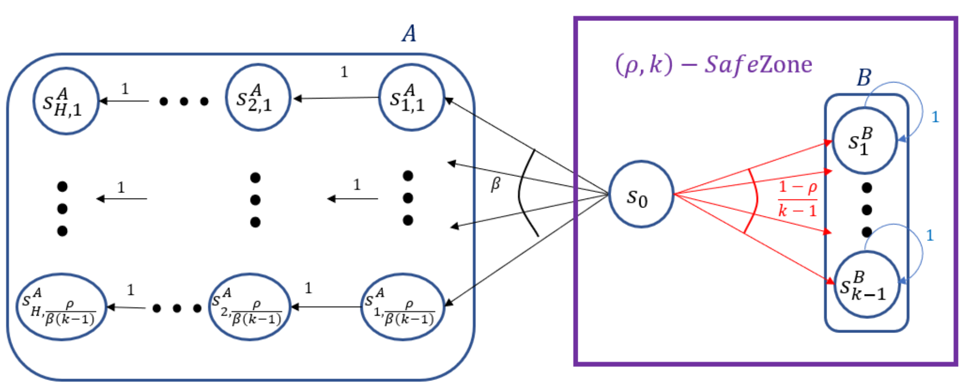


Figure 2: Lower bound for Greedy By Threshold Algorithm.

Algorithm 4 Simulation Algorithm

Input: $m = \frac{1}{\beta} \ln \frac{k^*}{0.005}$
$F \leftarrow \{s_0\}$
for $i = 1 \dots m$ **do**
  $\tau \leftarrow$ choose a random trajectory
  $F \leftarrow F \cup \tau$
end for
return F

B.2 Simulation Algorithm

Lemma 3.2. *Fix* $\rho, \beta \in (0, 1)$. *With probability at least* 0.99*,* SIMULATION *Algorithm returns a set that is* $\left(\rho + k^*\beta, O(k^* + \frac{\rho H \ln k^*}{\beta})\right) -$ SAFEZONE. *In particular, for* $\beta = \frac{\rho}{k^*}$*, this set is* $(2\rho, O(k^* H \ln k^*)) -$ SAFEZONE.

Proof. Denote by F^* the optimal $(\rho, k^*) -$ SAFEZONE set. By the law of total expectation, we can split $\mathbb{E}[|F|]$ into two parts, depending on whether trajectories are entirely in F^* or not:

- Trajectories that are entirely in F^* contribute at most k^* states to F.
- A trajectory that is not contained in F^* contributes at most H states to F.

Thus,

$$\mathbb{E}[|F|] \leq k^* + \rho \cdot \left(\frac{1}{\beta} \ln \frac{k^*}{0.005}\right) \cdot H = O\left(k^* + \frac{\rho H \ln k^*}{\beta}\right).$$

We use Markov's inequality to get the desired bound on $|F|$.

For the safety, we first denote the set of all states in F^* with probability at least β as $\Gamma = \{s \in F^* \mid p(s) \geq \beta\}$. We will show that with probability at least 0.9995, it holds that $\Gamma \subseteq F$, which will prove our claim, similarly to Lemma 3.1.

For a fixed state $s \in \Gamma$, the probability that $s \notin F$ is bounded by $(1 - p(s))^{\frac{1}{\beta} \ln \frac{k^*}{0.005}} \leq e^{-\frac{\beta}{\beta} \cdot \ln \frac{k^*}{0.005}} = \frac{0.005}{k^*}$. Using union bound, the probability that there is a state $s \in \Gamma$ which is not in F is bounded by $k^* \cdot \frac{0.005}{k^*} = 0.005$.

In other words, with probability at least 0.995, $\Gamma \subseteq F$, thus implementing the greedy approach in Algorithm 3 and proving that the probability that a random trajectory escapes F is bounded by $\rho + k^*\beta$. ☐

Lemma B.2. *For every* $\rho, \gamma \in (0, 1)$*,* $H, k \in \mathbb{N}$*, and* $\beta = \frac{\rho}{k}$*, there is an integer* $r \in \mathbb{N}$ *and MDP with* $(\rho, k)-$SAFEZONE*, but with probability* $\geq 1 - \gamma$*,* SIMULATION *algorithm returns* F *of size* $\mathbb{E}[|F|] \geq kH \ln k$ *with escape probability* $\Delta(F) = O(\rho)$*.*

Proof. Fix $\rho, \gamma \in (0, 1)$. Recall that $m = \frac{1}{\beta} \ln \frac{k^*}{0.005}$ and take $r = \lceil \frac{m^2}{\gamma} \rceil$. Define A to contain rH states, B to contain $k - 1$ states, and $\mathcal{S} = \{s_0\} \cup A \cup B$.

Consider the following MDP with states $\mathcal{S}$ and starting state s_0. The transition function is defined as follows:

- For every $i \in A$, $\Pr[s^A_{1,i} | s_0] = \frac{\rho}{r}$ and for every $j \in [H - 1]$, $\Pr[s^A_{j+1,i} | s^A_{j,i}] = 1$.
- For $s \in B$, $\Pr[s | s_0] = \frac{1-\rho}{k-1}$
- For $s \in B$, $\Pr[s|s] = 1$

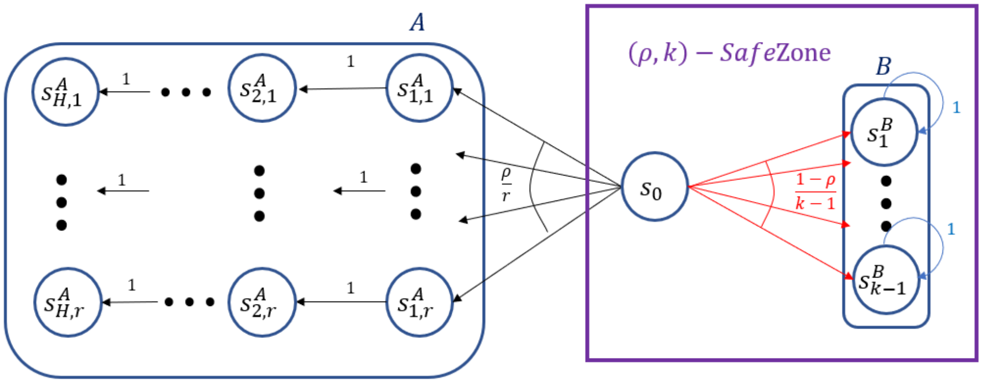


Figure 3: Lower bound for SIMULATION Algorithm.

The MDP is illustrated in Figure 3.

The set $B \cup \{s_0\}$ is $\rho-$safe with k states.

We will show that:

- After adding $\geq \frac{1}{\beta} \ln k = \frac{k}{\rho} \ln k$ random trajectories, with probability $\geq 1 - \gamma$ we have that $|F| \geq kH \ln k$.
- After adding m random trajectories, we have that with high probability $F^* \subseteq F$, thus $\Delta(F) \leq \Omega(\rho)$.

To prove the first property, we claim that with probability$\geq 1 - \gamma$, every time we add a trajectory τ such that $\tau \cap A \neq \emptyset$, we add H new states.

Notice that if we ignore s_0, trajectories in A are entirely unconnected, and each trajectory is chosen randomly with probability $\Pr[s^A_{1,i}|s_0] = \frac{\rho}{r}$. This yields that if $s^A_{1,i} \notin F$, then $s^A_{j,i} \notin F$ for every $j \in [H]$. As a result, every time we add a new $s^A_{1,i}$ to F, we add $H - 1$ more states to F. Let N denotes the amount of trajectories sampled with states from A. The probability that their intersection contains only s_0 is

$$\frac{r \cdot (r-1) \cdot \ldots \cdot (r-N)}{r^N} \geq \left(\frac{r-N}{r}\right)^N = \left(1 - \frac{N}{r}\right)^N \geq 1 - \frac{N^2}{r} = 1 - \gamma.$$

From the structure of the MDP, we have that $\mathbb{E}[N] = \rho m$. Therefore, with probability $\geq 1 - \gamma$,

$$\mathbb{E}[|F|] \geq \mathbb{E}[N] \cdot H = \rho \cdot m \cdot H \geq \rho \cdot \frac{1}{\beta} \ln k \cdot H = kH \ln k.$$

The second property follows from Lemma 3.2.

□

B.3 Greedy at Each Step

Lemma 3.3. *For any $\rho \in (0, 1)$, if the MDP is layered,* GREEDY AT EACH STEP ALGORITHM *returns a set that is $(\rho H, k^*) -$* SAFEZONE.

Proof. Take a random trajectory $\tau = (s_1, s_2, \ldots)$. For every $s_i \in \tau$, the probability that $s_i \notin F$ is bounded by ρ, thus using union bound, the probability that τ has state s_i such that $s_i \notin F$ is at most ρH.

Algorithm 5 Greedy at Each Step

Input: $\rho > 0, \{p(s)\}_{s\in\mathcal{S}}$
$F \leftarrow \{s_0\}$
for $i = 1 \dots H$ **do**
  Sort states in $\mathcal{S}_i$, $p(s_i^1) \geq \dots \geq p(s_i^{|\mathcal{S}_i|})$
  $j^* \leftarrow \arg\min_{j\in[|\mathcal{S}_i|]} \sum_{r=1}^{j} p(s_i^r) \geq 1-\rho$
  $F \leftarrow F \cup \left\{s_i^1, \dots s_i^{j^*}\right\}$
end for
return F

The construction of F guarantees that F is the minimal subset of states such that for every i, the probability that s_i is in the subset is at least $1-\rho$. Assume by contradiction that $|F| > k^*$. Then there is a time step i such that $\Pr[s_i \in F^*] < 1-\rho$, which is a contradiction, since $\Pr[\tau \in F^*] \leq \min_i \Pr[s_i \in F^*]$.

□

Lemma B.3. *For any $\rho \in (0,1)$, there is an MDP and an integer k such that there is a $(\rho,k)-$*SAFEZONE *, but* GREEDY AT EACH STEP *Algorithm returns F with escape probability $\Delta(F) \geq \Omega(H\rho)$.*

Proof. Fix $\rho \in (0,1)$ and take $k = 3H+1$.

Consider the MDP illustrated in Figure 4. The set $\{s_0\} \cup \{s_1^i\}_i \cup \{s_2^i\}_i \cup \{s_3^i\}_i$ form a $(\rho, 3H+1)-$SAFEZONE .

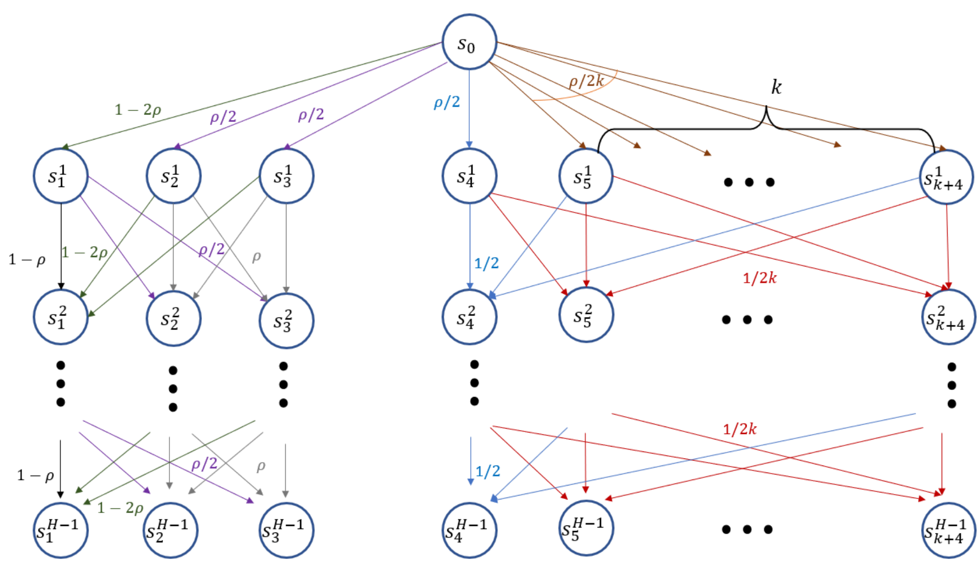


Figure 4: Lower bound for GREEDY AT EACH STEP Algorithm.

We will prove by induction that the for every time i,

- $p(s_1^i) = 1-2\rho$,
- $p(s_2^i) = p(s_3^i) = p(s_4^i) = \frac{\rho}{2}$, and
- For every $j \in \{5,\dots,k+4\}$, $p(s_j^i) = \frac{\rho}{2k}$.

It is easy to see that the two properties hold for $i=1$.

For $i > 1$,

$$p(s_1^i) = p(s_1^{i-1})(1-\rho) + p(s_2^{i-1})\frac{\rho}{2} + p(s_3^{i-1})\frac{\rho}{2} = (1-2\rho)(1-\rho) + 2(1-2\rho)\frac{\rho}{2} = 1-2\rho$$

$$p(s_2^i) = p_{i-1}(s_1^{i-1})\frac{\rho}{2} + p(s_2^{i-1})\rho + p(s_3^{i-1})\rho = (1-2\rho)\frac{\rho}{2} + \frac{\rho^2}{2} + \frac{\rho^2}{2} = \frac{\rho}{2}$$

Similarly, $p(s_3^i) = \frac{\rho}{2}$.

$$p(s_4^i) = \frac{1}{2}p(s_4^{i-1}) + \sum_{j=5}^{k+4}\frac{p(s_j^{i-1})}{2} = \frac{\rho}{4} + k\frac{\rho}{4k} = \frac{\rho}{2}$$

For every $j \in \{5, \ldots, k+4\}$,

$$p(s_j^i) = \frac{1}{2k}p(s_4^{i-1}) + \sum_{m=5}^{k+4}\frac{p(s_m^{i-1})}{2k} = \frac{\rho}{4k} + k\frac{\rho}{4k^2} = \frac{\rho}{2k}.$$

The algorithm might return $\{s_0\} \cup \{s_1^i\}_i \cup \{s_2^i\}_i \cup \{s_4^i\}_i$, i.e., instead of taking $\cup_i\{s_3^i\}_i$ it takes $\cup_i\{s_4^i\}_i$. Finally, the observation $\Delta(\{s_0\} \cup \{s_1^i\}_i \cup \{s_2^i\}_i \cup \{s_4^i\}_i) \geq \frac{\rho H}{4}$ completes the proof. □

C Proofs of Section 4

For convince, we state here Hoeffding's inequality.

Lemma C.1. *[Hoeffding's Inequality] Let $y_1, \ldots, y_N$ be independent random variables such that $y_i \in [a, b]$ for every y_i with probability 1. Then, for any $\epsilon > 0$,*

$$\Pr\left[\left|\frac{1}{N}\sum_{i=1}^{N} y_i - \mathbb{E}[y_i]\right| \geq \epsilon\right] \leq 2e^{-2N\epsilon^2/(b-a)^2}.$$

C.1 Proof of Theorem 4.1

In this section we provide a complete proof for Theorem 4.1. Throughout the section, we define a few terms and notions. We will start with proving guarantees regarding a single iteration of the while–loop.

Recall that F^* denotes a minimal $\rho-$safe set (of size k^*). If there are multiple optimal solutions, choose one arbitrarily. For the convince of analysis, we denote the values of the algorithm variables at the end of each iteration i of the while–loop by $\tau_i, F_i, accept_i$. Let $j(i)$ denote the value of variable j during the $i-$th call to *EstSafety* Subroutine. In addition, let N_i denote the number of trajectories sampled for the $j-$th time of calling Subroutine *EstSafety*, i.e., $N_i = \frac{1}{2\epsilon^2}\ln\frac{2}{\lambda_{j(i)}}$ for $j(i) \leq i$.

For ease of presentation, we recall some of the definitions from the proof technique description. We say that a trajectory τ is *good* if all the states in τ are in F^* and *bad* if it escapes it. I.e., a trajectory is good if $\tau \subseteq F^*$ and bad if $\tau \not\subseteq F^*$. Additionally, we say that a state $s \in \mathcal{S}$ is *good* if it is in F^* and *bad* otherwise. Namely, a state s is good if $s \in F^*$ and bad if $s \notin F^*$. Let $G_i(F_{i-1})$ and $B_i(F_{i-1})$ be the number of good and bad states added to F_{i-1} in iteration i, respectively (notice that $G_i(F_{i-1})$ and $B_i(F_{i-1})$ are random variables that depends on F_{i-1}). For short, whenever it is clear from the context, we write G_i and B_i respectively.

The following lemma bounds the error in approximating the escape probability.

Lemma C.2. *Let $F_{i-1} \subseteq \mathcal{S}$ be a subset of of states and $\epsilon, \lambda_j > 0$ be some parameters. Let S_i be a sample of $N_i \geq \frac{1}{2\epsilon^2}\ln\frac{2}{\lambda_{j(i)}}$ i.i.d. random trajectories. Then,*

$$\Pr_{S_i}\left[\left|\widehat{\Delta}(F_{i-1}) - \Delta(F_{i-1})\right| \geq \epsilon\right] \leq \lambda_j.$$

Also, as $\lambda_j = \frac{3\lambda}{2(\pi j)^2}$,

$$\Pr\left[\exists i \ \left|\widehat{\Delta}(F_{i-1}) - \Delta(F_{i-1})\right| \geq \epsilon\right] \leq \lambda/4,$$

Where the last probability is over all the samples S_i made by EstSafety Subroutine.

Proof. The first part follows directly from Hoeffding's inequality by taking $y_i = \mathbb{I}[\tau \not\subseteq F]$.

Assigning $\lambda_j = \frac{3\lambda}{2(\pi j)^2}$ and applying union bound, we get

$$\Pr\left[\exists i \, \left|\widehat{\Delta}(F_{i-1}) - \Delta(F_{i-1})\right| \geq \epsilon\right] \leq \sum_i \Pr_{S_i}\left[\left|\widehat{\Delta}(F_{i-1}) - \Delta(F_{i-1})\right| \geq \epsilon\right]$$

$$\leq_{(*)} \sum_{j(i)} \lambda_{j(i)} \leq \sum_{j=1}^{\infty} \lambda_j = \sum_{j=1}^{\infty} \frac{3\lambda}{2(\pi j)^2} = \frac{\lambda}{4}.$$

The inequality marked by $(*)$ follows from the fact that $\Delta(F)$ is estimated once for every time j increases. □

We define the event that *EstSafety* always provides good estimations by

$$\mathcal{E} = \{\forall i \, \left|\widehat{\Delta}(F_{i-1}) - \Delta(F_{i-1})\right| \leq \epsilon\}.$$

By the above we have that $\Pr[\mathcal{E}] \geq 1 - \lambda/4$.

In the following lemma we assume that if the current escape probability is at least 2ρ, then the fraction of bad trajectories that escape F_{i-1} is bounded from above by the fraction of good trajectories that escape F_{i-1}.

Lemma C.3. *Let $\rho > 0$ and assume that $\Delta(F_{i-1}) \geq 2\rho$. Then,*

$$\Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \not\subseteq F^*] \leq \Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \subseteq F^*],$$

where the probabilities are over random trajectories.

Proof. To prove the lemma, we will bound the probability $\Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \not\subseteq F^*]$ from above and the probability $\Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \subseteq F^*]$ from below. Since $\Delta(F^*) \leq \rho$,

$$\Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \not\subseteq F^*] \leq \Pr_\tau[\tau \not\subseteq F^*] \leq \rho. \quad (5)$$

The assumption $\Delta(F_{i-1}) \geq 2\rho$ implies that

$$2\rho \leq \Delta(F_{i-1}) = \Pr_\tau[new_{F_{i-1}}(\tau) \neq 0] = \Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \subseteq F^*] + \Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \not\subseteq F^*]$$

$$\leq \Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \subseteq F^*] + \Pr_\tau[\tau \not\subseteq F^*] \leq \Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \subseteq F^*] + \rho,$$

hence

$$\rho \leq \Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \subseteq F^*]. \quad (6)$$

Putting (5) and (6) together yields the statement. □

Now, as long as the algorithm is inside the while–loop (i.e., the escape probability holds $\widehat{\Delta}(F) > 2\rho + \epsilon$), it follows that $\Delta(F) \geq 2\rho$ with high probability from Lemma C.2. Combining it with Lemma C.3 would yield that with high probability over a random trajectory, if the trajectory escapes F then in expectation it is at least as likely to be good as it is to be bad.

We move on to show the main ingredient of the proof, namely that for any iteration, with high probability, the expected number of good states added to the current set F is larger or equal to the expected number of bad states.

For every iteration i in which we sample τ_i both G_i and B_i depends on the following:

1. The realizations of the sampled trajectory, τ_i, and in particular on $new_{F_{i-1}}(\tau_i)$.
2. The probability of adding it to F, i.e., $1/new_{F_{i-1}}(\tau_i)$.

Next, we prove Equation (4).

Lemma C.4. *Assume event $\mathcal{E}$ holds. Thus, for all iterations i inside the while–loop we have*

$$\mathbb{E}[B_i|F_{i-1}] \leq \mathbb{E}[G_i|F_{i-1}],$$

where the expectation is over the trajectory τ that is sampled from the MC dynamics and added to F_{i-1} according to $Q_{F_{i-1}}$.

Proof. Since event $\mathcal{E}$ holds, we have that $\Delta(F_{i-1}) \geq 2\rho$ as long as we do not terminate in iteration i. We can use it to bound $\mathbb{E}_\tau[B_i|F_{i-1}]$ by

$$\begin{aligned}
\mathbb{E}_\tau[B_i|F_{i-1}] &\leq \sum_{h=1}^{H} \frac{\Pr_\tau[new_{F_{i-1}}(\tau) = h \wedge \tau \not\subseteq F^*]}{h} \cdot h \\
&= \Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \not\subseteq F^*] \underbrace{\leq}_{Lemma\ C.3} \Pr_\tau[new_{F_{i-1}}(\tau) \neq 0 \wedge \tau \subseteq F^*] \\
&= \sum_{h=1}^{H} \frac{\Pr_\tau[new_{F_{i-1}}(\tau) = h \wedge \tau \subseteq F^*]}{h} \cdot h \leq \mathbb{E}_\tau[G_i|F_{i-1}].
\end{aligned}$$

□

Theorem 4.1. *Given $\rho, \epsilon, \lambda \in (0,1)$,* FINDING SAFEZONE *Algorithm returns a subset $F \subseteq \mathcal{S}$ such that:*

1. *The escape probability is bounded from above by $\Delta(F) \leq 2\rho + 2\epsilon$, with probability $1-\lambda$.*
2. *The expected size of F given $\mathcal{E}$ is bounded by $\mathbb{E}[|F| \mid \mathcal{E}] \leq 2k^*$.*
3. *The sample complexity of the algorithm is bounded by $O\left(\frac{k^*}{\lambda\epsilon^2}\ln\frac{k^*}{\lambda} + \frac{Hk^*}{\rho\lambda}\right)$, and the running time is bounded by $O\left(\frac{Hk^*}{\lambda\epsilon^2}\ln\frac{k^*}{\lambda} + \frac{H^2k^*}{\rho\lambda}\right)$, with probability $1-\lambda$.*

Proof. Assume that the event $\mathcal{E}$ holds, and recall that

$$\Pr[\mathcal{E}] \geq 1 - \lambda/4. \tag{7}$$

We start with the first clause. Since event $\mathcal{E}$ holds, Lemma C.2 in particular implies that $\Delta(F) \leq 2\rho + 2\epsilon$, hence the first clause holds.

For second clause, we will bound $\mathbb{E}[|F| \mid \mathcal{E}]$ from above by $2k^*$. Since $\mathcal{E}$ holds, we have that $\Delta(F_{i-1}) \geq 2\rho$, for every i inside the while–loop, thus Lemma C.4 yields

$$\mathbb{E}[B_i|F_{i-1}] \leq \mathbb{E}[G_i|F_{i-1}].$$

This implies that

$$\mathbb{E}[|F| \mid \mathcal{E}] \leq 2\sum_i \mathbb{E}_{F_{i-1}}[\mathbb{E}[G_i|F_{i-1}]]|\mathcal{E}] \leq 2k^*, \tag{8}$$

where the last inequality follows from the definition of G_i, as $\sum_i G_i \leq |F^*| = k^*$.

We continue with the third clause of the theorem. Let M denote the sample complexity of the algorithm, namely $M = M_F + M_E$ where M_F is the expected total number of trajectories sampled within the FINDING SAFEZONE Algorithm (without the samples made by *EstSafety* Subroutine) and M_E is total number of trajectories sampled using *EstSafety*. We will bound each term separately.

Since $\mathcal{E}$ holds, whenever we are inside the while–loop, $\Delta(F_i) \geq 2\rho$, which implies that it takes at most $1/2\rho$ trajectories in expectation to sample a trajectory that escapes F_i, and such trajectory is accepted with probability at least $1/H$. Thus, from Wald's identity, it follows that

$$\mathbb{E}\left[M_F | \, \mathcal{E}\right] = \frac{H}{2\rho} \cdot \mathbb{E}[|F| \, |\mathcal{E}] \leq \frac{Hk^*}{\rho}.$$

From Markov's inequality on the above inequality, with probability at least $1 - \frac{\lambda}{4}$,

$$\Pr\left[M_F \geq \frac{4Hk^*}{\rho\lambda} \big| \mathcal{E}\right] \leq \frac{\lambda}{4}. \tag{9}$$

Moving on to bound M_E. Since $\mathcal{E}$ holds, it follows from Equation (8) and Markov's inequality that

$$\Pr\left[|F| \geq \frac{8k^*}{\lambda} \mid \mathcal{E}\right] = \Pr\left[|F| \geq 2k^* \cdot \frac{4}{\lambda} \mid \mathcal{E}\right] = \Pr\left[|F| \geq \mathbb{E}[|F| \mid \mathcal{E}] \cdot \frac{4}{\lambda} \mid \mathcal{E}\right] \leq \frac{\lambda}{4}. \tag{10}$$

If $|F| \leq \frac{8k^*}{\lambda}$, the number of calls for Subroutine *EstSafety* is also bounded by $8\pi k^*/\lambda$ (we only call *EstSafety* after we added states to F). It also implies that $\frac{3\lambda^3}{2(8\pi k^*)^2} \leq \lambda_j$ for every $j \geq 1$. Thus, if $|F| \leq \frac{8k^*}{\lambda}$,

$$M_E = \sum_{j=1}^{|F|} N_i \leq \sum_{j}^{\frac{8k^*}{\lambda}} \frac{1}{2\epsilon^2} \ln \frac{2}{\lambda_j} \leq \sum_{j}^{\frac{8k^*}{\lambda}} \frac{1}{2\epsilon^2} \ln \frac{2}{\frac{3\lambda^3}{2(8\pi k^*)^2}} \leq \sum_{j}^{\frac{8k^*}{\lambda}} \frac{1}{2\epsilon^2} \ln \frac{86(\pi k^*)^2}{\lambda^3}$$
$$= \frac{8k^*}{2\lambda\epsilon^2} \ln \frac{86(\pi k^*)^2}{\lambda^3} = \frac{4k^*}{\lambda\epsilon^2} \ln \frac{86(\pi k^*)^2}{\lambda^3}$$

Combining the above with Equation (10), we get

$$\Pr\left[M_E > \frac{4k^*}{\lambda\epsilon^2} \ln \frac{86(\pi k^*)^2}{\lambda^3} \mid \mathcal{E}\right] \leq \frac{\lambda}{4} \tag{11}$$

As $M = M_F + M_E$, union bound over Equation (7), Equation (9) and Equation (11) implies that with probability $\geq 1 - 3\lambda/4 > 1 - \lambda$,

$$M = O\left(\frac{k^*}{\lambda\epsilon^2} \ln \frac{k^*}{\lambda} + \frac{Hk^*}{\rho\lambda}\right) \tag{12}$$

For each trajectory we sample we run in time $O(H)$, e.g., by using a lookup table for maintaining the current set F. Consequently, if the event in Equation (12) holds then the running time of the algorithm is bounded by

$$O\left(\frac{Hk^*}{\lambda\epsilon^2} \ln \frac{k^*}{\lambda} + \frac{H^2 k^*}{\rho\lambda}\right).$$

Overall, all the clauses in the lemma hold with probability $\geq 1 - \lambda$.

□

C.2 Proof of Theorem 4.2

Theorem 4.2. *(main theorem) Given $\epsilon, \rho, \delta > 0$, if we run* FINDING SAFEZONE *for $\Theta(\frac{1}{\delta})$ times and return the smallest output set, $F \subseteq \mathcal{S}$, then with probability ≥ 0.99*

1. *The escape probability is bounded by $\Delta(F) \leq 2\rho + 2\epsilon$.*
2. *The size of F is bounded from above by $|F| \leq (2 + \delta)k^*$.*
3. *The total sample complexity and running time are bounded by $O(\frac{k^*}{\delta^2\epsilon^2} \ln \frac{k^*}{\delta} + \frac{Hk^*}{\rho\delta^2})$, and $O(\frac{Hk^*}{\delta^2\epsilon^2} \ln \frac{k^*}{\delta} + \frac{H^2 k^*}{\rho\delta^2})$, respectively.*

Proof. Assume we run FINDING SAFEZONE Algorithm for $m = \frac{2\ln 300}{\delta}$ times and denote each algorithm output by F^i. Return the smallest set $F = \text{argmin}_{F^i} |F^i|$.

It follows from Theorem 4.1 that for every $\lambda \in (0, 1)$, each F^i is of expected size $\mathbb{E}[|F^i|] \leq 2k^*$, and is $(2\rho + 2\epsilon)-$safe with probability $\geq 1 - \lambda$. Choosing $\lambda = \frac{0.01}{3m}$ implies

$$\Pr[\Delta(F) > 2\rho + 2\epsilon] \leq \frac{0.01}{3}. \tag{13}$$

In addition, from Markov's inequality it follows that for every $\delta > 0$,

$$\begin{aligned}
\Pr\left[|F^i| > (2+\delta)k^*\right] &\leq \Pr\left[|F^i| > (2+\delta)k^* | \mathcal{E}\right] + \Pr[\mathcal{E}] \\
&\leq \frac{2k^*}{(2+\delta)k^*} + \lambda \\
&= 1 - \frac{\delta/2}{1+\delta/2} + \lambda \\
&= 1 - \frac{\delta/2 - \lambda - \lambda\delta/2}{1+\delta/2}
\end{aligned}$$

From the independence of the algorithm runs, for $m = \frac{2\ln 300}{\delta}$,

$$\begin{aligned}\Pr[|F| > (2+\delta)k^*] &\le \Pr[\forall i : (|F^i| > (2+\delta)k^*)] \\ &\le \prod_{i\in[m]} \Pr[|F^i| > (2+\delta)k^*] \\ &\le \left(1 - \frac{\delta/2 - \lambda - \lambda\delta/2}{1+\delta/2}\right)^m \\ &\le e^{-m(\frac{\delta/2-\lambda-\lambda\delta/2}{1+\delta/2})} \le \frac{0.01}{3}.\end{aligned}$$

Hence

$$\Pr[|F| > (2+\delta)k^*] \le \frac{0.01}{3}. \tag{14}$$

As for the sample complexity, let M_i denote the (random) sample complexity of the $i-$th run, and let us denote

$$\bar{M} = \frac{4k^*}{\lambda\epsilon^2}\ln\frac{86(\pi k^*)^2}{\lambda^3} + \frac{4Hk^*}{\rho\lambda}.$$

From Theorem 4.1, $M_i > \bar{M}$ with probability $< \lambda$.

By taking union bound on the sample complexity bound per one run, we get

$$\Pr\left[\exists i : M_i > \bar{M}\right] \le \sum_{i\in[m]} \Pr\left[M_i > \bar{M}\right] \le m\cdot\lambda = \frac{0.01}{3}.$$

Where the last inequality follows from Theorem 4.1, and $\lambda = \frac{0.01}{3m}$.

Assigning $m = \frac{2\ln 300}{\delta}$ and $\lambda = \frac{0.01}{3m} = \frac{0.01\delta}{6\ln 300}$, we get that with probability $\ge 1 - \frac{0.01}{3}$,

$$\sum_{i=1}^{m} M_i = O\left(\frac{mk^*}{\lambda\epsilon^2}\ln\frac{k^*}{\lambda} + \frac{mHk^*}{\rho\lambda}\right) = O\left(\frac{k^*}{\delta^2\epsilon^2}\ln\frac{k^*}{\delta} + \frac{Hk^*}{\rho\delta^2}\right) \tag{15}$$

Since the algorithm runs in time $O(H)$ for every trajectory sampled, if the sample complexity is bounded by the above term, then the total running time is bounded by $O\left(\frac{Hk^*}{\delta^2\epsilon^2}\ln\frac{Hk^*}{\delta} + \frac{Hk^*}{\rho\delta^2}\right)$.
Finally, from union bound over Equation (13), Equation (14) and Equation (15) all the theorem properties hold with probability ≥ 0.99. $\square$

D Proofs of Section 6

Theorem 6.2. *For every graph $G = (V, E)$ and an integer k_c there exists a clique of size k_c in G $\iff$ SAFEZONE$(M(G), k_c, \rho)$ answers YES.*

Proof. ($\Longrightarrow$) If there is a clique of size k_c, then we can take the corresponding k states. The probability to remain in this subset is at least $\left(\frac{k-1}{d}\right)^2$. Thus, an exact solver for SAFEZONE must return YES.

($\Longleftarrow$) Suppose there is no clique of size k. Assume by contradiction that the reduction (algorithm) returns YES. Let s_0 be a vertex which was the starting state from the running instance which the YES came from and let $\hat{F}$ denote the output of SAFEZONE . We will show that the probability to remain in any subset of size k is smaller than $\left(\frac{k-1}{d}\right)^2$.

Since there is no clique of size k in G, we know that $\hat{F}$ is not a clique. It therefore follows that there exists at least two vertexes, $s_a, s_b \in V$ such that $(s_a, s_b) \notin E$.

We will now bound the probability of escape from state s_0 by exhaustion.

1. If $s_0 \neq s_a$, then

$$\Pr[escape\ from\ s_0] \geq \Pr[t = 1 : (s_0, s'), s' \notin \hat{F}]$$

$$+\Pr[t = 1 : (s_0, s), s \neq s_a] \cdot \Pr[t = 2 : (s, s'), s' \notin \hat{F} | t = 1 : (s_0, s), s \neq s_a]$$

$$+\Pr[t = 1 : (s_0, s_a)] \cdot \Pr[t = 2 : (s_a, s'), s' \notin \hat{F} | t = 1 : (s_0, s_a)]$$

$$= \frac{d-(k-1)}{d} + \frac{k-2}{d} \cdot \frac{d-(k-1)}{d} + \frac{1}{d} \cdot \frac{d-(k-2)}{d}$$

$$= 1 - \frac{k-1}{d} + \frac{k-2}{d} - \frac{(k-2)(k-1)}{d^2} + \frac{1}{d} - \frac{k-2}{d^2} =$$

$$1 - \frac{k-2}{d^2}(k-1+1) = 1 - \frac{k(k-2)}{d^2}$$

Hence

$$\Pr[staying] \leq \frac{k(k-2)}{d^2} < \frac{(k-1)^2}{d^2}.$$

2. If $s_0 = s_a$, then

$$\Pr[escape\ from\ s_0] \geq \Pr[t = 1 : (s_0, s'), s' \notin \hat{F}]$$

$$+\Pr[t = 1 : (s_0, s), s \in \hat{F}] \cdot \Pr[t = 2 : (s, s'), s' \notin \hat{F} | t = 1 : (s_0, s), s \in \hat{F}]$$

$$= \frac{d-(k-2)}{d} + \frac{k-2}{d} \cdot \frac{d-(k-1)}{d}$$

$$= 1 - \frac{k-2}{d} + \frac{k-2}{d} - \frac{(k-2)(k-1)}{d^2}$$

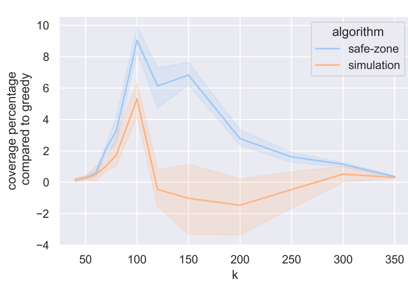
$$= 1 - \frac{(k-2)(k-1)}{d^2}$$

Hence

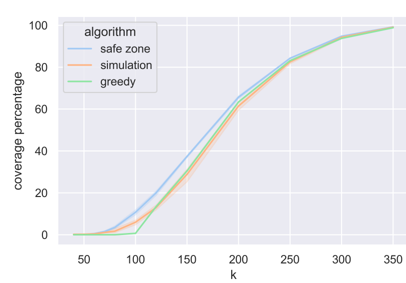
$$\Pr[staying] \leq \frac{(k-2)(k-1)}{d^2} < \frac{(k-1)^2}{d^2}.$$

□

E Additional Figures for Section A



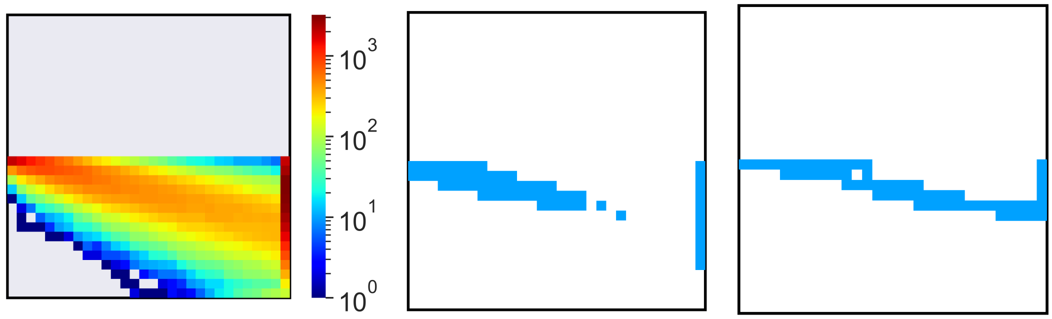
(a) %Coverage: difference from GREEDY BY THRESHOLD Algorithm.



(b) %Coverage: absolute values.

E.1 Solution illustrations

Figures 5(d),5(e) show the sets found for $k = 60$ both by the *Finding* SAFEZONE Algorithm and GREEDY BY THRESHOLD. We see that GREEDY BY THRESHOLD choose an unconnected set for this small k, leading to a coverage (safety) of 0. While the new algorithm, choose a few states which consists of a several trajectories, thus leading to a coverage (safety) larger than 0.



(c) Total number of visits at each state from 2000 episodes. Zero visits in grey.

(d) In blue: set chosen by GREEDY BY THRESHOLD Algorithm.

(e) In blue: set chosen by SAFEZONE Algorithm.

Figure 5: Empirical results regarding Coverage of the different algorithms, FINDING SAFEZONES and state visit frequency.

E.2 Comparing SAFEZONE of two policies

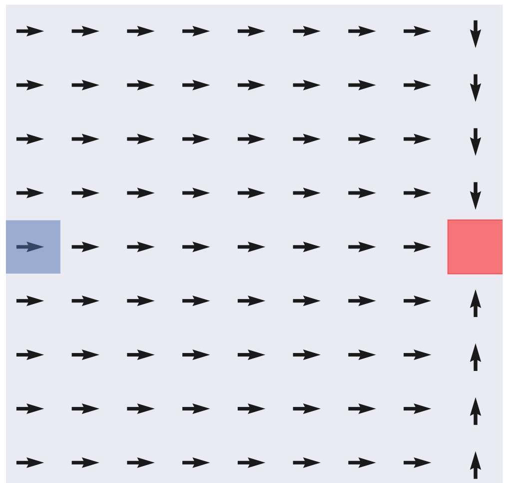
In this section we empirically explore the SAFEZONE of two different policies within the same MDP. The first policy, described in the previous section, first goes right and then to the middle, and the second policy first goes to the middle and then goes right. See Figure 6. These seemingly similar policies induce very different SAFEZONES as can be seen in Figure 8 that depict the number of visits in each state. We clearly see that the second policy requires less states to achieve the same level of safety, even though in terms of minimizing the number of steps to get to the goal state it is outperformed by the first policy (intuitively, the second policy have more fail attempts to go up in expectation since the lowest row of the grid cannot get worst). In Figure 7 we see that already with 14% of the states, all three algorithms achieve trajectory coverage of more than 85%.

Figure 8 shows the visits of the policies described in the main paper for $N = 30$. It is immediately clear that the SAFEZONE of the two policies are fundamentally different. As mentioned, this affects their SAFEZONE sizes. Namely, when trying to go right from a current state in the lowest row it is impossible to get to square which is lower than that, and the first policy takes advantage of this. In contrast, the second policy keeps trying to go up from lowest row, which implies that in expectation it goes down more times compared to the first.

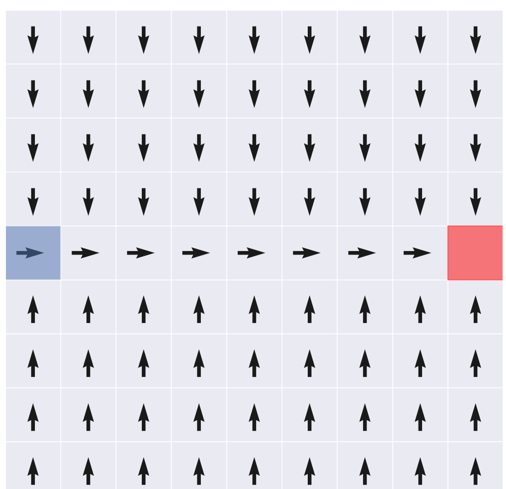
Figure 6 depicts the two policies discussed in the paper when $N = 7$.

Figure 7 depicts coverage percentage for the different algorithms discussed in the paper when applied to the second policy.

Similarly to Figures 5(d) and 5(e), we provide for completeness, the same figures for the policy "Go to the middle and then right". Namely, Figures 9(a),9(b) show the sets found for $k = 60$ both by the *Finding* SAFEZONE and GREEDY BY THRESHOLD algorithms w.r.t. this policy.



(a) Go right and then to the goal state.



(b) Go to the middle and then right.

Figure 6: Two policies for the same MDP with $N = 7$. Starting state, s_0, in blue, goal state in red.

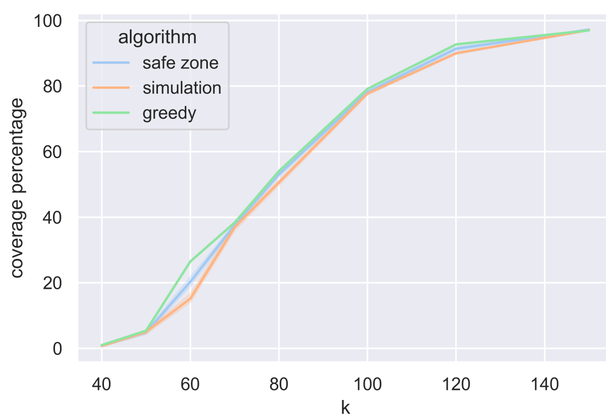
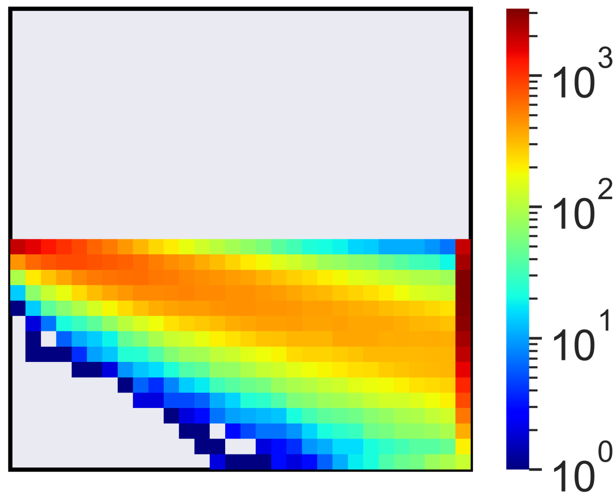
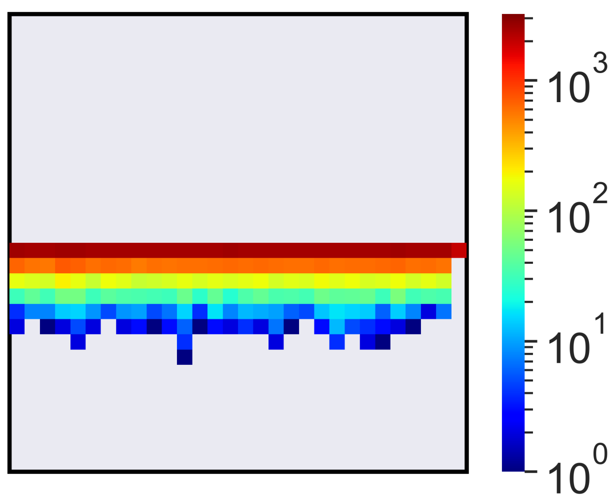


Figure 7: SAFEZONE coverage for the second policy.

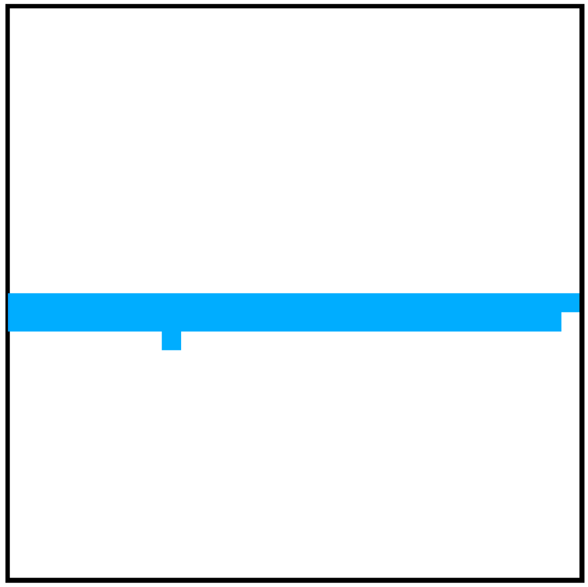


(a) Number of visits at each state for policy “Go right and then to the middle”

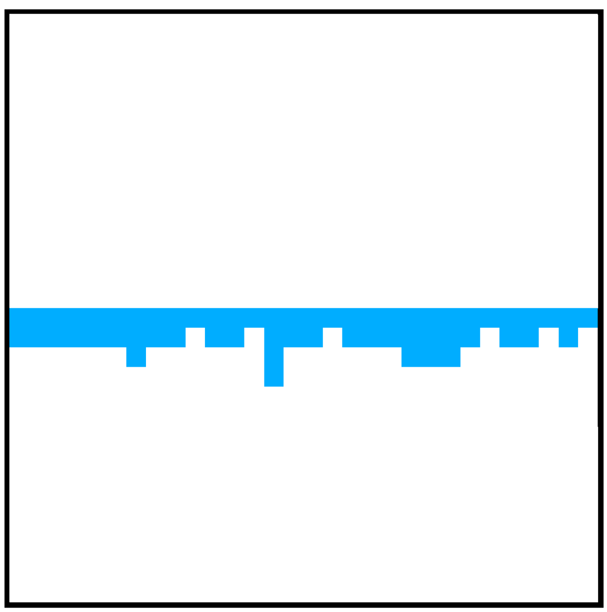


(b) Number of visits at each state for policy “Go to the middle and then right”

Figure 8: Total number of visits for the two policies.



(a) In blue: set chosen by GREEDY AT EACH STEP Algorithm on the policy “Go to the middle and then right”



(b) Number of visits at each state for policy “Go to the middle and then right”

Figure 9: Empirical results regarding Coverage of the different algorithms, FINDING SAFEZONES and state visit frequency.

F Exact Computation

In this section we assume that the transition function is known to the algorithm and show how to compute $\Delta(F)$.

Given a Markov Chain $\langle \mathcal{S}, P, s_0 \rangle$ and a set $F \subseteq \mathcal{S}$ we create a new Markov Chain $\langle \mathcal{S}', P', s_0 \rangle$ as follows. We add a new state $s_{sink} \notin \mathcal{S}$, and set $\mathcal{S}' = F \cup \{s_{sink}\}$. Each transition from a state $s \in F$ to a state $s' \notin F$ we modify and make the transition in P' to the sink s_{sink}. In P', when we are in s_{sink} we always stay in s_{sink}. More formally: (1) if $s, s' \in F$ then $P'(s'|s) = P(s'|s)$, (2) we set $P'(s_{sink}|s) = \sum_{s' \notin F} P(s'|s)$ and (3) $P'(s_{sink}|s_{sink}) = 1$ and $P'(s|s_{sink}) = 0$ for $s \neq s_{sink}$.

Now we claim that $\Delta(F) = \Pr_{P'}[s_H = s_{sink}]$, since any trajectory that reaches a state not in F will reach the sink in P' and stay there. We can compute $\Pr_{P'}[s_H = s_{sink}]$ using standard dynamics programming.

The running time of constructing $\langle \mathcal{S}', P', s_0 \rangle$ is $O(|\mathcal{S}|^2)$. Computing the probability of $\Pr_{P'}[s_H = s_{sink}]$ takes $O(H|\mathcal{S}|^2)$. Therefore we have established the following.

Lemma F.1. *Given a Markov chain $\langle \mathcal{S}, P, s_0 \rangle$ and a set $F \subseteq \mathcal{S}$ we can compute $\Delta(F)$ in time $O(|\mathcal{S}|^2 H)$.*

Note that the above lemma implements an exact version of the *EstSafety* Subroutine.

G MC with Traps

Consider a MC with countable state space and fixed absorbing probability $p(s)$ for each state s, where the absorbing states are either sampled at the beginning (Quenched problem), or after each step (Annealed problem). In both versions, the goal of MC with traps (den Hollander et al. (1995)) is to decide whether or not the reaching probability at a (stochastic) trapping state is 1, when starting from a specific state, x.

The main challenge of MC with traps is to handle a (possibly infinite) countable state space and an infinite horizon. In contrasts, SAFEZONE is defined over a finite state space and a finite horizon. Handling the SAFEZONE via trapping states problem is pointless, as it is most likely to return a negative answer for finite setting.

Given a MC, a trivial exponential time algorithm to find its SAFEZONE is to enumerate over all possible subsets of states, and compute their safety (as done in Lemma F.1). In general, the main challenges of the SAFEZONE problem are computational and sample complexity minimization (we address both in the paper).

We highlight some additional differences between the two problems:

1. The trapping states problem mainly addresses infinite-sized input, and the goal is to **decide** whether some absorbing state is eventually reached, or not. In contrast, in the SafeZone problem, we consider the **algorithmic** problem of computing a subset of states from which the escape probability within the H steps is small using trajectory samples alone. As a result, we do not see how one of these problems could help solve the other.
2. Even if there are no absorbing states within the MC (thus the trapping probability is 0), the SafeZone problem is still challenging (in particular, the hardness result still stands).
3. The safety of a subset of states depends on the subset itself, which is selected by the algorithm. In contrast, trapping states are sampled from a known distribution and induce a probability over reaching some absorbing state.
4. Our main challenge is to efficiently find a "good" subset of states. Given a finite-horizon MC and a subset of states, Lemma $E.1$ computes the escape probability from the subset. Computing this probability is not a significant challenge, unlike in the case of trapping states.
5. Finally, unlike the SafeZone problem, in trapping states problems, access to the MC model is assumed.