Dynamic Shielding for Reinforcement Learning in Black-Box Environments

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Abstract. It is challenging to use reinforcement learning (RL) in cyber-physical systems due to the lack of safety guarantees during learning. Although there have been various proposals to reduce undesired behaviors during learning, most of these techniques require prior system knowledge, and their applicability is limited. This paper aims to reduce undesired behaviors during learning without requiring any prior system knowledge. We propose dynamic shielding: an extension of a model-based safe RL technique called shielding using data-driven automata learning. The dynamic shielding technique constructs an approximate system model in parallel with RL using a variant of the RPNI algorithm and suppresses undesired explorations due to the shield constructed from the learned model. Through this combination, potentially unsafe actions can be foreseen before the agent experiences them. Experiments show that our dynamic shield significantly decreases the number of undesired events during training.

Keywords: reinforcement learning, shielding, automata learning

1 Introduction

Reinforcement learning (RL) [28] is a powerful tool for learning optimal (or near-optimal) controllers, where the performance of controllers is measured by their long-term cumulative rewards. An agent in RL explores the environment by taking actions at each visited state, each of which yields a corresponding reward: RL aims for an efficient exploration by prioritizing actions that maximize the

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Environment
Learning Agent
observation
reward
safe action according to $M$

Shield $S$
safe actions according to $M$

System Model $M$
a priori construction

Automata Learner
observation
reward
Learning Agent
safe action according to $M$

Fig. 1: Comparison of the conventional shielding and our dynamic shielding.

(a) Conventional shielding [1] based on a system model $M$ given by a user. The shield is constructed before starting RL.

(b) Our dynamic shielding. An approximate model $M$ is learned and updated in parallel with RL, and the shield is regularly updated.

subsequent cumulative reward. RL is particularly advantageous when the system model is unavailable [21] or too large for an exhaustive search [27].

Since an RL agent learns a controller through trial and error, the exploration can lead to undesired behavior for the system. For instance, when the learning is conducted on a cyber-physical system, such undesired behaviors can be harmful because they can damage the hardware, e.g., by crashing into a wall. **Shielding** [1] is actively studied to address this problem. A shield is an external component that suggests a set of safe actions to an RL agent so that the agent can explore the environment with fewer encounters with undesired behaviors (Fig. 1a).

**Example 1 (WaterTank).** Consider a 100 liter water tank with valves to control the water inflow. The controller opens and closes the valve, and tries to prevent the water tank from becoming empty or full. The exact inflow cannot be controlled but can be observed, s.t. inflow $\in \{0, 1, 2\}$. The tank also has a random outflow, s.t. outflow $\in \{0, 1\}$. A good shield prevents opening (resp. closing) the valve when the water tank is almost full (resp. empty). Moreover, there must be at least three time steps between two consecutive valve position changes to prevent hardware failure. Hence, the shield should also prevent changing the valve position when the last change was too recent.

Most of the existing shielding techniques [1,2,15,8,13] for RL assume that the system model is at least partially available, and its formal analysis is feasible. Thus, with few exceptions (e.g., [12]), black-box systems have been beyond existing techniques. However, this assumption of conventional shielding techniques limits the high applicability of RL, which is one of the major strengths of RL.

**Dynamic shielding** To improve the applicability of shielding for RL, we propose the dynamic shielding scheme (Fig. 1b). Our goal is to prevent actions similar

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6 The shield we use in this paper is the variant called preemptive shield in [1]. It is straightforward to apply our framework to the classic shield called post-posed shield. See Appendix A for the detail.
to those ones that led to undesired behavior in previous explorations. In our dy-
namic shielding scheme, the shield is constructed and regularly updated using an
approximate system model learned by a variant of the RPNI algorithm [22]
for passive automata learning [18]. Since the RPNI algorithm generates a sys-
tem model consistent with the agent’s experience, a dynamic shield can prevent
previously experienced undesired actions. Moreover, since the RPNI algorithm
can deem some of the actions similar, a dynamic shield can prevent undesired
actions even without experiencing if the action is deemed unsafe.

It is, however, not straightforward to use a system model constructed by
the original RPNI algorithm for shielding. At the beginning of the learning,
our knowledge of the system is limited, and the RPNI algorithm often deems
a safe action as unsafe, which prevents necessary exploration for RL. To in-
fer the (un)safety of unexplored actions with higher accuracy, we introduce a
novel variant of the RPNI algorithm tailored for our purpose. Intuitively, our
algorithm deems two actions in the training data similar only if there is a long
example supporting it, while the original RPNI algorithm deems two actions
similar unless there is an explicit counter example. We also modified the shield
construction to optimistically enable not previously seen actions, as otherwise,
necessary explorations are also prevented.

We implemented our dynamic shielding scheme in Python and conducted
experiments to evaluate its performance compared to two baselines: the plain
RL without shielding and safe padding [12], one of the shielding techniques
applicable to black-box systems. Our experiments suggest that dynamic shielding
prevents undesired exploration during training and often improves the quality
of the resulting controller. Although the construction and the use of dynamic
shielding require some extra time, it is not prohibitive.

Contributions The following list summarizes our contributions.

- We introduce the dynamic shielding scheme (Fig. 1b) using a variant of the
  RPNI algorithm for passive automata learning.
- We modify the RPNI algorithm and the shield construction so that the shield
does not prevent necessary exploration, even if our prior system knowledge
is limited.
- We experimentally show that our dynamic shielding scheme significantly
  reduces the number of undesired explorations during training.

1.1 Related works

The notion of shield is originally proposed in [5] as an approach for runtime
enforcement. In this line of research [3,4,29], a shield takes the role of an enforcer
that overwrites the output of the system when the specification is violated at
runtime. Shielding in this context is fundamentally different from ours, where
shields are used to block system inputs that incur unsafe outputs of the system.

Shielding for RL (or simply shielding) is categorized as a technique of safe
RL. Using the taxonomy of [11], shielding is an instance of “teacher provides
To the best of our knowledge, the existing work closest to ours is cautious RL [12]; it is also a shielding-based safe RL that does not require a system model (but can perform better with a system model). To avoid unsafe events under uncertainty, cautious RL learns an MDP in parallel with the RL process, and its safe padding blocks actions that let the agent come too close to an area where an action may lead to undesired behavior according to the learned MDP. That strong blocking policy works as a safety buffer against unexpected transitions.

A major difference between our technique and safe padding is in the approximate model learning: in safe padding, the observation space is directly used as the state space of the learned MDP, while we merge some of them based on similarity of the suffixes to generalize observations. It is demonstrated in [12] that safe padding offers a promising safety assurance when prior knowledge of the system (e.g., the system’s dynamics without disturbance) is available. However, it is unclear if, without generalization, it also reduces safety violations during learning when such knowledge is unavailable in the beginning. In experiments, we demonstrate that generalization by automata learning effectively reduces safety violations.
2 Preliminaries

For a set $X$, we denote the set of probability functions over $X$ by $\mathcal{D}X$. For a set $\Sigma$, let $\Sigma^*$ be the set of finite sequences over $\Sigma$. We denote the empty sequence by $\varepsilon$. For any $w \in \Sigma^*$, the length is denoted by $|w|$.

We use Mealy machines to formalize an abstract system model and a shield.

**Definition 2 (Mealy machine).** A Mealy machine is a 6-tuple $M = (S, s_0, \Sigma_{in}, \Sigma_{out}, E, \Lambda)$, where:
- $S$ is a finite set of states,
- $s_0 \in S$ is the initial state,
- $\Sigma_{in}$ and $\Sigma_{out}$ are finite alphabets for inputs and outputs, respectively,
- $E: S \times \Sigma_{in} \rightarrow S$ is a partial transition function, and
- $\Lambda: S \times \Sigma_{in} \rightarrow \Sigma_{out}$ is a partial output function such that $\Lambda(s, a)$ is defined if and only if $E(s, a)$ is defined.

**Definition 3 (path, run, output).** Let $M = (S, s_0, \Sigma_{in}, \Sigma_{out}, E, \Lambda)$ be a Mealy machine and let $w_{in} = a_1, a_2, \ldots, a_n \in \Sigma_{in}^*$ be an input word. For a state $s \in S$ of $M$, the path $\rho$ of $M$ from $s$ over $w_{in}$ is the alternating sequence $\rho = s, a_1, s_1, a_2, \ldots, a_n, s_n$ of states $s_i \in S$ and input actions $a_i \in \Sigma_{in}$ satisfying $E(s, a_1) = s_1$ and $E(s_{i-1}, a_i) = s_i$ for each $i \in \{2, \ldots, n\}$. A run of a Mealy machine $M$ is a path of $M$ from the initial state $s_0$. For a state $s \in S$ of $M$, we write $E(w_{in}, s)$ to denote the last state $s_n$ of the path $\rho = s, a_1, s_1, a_2, \ldots, a_n, s_n$ of $M$ from $s$ over $w_{in}$. The output $M(w_{in}, s) \in \Sigma_{out}$ of a Mealy machine $M$ is defined by $M(w_{in}, s) = \Lambda(s_{n-1}, a_n)$, where $s_{n-1} = E(w_{in}', s)$ and $w_{in}' = a_1, a_2, \ldots, a_{n-1}$. We write $E(w_{in}) = E(w_{in}, s_0)$ and $M(w_{in}) = M(w_{in}, s_0)$.

2.1 Automata and games for system modeling

As shown in Fig. 2, we assume that the system is representable as a Markov decision process (MDP), and we use finite-state reactive systems (FSRSs) [1] to abstract the MDP. More precisely, an FSRS is a two-player deterministic game of the controller (Cont) and the environment (Env), where MDPs’ probabilistic transitions are represented by Env transitions. Note that MDPs are only used for the theoretical discussion in this paper.

**Definition 4 (Markov decision process (MDP)).** An MDP is a 5-tuple $(S, s_0, \Sigma_{in}, \Sigma_{out}, \Delta)$ such that:
- $S$ is a finite set of states,
- $s_0 \in S$ is the initial state,
- $\Sigma_{in}$ and $\Sigma_{out}$ are the finite set of input and output alphabets, respectively, and
- $\Delta: S \times \Sigma_{in} \rightarrow \mathcal{D}(S \times \Sigma_{out})$ is the probabilistic transition function.

**Definition 5 (finite-state reactive system (FSRS)).** An FSRS is a Mealy machine $M = (S, s_0, \Sigma_{in}, \Sigma_{out}, E, \Lambda)$ that satisfies the following:
− $\Sigma_{in} = \Sigma_{in}^1 \times \Sigma_{in}^2$, where $\Sigma_{in}^1$ (resp. $\Sigma_{in}^2$) is the set of actions of $\text{Cont}$ (resp. $\text{Env}$);

− for each $s \in S$ and $a^1 \in \Sigma_{in}^1$, there is $a^2 \in \Sigma_{in}^2$ for which $E(s,(a^1,a^2))$ is defined.

**Definition 6 (strategy).** For an FSRS $\mathcal{M} = (S,s_0,\Sigma_{in}^1 \times \Sigma_{in}^2,\Sigma_{out},E,\Lambda)$, strategies of $\text{Cont}$ and $\text{Env}$ are functions $\sigma: \Pi_{\mathcal{M}} \rightarrow \Sigma_{in}^1$ and $\tau: \Pi_{\mathcal{M}} \times \Sigma_{in}^1 \rightarrow \Sigma_{out}$, respectively, where $\Pi_{\mathcal{M}}$ is the set of runs of $\mathcal{M}^\tau$. For strategies $\sigma$ of $\text{Env}$, we also require that $\sigma(p,a^1)(\{a^2\}) > 0$ holds only if $E(p_{last},(a^1,a^2))$ is defined, where $p_{last}$ is the last state of $p$. A strategy is memoryless if it is independent of the run except for the last state.

We use an FSRS as an abstraction of an MDP because for an FSRS $\mathcal{M}$ and a memoryless strategy $\tau$ of $\text{Env}$, there is a canonical MDP $\mathcal{M}^\tau$, where the actions of $\text{Env}$ are chosen by $\tau$. Formally, for $\mathcal{M} = (S,s_0,\Sigma_{in}^1 \times \Sigma_{in}^2,\Sigma_{out},E,\Lambda)$ and $\tau$, $\mathcal{M}^\tau$ is $\mathcal{M}^\tau = (S,s_0,\Sigma_{in}^1,\Sigma_{out},\Delta)$, where for each $s,s' \in S$, $a^1 \in \Sigma_{in}^1$, and $b \in \Sigma_{out}$, $\Delta(s,a^1)$ is such that

$$(\Delta(s,a^1))(s',b) = (\tau(s,a^1))(\{a^2 \in \Sigma_{in}^2 \mid E(s,(a^1,a^2)) = s' \land \Lambda(s,(a^1,a^2)) = b\}).$$

By fixing both $\text{Cont}$ and $\text{Env}$ strategies $\sigma$ and $\tau$ of an FSRS $\mathcal{M}$, we obtain a (purely) stochastic structure $\mathcal{M}^{\sigma,\tau}$. We define the language $L(\mathcal{M}^{\sigma,\tau}) \subseteq (\Sigma_{in}^1 \times \Sigma_{in}^2 \times \Sigma_{out})^*$ of $\mathcal{M}^{\sigma,\tau}$ as the set of sequences of input/output actions $((a^1,a^2),b) \in (\Sigma_{in}^1 \times \Sigma_{in}^2) \times \Sigma_{out}$ in the runs of $\mathcal{M}^{\sigma,\tau}$.

**Example 7 (WaterTank FSRS).** The Water Tank in Example 1 is formalized as an FSRS $\mathcal{M} = (S,s_0,\Sigma_{in}^1 \times \Sigma_{in}^2,\Sigma_{out},E,\Lambda)$, where:

− $S = \{0,1,\ldots,100\}$;

− $\Sigma_{in}^1 = \{\text{open,close}\}$;

− $\Sigma_{in}^2$ is inflow $\times$ outflow, where inflow = $\{0,1,2\}$ and outflow = $\{0,1\}$;

− $\Sigma_{out} = \{\text{low, safe, high}\}$;

− $\Delta(s,(a^1,(n,m)))$ is defined if either $a^1 = \text{open}$ and $n \in \{1,2\}$ or $a^1 = \text{close}$ and $n = 0$;

− $\Delta(s,(a^1,(n,m))) = \max\{0,\min\{s+n-m,100\}\}$;

− For any $(a^1,(n,m)) \in \Sigma_{in}^1 \times \Sigma_{in}^2$, we have $\Lambda(0,(a^1,(n,m))) = \text{low}$, $\Lambda(100,(a^1,(n,m))) = \text{high}$, and $\Lambda(s,(a^1,(n,m)))$ = safe otherwise.

The probabilistic behavior of the WaterTank environment (i.e., $\text{Env}$) is such that:

1. the inflow of water is randomly chosen from $\{1,2\}$ when $a^1 = \text{open}$, and

2. the outflow of the water is randomly chosen from $\{0,1\}$.

Such a behavior is formalized by a $\text{Env}$ strategy $\tau$ such that:

− $\tau(s,\text{open})((n,m)) = 0.25$ for each $(n,m) \in \{1,2\} \times \{0,1\}$, and

− $\tau(s,\text{close})(((0,m))) = 0.5$ for each $m \in \{0,1\}$.

\(^7\) This definition implies that we understand FSRSs as turn-based games rather than concurrent ones.
2.2 Safety automata for specifications

In the shielding methodology, the shield’s specification is given as a safety automaton. As shown in Fig. 2, typically, this automaton is automatically generated from a temporal logic formula, e.g., linear temporal logic (LTL). See, e.g., [16] for the construction of an automaton from an LTL formula.

Definition 8 (Safety Automata). A safety automaton is a 5-tuple \( A = (Q, q_0, F, \Sigma, N) \), where:

- \( Q \) is a finite set of states,
- \( q_0 \in Q \) is the initial state,
- \( F \subseteq Q \) is the set of safe states,
- \( \Sigma \) is the finite set of alphabet, and
- \( N: Q \times \Sigma \rightarrow Q \) is the transition function satisfying \( N(q, a) \in F \) only if \( q \in F \).

A run of a safety automaton is defined similarly to that of a Mealy machine.

For a safety automaton \( A \), the language \( L_A \subset \Sigma^* \) of \( A \) is the set of words \( w = a_1, a_2, \ldots, a_n \) such that the unique run \( q_0, a_1, q_1, \ldots, a_n, q_n \) over \( w \) satisfies \( q_n \in F \). By the definition of \( N \) and \( F \), \( L_A \) is prefix-closed. We call \( \varphi \subset \Sigma^* \) a safety specification if there is a safety automaton recognizing it. For an FSRS \( M \) over \( \Sigma_{in} \) and \( \Sigma_{out} \), a Cont strategy \( \sigma \) of \( M \), and a specification \( \varphi \subset (\Sigma_{in} \times \Sigma_{out})^* \), we say \( M \) satisfies \( \varphi \) under \( \sigma \) if for any Env strategy \( \tau \), we have \( L(M^{\sigma, \tau}) \subset \varphi \).

2.3 Shielding for safe reinforcement learning

We use an FSRS and a safety automaton to define a safety game which we use to create a shield for safe RL. First, we show the formal definition of shields.

Definition 9 ((Preemptive) Shield [1]). Let \( M \) be an FSRS as above. A shield for \( M \) is a Mealy machine \( S = (S_S, s_0, S_{in}^1 \times S_{in}^2, 2^{S_{in}^1}, \Delta_S, \Lambda_S) \) s.t. for any \( s \in S \) and input actions \( a, a' \in S_{in}^1 \times S_{in}^2 \), we have \( \Lambda_S(s, a) = \Lambda_S(s, a') \).

For any input word \( w \in (S_{in}^1 \times S_{in}^2)^* \), the shield \( S \) returns \( \Lambda_S(w) \) as the set of safe actions for Cont after \( w \) is processed in \( M \). A shield \( S \) canonically induces a strategy \( \sigma \) for an MDP \( M_S^T \) generated by any \( \tau \), namely a strategy \( \sigma \) such that \( \sigma(s_0, a_1, s_1, \ldots, a_k, s_k) \) is the discrete uniform distribution over \( \Lambda_S(w) \).

Given an FSRS \( M \) and a specification \( \varphi \) realized by a safety automaton \( A^\varphi \) (i.e., \( \mathcal{L}(A^\varphi) = \varphi \)), our goal is to construct a shield \( S \) such that for any Env strategy \( \tau \), the MDP \( M_S^T \) satisfies \( \varphi \) under any Cont strategy \( \sigma \) compatible with \( S \). To this end, we consider a safety game constructed by \( M \) and \( A^\varphi \).

Definition 10 (Safety Game). A 2-player safety game is an FSRS \( G = (G, g_0, \Sigma_{in}^1 \times \Sigma_{in}^2, \{0, 1\}, E^G, F^G) \).
For an FSRS $\mathcal{M}$ and a safety automaton $A^p$, the parallel composition $\mathcal{M} \parallel A^p$ is the safety game $\mathcal{M} \parallel A^p = (G, (s, q), \Sigma^1_{\text{in}} \times \Sigma^2_{\text{in}}, [0, 1], E^G, F^G)$, where $G = S \times Q$, $E^G((s, q), (a^1, a^2)) = (s', q')$, $s' = E(s, (a^1, a^2))$, $q' = N(q, (a, A(s, (a^1, a^2))))$, and $F^G$ is such that $F^G((s, q), (a^1, a^2)) = 1$ if and only if $N(q, (a^1, a^2)), A(s, (a^1, a^2))) \in F$.

We say $g \in G$ is a safe state if there is a Cont strategy $\sigma$ such that, for any Env strategy $r$ and $w = ((a_1, a_1^2), b_1), ((a_2, a_2^2), b_2), \ldots, ((a_n, a_n^2), b_n) \in L(M^{r, r})$, the unique run $g_0, (a_1^1, a_1^2), g_1, \ldots, (a_n^1, a_n^2), g_n$ of $M$ over $w$ satisfies $g_n \in F^G$.

Intuitively, a state $g$ is safe if there is a Cont strategy $\sigma$ such that the run always remains in safe states, regardless of the Env actions.

We utilize the shield construction algorithm in [1] to the above safety game $\mathcal{G}$. Namely, the shield generated from $\mathcal{G}$ is an FSRS $S = (G, g_0, \Sigma^1_{\text{in}} \times \Sigma^2_{\text{in}}, \Sigma^1_{\text{out}}, E^G, \Lambda_S)$, where for each state $s \in G$, $\Lambda_S$ assigns the set of Cont actions such that for any Env strategy, we remain in the safe states forever.

### 2.4 The RPNI algorithm for passive automata learning

We use a variant of the regular positive and negative inference (RPNI) algorithm [22] to learn an approximate system model in parallel with RL. See, e.g., [18] for the detail. Given a finite training data $D \subseteq \Sigma^1_{\text{in}} \times \Sigma^2_{\text{out}}$, the RPNI algorithm constructs a Mealy machine $M$ that is consistent with the training data $D$, i.e., for any $(w_{in}, b) \in D$, we have $M(w_{in}) = b$. For simplicity, we assume that the training data is prefix-closed, i.e., if $D$ contains $(w_{in}, b)$, for any prefix $w'_{in}$ of $w_{in}$ and for some $b' \in \Sigma^2_{\text{out}}$, $D$ contains $(w'_{in}, b')$. This assumption holds in our dynamic shielding scheme and does not harm its applicability. Since we learn a Mealy machine, we assume that the output in the training data is uniquely determined by the input word, i.e., for each $(w_{in}, b), (w'_{in}, b') \in D$, $w_{in} = w'_{in}$ implies $b = b'$.

The RPNI algorithm creates the prefix tree Mealy machine (PTMM) $M_D$ from the training data $D$ and constructs a Mealy machine $M$ by merging the states of $M_D$. The PTMM $M_D$ is the Mealy machine such that the states are the input words in the training data, and the transition and output functions are $E(w_{in}, a) = w_{in} \cdot a$ and $A(w_{in}, a) = b$ if $(w_{in}, a, b) \in D$ for some $b \in \Sigma^2_{\text{out}}$, and otherwise, undefined. When merging states $s$ and $s'$ of $M_D$, we require them to be compatible, i.e., the merging of $s$ and $s'$ must not cause any nondeterminism to make the learned Mealy machine the consistent with the training data. The RPNI algorithm greedily merges states $s$ and $s'$ of $M_D$ as far as they are compatible.

### 3 Dynamic shielding with online automata inference

Here, we introduce our dynamic shielding scheme in Fig. 1b, where the shield is constructed from the FSRS inferred in parallel with the RL process. Since our dynamic shielding scheme does not require the system model, we can apply it to black-box systems.
3.1 Dynamic shielding scheme

In conventional shielding (Fig. 1a), the shield is constructed from the system model and provides safe actions to the learning agent. See also Fig. 2 for the shield creation schema. By shielding, we can ensure the safety of the exploration in RL if the given system model correctly abstracts the actual system. However, the use of a predefined system model limits the applicability of shielding. Specifically, we cannot use the conventional shielding scheme for black-box systems.

In dynamic shielding (Fig. 1b), using the RPNI algorithm, we learn a system model in parallel with RL, and prevent exploring undesired actions according to the learned model. More precisely, all the inputs and the outputs in RL are given to the RPNI algorithm, and we obtain an FSRS \( \mathcal{M} \) in Fig. 2. From \( \mathcal{M} \) and the given specification \( \varphi \), we generate a shield \( \mathcal{S} \), and prevent undesired exploration using \( \mathcal{S} \). We continuously reconstruct the shield along with the RL process. Since we learn FSRS from observations, the learned FSRS may be incomplete or inconsistent with the actual system, which causes the following challenges.

3.2 Challenge 1: Incompleteness of the learned FSRS

Since the RPNI algorithm is based on merging of nodes of the prefix tree representing the training data, the inferred FSRS \( \mathcal{M} \) has partial transitions when there are unexplored actions from some of the states of \( \mathcal{M} \). Specifically, there may be a state \( s \in S \) of the FSRS \( \mathcal{M} \) and a Cont action \( a^1 \) such that \( E(s, (a^1, a^2)) \) is undefined for any Env action \( a^2 \). If we construct a shield from such an FSRS by the algorithm in [1], the shield prevents the Cont action \( a^1 \) because there is no transition labeled with \( a^1 \) to stay in the safe states. However, since we have no evidence of safety violation by the Cont action \( a^1 \), this interference is against the “minimum interference” policy of shielding [1]. Moreover, such interference can harm the performance of the synthesized controller because it limits the exploration in RL.

To minimize the interference, we modify the safety game construction so that the undefined destinations in the FSRS are deemed safe. More precisely, we create a fresh sink state \( s_{\perp} \) that is safe in the safety game, and make it the destination of the undefined transitions in the FSRS. We remark that the use of such an additional sink state does not allow any Cont action with evidence of safety violation because even if a Cont action \( a^1 \) leads to a safe state for one Env action \( a^2 \), the Cont action \( a^1 \) is prevented if there is another Env action \( \tilde{a}^2 \) leading to a violation of the specification \( \varphi \).

The safety game construction is formalized as follows.

**Definition 11.** For an FSRS \( \mathcal{M} = (S, s_0, \Sigma_{{\text{in}}}^1 \times \Sigma_{{\text{in}}}^2, \Sigma_{{\text{out}}}, E, \Lambda) \) and a safety automaton \( \mathcal{A}^\varphi = (Q^\varphi, q_0^\varphi, F, \Sigma_{{\text{out}}}, N^\varphi) \), their compositions is the safety game \( \mathcal{G} = (G, g_0, \Sigma_{{\text{in}}}^1 \times \Sigma_{{\text{in}}}^2, \{0, 1\}, E^G, F^G) \) such that:

- \( G = (S \cup \{s_{\perp}\}) \times Q^\varphi \);
- \( g_0 = (s_0, q_0^\varphi) \);
– $E^G$ is $E^G((s, q^p), (a^1, a^2)) = (E(s, (a^1, a^2)), N^p(q^p, A(s, (a^1, a^2))))$ if $E(s, (a^1, a^2))$ is defined, and otherwise, $E^G((s, q^p), (a^1, a^2)) = (s_\bot, N^p(q^p, A(s, (a^1, a^2))))$;
– $F^G = (S \times F) \cup (\{s_\bot\} \times Q^p)$.

### 3.3 Challenge 2: Precision in automata learning

In the RPNI algorithm, the generalization of the training data is realized by the state merging. Such generalization allows a dynamic shield to foresee potentially unsafe actions before the learning agent experiences them.

Since the RPNI algorithm aims to construct a minimal FSRS, it greedily merges the states as long as there is no evidence of inconsistency. However, when the training data is limited, there may not be evidence of the inconsistency of states, even if they must be distinguished according to the (black-box) ground truth. In such a case, the greedy merging in the RPNI algorithm may decrease the precision of the learned FSRS. This is especially the case at the beginning of the training because the training data $D$ is small. Moreover, such an imprecise dynamic shield may even harm the quality of the controller synthesized by RL because the dynamic shield may prevent necessary exploration when it deems a safe action to be unsafe.

To prevent such too aggressive merging, we require additional evidence in the state merging. Namely, we modify the RPNI algorithm so that states $s$ and $s'$ can be merged only if there are paths from $s$ and $s'$ over a common word $w \in (\Sigma_{in} \times \Sigma_{out})^*$ longer than a threshold $\text{MINDEPTH}$. This idea is related to the evidence-driven state merging (EDSM) [17], where similar evidence is used in prioritizing the merged states. In our implementation, we adaptively decide the threshold $\text{MINDEPTH}$ so that $\text{MINDEPTH}$ is large when the mean length of the episodes is short. This typically makes the merging more aggressive through the learning process. Nevertheless, further investigation of $\text{MINDEPTH}$ is future work.

### 3.4 Theoretical validity of our dynamic shielding

We show that our dynamic shielding scheme assures the safety of RL when the training data is large enough to construct an abstraction of the actual system.

**Definition 12 (abstraction).** For FSRSs $\mathcal{M} = (S, s_0, \Sigma_{in}, \Sigma_{out}, E, A)$ and $\mathcal{M}' = (S', s'_0, \Sigma_{in}^1 \times \Sigma_{in}^2, \Sigma_{out}, E', A')$, $\mathcal{M}'$ abstracts $\mathcal{M}$ if for each $w \in (\Sigma_{in}^1 \times \Sigma_{in}^2)^*$ if $E(w)$ is defined, $E'(w)$ is also defined, and $A(w) = A'(w)$ holds.

**Theorem 13 (safety assurance by a dynamic shield).** Let $\mathcal{M}$ be an FSRS, let $\mathcal{M}'$ be its abstraction, let $\varphi$ be a specification realized by $A^\omega$, and let $S$ be a shield generated by $\mathcal{M}'$ and $A^\omega$. For any strategy $\tau$ of $\text{Env}$ in $\mathcal{M}$, the MDP $\mathcal{M}'$ satisfies $\varphi$ under any strategy $\sigma$ generated by $S$.
Proof (sketch). Let \( \sigma \) be a \text{Cont} strategy of \( \mathcal{M}' \times \mathcal{A}^2 \), and let \( \sigma' \) be a \text{Cont} strategy of \( \mathcal{M}' \) obtained by taking the obvious projection of \( \sigma \). It is well known that if a state \((s, q)\) of the product game is winning for \text{Cont} under \( \sigma \), in \( \mathcal{M}' \), any path from \( s \) satisfies \( \varphi \) under \( \sigma' \). Since \( \mathcal{M}' \) is an abstraction of \( \mathcal{M} \), if any path from the initial state \( s_0 \) of \( \mathcal{M}' \) satisfies \( \varphi \) under \( \sigma' \), any path from the initial state \( s_0 \) of \( \mathcal{M} \) also satisfies \( \varphi \) under \( \sigma' \). Therefore, for any \text{Env} strategy \( \tau \), the MDP \( \mathcal{M}' \) satisfies \( \varphi \) under any strategy \( \sigma \) generated by \( S \).

Let \( \mathcal{M}' \) be the MDP representing the actual system in Fig. 2, where \( \mathcal{M} \) is an FSRS and \( \tau \) is a \text{Env} strategy in \( \mathcal{M} \). By Theorem 13, if the learned FSRS \( \mathcal{M}' \) abstracts the FSRS \( \mathcal{M} \), the dynamic shield \( S \) assures the safety of the exploration in \( \mathcal{M}' \). When the training data is large and includes a certain set of words called \text{characteristic set}, the RPNI algorithm is guaranteed to learn the abstraction correctly [18]. However, in our dynamic shielding scheme, the training data may not be a superset of the characteristic set even in the limit because the dynamic shield interferes with the exploration. Nevertheless, suppose the learning algorithm eventually explores all available actions, and the maximum length of each episode in RL is long enough to cover all states of \( \mathcal{M} \). In that case, the training data eventually includes the characteristic set of \( \mathcal{M} \) restricted to the safe actions according to the dynamic shield \( S \). Since the dynamic shield constructed from such training data prohibits all the unsafe actions, our dynamic shielding assures the safety in the limit.

4 Experimental evaluation

To show the applicability of dynamic shielding and the viability of our approach, we conducted a series of experiments. The following research questions guided our experiments on our dynamic shielding scheme for RL.

\textbf{RQ1} Does dynamic shielding reduce the number of undesired behaviors?
\textbf{RQ2} How does dynamic shielding affect the quality of the controller synthesized by RL?
\textbf{RQ3} What is the computational overhead of dynamic shielding, and is it prohibitively large?

4.1 Implementation and experiments

We implemented our dynamic shielding scheme in Python 3 and Java using LearnLib [14] for the RPNI algorithm\(^8\). For deep RL, we used Stable Baselines 3 [25] (for \textit{proximal policy optimization algorithm} (PPO) [26]) and Keras-RL [23] (for \textit{deep Q learning} (DQN) with Boltzmann exploration [20]). We used two libraries and learning algorithms to demonstrate that our dynamic shielding scheme is independent of the RL algorithm.

\(^8\) The artifact is publicly available at https://doi.org/10.5281/zenodo.6906673.
Table 1: Summary of the benchmarks we used. MLP and CNN are abbreviations of “multilayer perceptron” and “convolutional neural network”.

| Benchmark’s origin | Observation space (size) | Network | Learning algorithm | # of steps |
|--------------------|---------------------------|---------|--------------------|------------|
| WATER Tank         | Discrete (714)            | MLP     | PPO                | 500,000    |
| Grid World         | Discrete (625)            | MLP     | PPO                | 100,000    |
| Taxi               | Discrete (500)            | MLP     | PPO                | 200,000    |
| Cliff Walk         | Discrete (48)             | MLP     | PPO                | 200,000    |
| Self Driving Car   | Continuous ([-1.1]^4)     | MLP     | DQN with Boltzmann exploration | 200,000 |
| Side Walk          | Image (80 x 60 x 3 x 256) | CNN     | PPO                | 100,000    |
| Car Racing         | Image (96 x 96 x 3 x 256) | CNN     | PPO                | 200,000    |

To answer the research questions, we compared the performance of RL with dynamic shielding (denoted as SHIELDING) with the standard RL process without shielding (denoted as Plain) and the RL process with safe padding [12] (denoted as SafePadding).

Learning of each controller consists of the training and the test phases. The training phase is the main part of the learning, and the testing phase is invoked once every 10,000 training steps to evaluate the learned controller and choose the resulting one. We finish the learning when the total number of steps in the training phase exceeds the predetermined bound, which is one of the commonly used criteria. See Table 1 for the bounds for each benchmark.

To evaluate the RL training, we measure the total number of training episodes with undesired behaviors and the total execution time, including both training and testing phases. To evaluate each controller, we run it for 30 episodes and measure the mean reward and the safe rate, i.e., the rate of the episodes without undesired behaviors in the 30 episodes.

We ran experiments on a GPU server with AMD EPYC 7702P, NVIDIA GeForce RTX 2080 Ti, 125GiB RAM, and Ubuntu 20.04.3 LTS. We used eight CPUs and one GPU for each execution. We ran each instance of the experiment 30 times, i.e., we trained 7 x 3 x 30 controllers in total. For each metric, we report the mean of the 30 executions, i.e., we have 7 x 3 reported values.

4.2 Benchmarks

We chose seven benchmarks for our experiments. Table 1 summarizes them. Most of them are common and openly available. We modified them to fit to dynamic shielding: randomness except for those observable as Env actions are removed; the actions are discretized; the observations for the RL agent is not changed, while the observation for the dynamic shield is discretized. We used CNN for the benchmarks with graphical observation and MLP for the others.

WATER Tank implements the benchmark already used for shielding in [1]. Examples 1 and 7 show the details of the system. The undesired behavior used in the shield construction is:

1. to make the water tank empty or full, or
2. to change the status of the switch too often.
Table 2: Mean of 1) the number of episodes with undesired behavior in training phases and 2) the execution time (in seconds), including both training and testing phases. The cells with the best results are highlighted.

|                  | Undesired episodes | Total time |
|------------------|---------------------|------------|
|                  | Plain   | SafePadding | Shielding | Plain   | SafePadding | Shielding |
| WaterTank        | 1883.67 | 1892.40     | 177.13    | 1860.46 | 1947.09     | 6080.89   |
| GridWorld        | 6996.40 | 7322.23     | 5623.43   | 177.18  | 1487.10     | 4548.70   |
| CliffWalk        | 1493.20 | 1528.67     | 478.20    | 355.18  | 365.54      | 839.06    |
| Taxi             | 8723.13 | 2057.33     | 37.77     | 336.04  | 349.78      | 611.87    |
| SelfDrivingCar   | 6403.07 | 427.93      | 273.37    | 7650.38 | 16694.63    | 12532.94  |
| SideWalk         | 373.60  | 427.93      | 273.37    | 7650.38 | 16694.63    | 12532.94  |
| CarRacing        | 180.13  | 141.17      | 41.73     | 7650.38 | 16694.63    | 12532.94  |

GRIDWorld is a high-level robot control example of two robots in a 5×5 grid arena. One of them is the ego robot we control, and the other robot randomly moves. The objective of the ego robot is to reach the goal area, without touching the arena walls or the other robot.

Taxi is a benchmark to pick up passengers and drop them off at another place in a 5×5 grid arena. As criteria of a safety violation, we measured the number of episodes where the taxi is broken, which randomly occurs when it hits the wall. The undesired behavior used in the shield construction is hitting the wall, picking up or dropping off the passenger at an inappropriate location.

CliffWalk is a benchmark to move ego to the goal area without stepping off the cliff in a 3×12 grid arena. The undesired behavior used in the shield construction is to step off the cliff.

SelfDrivingCar is a benchmark to drive a car in a 480×480 arena around a blocked area in a clockwise direction without hitting the walls. The undesired behavior used in the shield construction is to hit the walls in the arena.

SideWalk is a benchmark for 3D robot simulation. Its objective is to reach the goal area on the sidewalk without entering the roadway. The undesired behavior used in the shield construction is to enter the roadway.

CarRacing is a benchmark to drive a car on a predetermined racing course. The physical dynamics is simulated by Box2D, which is a 2D physics engine for games. As criteria of a safety violation, we measured the number of episodes with spin behavior, i.e., ego drives off the road and keeps rotating indefinitely. The undesired behavior used in the shield construction is to deviate from the road for any consecutive steps, which is not yet a safety violation but tends to lead to it.

4.3 RQ1: Safety by dynamic shielding in the training phase

To evaluate the safety by dynamic shielding, we measured the number of training episodes with undesired behaviors (“Undesired episodes” columns in Table 2), and the relationship between the number of undesired training episodes before each testing phase and the highest mean reward by the testing phase (Fig. 3).
Fig. 3: The mean of the number of undesired episodes before each testing phase and the reward of the best controller obtained in the testing phase.
In Table 2, we observe that, for all benchmarks, the training episodes with undesired behavior were, on average, the lowest when we used dynamic shielding. For example, for CarRacing, the mean number of the training episodes with undesired behavior was reduced by about 77% compared to Plain and about 70% compared to SafePadding. In Fig. 3, we observe that for all benchmarks, the curve of Shielding is growing faster than the curves of Plain and SafePadding. This suggests that dynamic shielding decreased the number of undesired explorations to obtain a controller with similar performance.

Answer to RQ1: Overall, we conclude that dynamic shielding can significantly reduce undesired behaviors during exploration.

Compared to Plain, Shielding decreases such undesired training episodes because it prevents exploration of actions known to cause undesired behavior, while the plain RL may repeatedly explore such actions. Although SafePadding also prevents such an undesired exploration, the number of the undesired training episodes of Shielding was smaller than that of SafePadding. This is because, with Shielding, the undesired explorations are generalized by state merging in the RPNI algorithm, while in SafePadding, the state space of the learned MDP is identical to the observation space in the RL, and the undesired explorations are not often generalized. Another reason is that in SafePadding, a state is deemed to be safe only if the agent can be in the safe states after taking any action. For example, a state is deemed to be unsafe if there is a bad action causing an undesired behavior even if the other actions are totally harmless. This definition of safe states is too pessimistic, and in many cases, SafePadding cannot provide any safe actions, in which case the RL agent explores in the same way as Plain.

4.4 RQ2: Performance of the resulting controller

To evaluate the performance of the resulting controller, for each instance of the experiments, we measured the mean reward and the safe rate using the controller that achieved the highest mean reward in the testing phases (Table 3). In Table 3, we observe that dynamic shielding does not significantly decrease the safe rate for most of the benchmarks. Moreover, the reward was the highest when we used dynamic shielding for most of the benchmarks. This is likely because dynamic shielding prevents explorations with undesired behaviors and leads the learning agent to achieve the task.

In Table 3, we also observe that for GridWorld and SideWalk, the performance of the controllers obtained by Shielding was the worst. This is likely because when a dynamic shield prevents undesired explorations, some of the useful explorations may also be prevented if they are deemed undesired when generalizing undesired behavior. Note that such generalization is useful since it can prevent undesired explorations even if we have not experienced exactly the same exploration. Nevertheless, Table 3 also shows that the average degradation of the safe rate due to dynamic shielding is at most 12% (GridWorld). This is not prohibitively large considering the reduction of undesired explorations (e.g., from 6996.40 to 5623.43 for GridWorld in Table 3).
Table 3: Mean of the performance of the best controllers obtained in the 30 executions. The cells with the best results are highlighted.

|               | Mean reward | Safe rate |
|---------------|-------------|-----------|
|               |             | Plain     | SafePadding | Shielding |
| WaterTank     | 918.89      | 919.81    | 921.81      | 1.00      |
| GridWorld     | 0.37        | 0.46      | 0.07        | 0.80      | 0.85      | 0.73      |
| CliffWalk     | -69.13      | -66.00    | -65.93      | 1.00      | 1.00      |
| Taxi          | -147.61     | -139.62   | -92.93      | 1.00      | 0.67      | 1.00      |
| SelfDrivingCar| 28.83       | 28.86     | 29.81       | 1.00      | 1.00      |
| SideWalk      | 0.93        | 0.90      | 0.67        | 0.93      | 0.89      | 0.89      |
| CarRacing     | 375.53      | 569.25    | 622.07      | 1.00      | 1.00      | 1.00      |

Answer to RQ2: Overall, we conclude that dynamic shielding usually improves the performance of the resulting controller.

4.5 RQ3: Time efficiency of dynamic shielding

To evaluate the overhead of dynamic shielding, we measured the execution time, including both training and testing phases ("Total time" columns in Table 2).

In Table 2, we observe that Plain was the fastest on average for all benchmarks. This is mainly because of the computation cost to construct the set of safe actions. We also observe that SafePadding is usually faster than Shielding. This is due to the combinatorial exploration in the RPNI algorithm to choose the merged states, while SafePadding does not conduct such state merging and directly uses the observation space in the RL as the state space of the learned MDP. We again remark that the generalization by the state merging contributes to the safety of Shielding.

In Table 2, we also observe that the overhead of Shielding is at most about 2.5 hours (153.7 minutes in SelfDrivingCar). This is not negligible but still acceptable for many common usage scenarios, e.g., learning a controller during non-working hours. Moreover, Table 2 also shows that the overhead is not very sensitive to the cost of each execution and the observation space. For example, the overhead of Shielding for WaterTank was close to that for CarRacing. This indeed makes the relative overhead for CarRacing small.

Answer to RQ3: Overall, we conclude that the overhead of dynamic shielding is not prohibitively large, especially when the RL is time-consuming even without shielding.

5 Conclusions and perspectives

Based on passive automata learning, we proposed a new shielding scheme called dynamic shielding for RL. Since dynamic shielding does not require a predetermined system model, it is applicable to black-box systems. The experiment results suggest that
1. dynamic shielding prevents undesired exploration during training,
2. dynamic shielding often improves the quality of the resulting controller, and
3. the overhead of dynamic shielding is not prohibitively large.

In dynamic shielding, we assume that the system behaves deterministically once the actions of the controller and the environment are fixed. Extending our approach, for example, utilizing a probabilistic model identification [19] to support probabilistic systems is a future direction.

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A Post-posed shielding with online automata inference

Here, we show how to apply our dynamic shielding scheme for post-posed shielding in [1, §5.2]. A post-posed shield is similar to a (preemptive) shield in Definition 9, but instead of returning the set of safe actions of Cont, a post-posed shield modifies an unsafe action of Cont to enforce the given specification.

Definition 14 (post-posed shield). Let \( M = (S, s_0, \Sigma_{in}, \Sigma_{out}, E, \Lambda) \) be an FSRS. A post-posed shield for \( M \) is a Mealy machine \( S = (S_p, s_p, S_{in}, \Sigma_{in}, \Delta_S, \Lambda_S) \) s.t. for any \( sS \in S_S \), Cont action \( a^1 \in \Sigma_{in} \), and Env actions \( a^2, a^2' \in \Sigma_{in} \), we have \( \Lambda_S(sS,(a^1,a^2)) = \Lambda_S(sS,(a^1,a^2')) \).

For any input word \( w_{in} \in \Sigma_{in}^* \), a post-posed shield \( S \) returns \( \Lambda_S(w_{in}) \) as a safe action for Cont after \( w_{in} \) is processed in \( M \). A shield \( S \) canonically induces a strategy \( \sigma \) for an MDP \( M^\tau \) generated by any \( \tau \), namely a strategy \( \sigma \) such that \( \sigma(s_0,a_1,s_1,\ldots,a_k,s_k) = \delta(k) \).

The construction of a post-posed shield is almost the same as that of a preemptive shield. We obtain a post-posed shield by taking one of the actions returned by a preemptive shield. We note that to minimize the interference, it is preferred to have \( \Lambda_S(sS,(a^1,a^2)) \) if \( a^1 \) is a safe action.

Since constructing a post-posed shield does not require any other information than that of a preemptive shield, it is straightforward to construct a post-posed shield with online automata inference.

B Detail of the RPNI algorithm

The following shows the formal definition of PTMMs.

Definition 15 (Prefix tree Mealy machine (PTMM)). For a finite training data \( D \subseteq \Sigma_{in}^* \times \Sigma_{out} \), the PTMM is the Mealy machine \( M = (S, s_0, \Sigma_{in}, \Sigma_{out}, E, \Lambda) \) such that:

- \( S \) consists of the set of the input words in \( D \), i.e., \( S = \{ w | \exists b \in \Sigma_{out}, (w,b) \in D \} \);
- the initial state \( s_0 \) is \( s_0 = \varepsilon \);
- the transition function \( E \) and the labeling function \( \Lambda \) are such that for each \( s \in S \) and \( (a,b) \in \Sigma_{in} \times \Sigma_{out} \), if \( s \cdot a \in S \) holds, \( \Delta(s,a) = s \cdot a \) and \( \Lambda(s,a) = b \), and undefined otherwise.

Algorithm 1 outlines the RPNI algorithm. In the RPNI algorithm, we have two sets, red and blue, of the states of the intermediate Mealy machine \( M \): red is the set of the states in the resulting Mealy machine; blue is the set of the states that may not be in the resulting Mealy machine. In the loop from lines 3 to 8, for each \( s_0 \in \text{blue} \), we try to find \( s_r \in \text{red} \) such that we can merge \( s_0 \) to \( s_r \). For the convergence of the RPNI algorithm, we try merging from the root to the leaves of the PTMM. Therefore, in line 4, we examine the minimum state
in blue according to the following order \( \preceq \): we have \( s \preceq s' \) if there is \( w_{in} \in \Sigma_{in}^* \) satisfying \( s_0 \xrightarrow{w_{in}} s \) and for any \( w_{in}' \in \Sigma_{in}^* \) satisfying \( s_0 \xrightarrow{w_{in}'} s' \), we have either \( |w_{in}| < |w_{in}'| \) or \( |w_{in}| = |w_{in}'| \) and \( w_{in} \) is smaller than \( w_{in}' \) in the lexicographical order.

C Detail of our definition of MinDepth

Here, we show how we decide MinDepth in our implementation. Let \( R \) be the set of the runs we have experienced before we evaluate MinDepth, MaxEpLen be the maximum length of each episode, and MinDepth\(_{max} \) be the maximum bound of MinDepth. The use of MinDepth\(_{max} \) is to prevent MinDepth from being very large at the beginning of the learning. In our experiments, we used MinDepth\(_{max} = 5 \). Eq. (1) shows the definition of MinDepth in our implementation, where \(|A|\) is the ceiling function.

\[
\text{MinDepth} = \min \left( |R| \left[ \frac{\text{MaxEpLen} - \frac{1}{|A|} \sum_{\rho \in R} |\rho|}{\sum_{\rho \in R} |\rho|} \right], \text{MinDepth}_{\max} \right)
\]

As we discussed in Section 3.3, MinDepth is large when the mean length of the episodes is short.

D Detail of the benchmarks

Here we show the detail of the benchmarks used in our experiments.

D.1 WaterTank

WATERTANK is the benchmark described in Examples 1 and 7. The input space is open and close. The output space is \{open, close\} \times \{low, safe, high\} \times \{valve violation, no violation\}. As explained in Example 1, the source of nondeterminism is the inflow and outflow of water. In this example, the undesired behavior is either having a switch violation or making the tank full or empty.

\[
\text{Algorithm 1: Outline of the RPNI algorithm}
\]

\[
\begin{array}{l}
\text{input : Training data } D \subseteq \Sigma_{in}^* \times \Sigma_{out} \\
\text{output : A Mealy machine } M \text{ compatible with the training data } D \\
1 \quad M \leftarrow M_D \quad /\!\!/ \text{ Initialize } M \text{ by the PTMM of } D \\
2 \quad \text{red } \leftarrow \emptyset; \text{ blue } \leftarrow S \\
3 \quad \text{while } \text{blue } \neq \emptyset \text{ do} \\
4 \quad \quad \text{pop the smallest element } s_b \text{ from blue} \\
5 \quad \quad \text{if } \exists s_r \in \text{red. compatible}(s_r, s_b) \text{ then} \\
6 \quad \quad \quad \text{merge } s_b \text{ to } s_r \\
7 \quad \quad \text{else} \\
8 \quad \quad \quad \text{push } s_b \text{ to red} \\
\end{array}
\]
D.2 GridWorld

GridWorld is a high-level robot control example in a $5 \times 5$ grid arena. Two robots are in the arena; one of them is the ego robot we control, and the other robot randomly moves. We note that the move of the other robot is encoded by actions of $\text{Env}$, and the system is still deterministic in the sense that it is represented by an FSRS. The objective of the ego robot is to reach the goal area without hitting either the wall or the other robot.

The propositions used for shielding are as follows.

- Either the ego robot hits the wall or not
- Either the ego robot hits the other robot or not

The undesired behavior used in the shield construction is to hit either the wall or the other robot.

D.3 Taxi

Taxi[10] is a $5 \times 5$ grid map in which a taxi has to pick up a passenger from a location and drop it at a different one. The map has some barriers that the taxi can not cross (see Fig. 5). In our extended version of the problem, the taxi can break nondeterministically when hitting a barrier. Every time the taxi hits a barrier, it gets damaged. Each of these damages increases the likelihood of breaking the car at the next hit to a barrier. Although the taxi nondeterministically becomes broken, our assumption on the system determinism still holds by letting the $\text{Env}$'s action be “Break” when the taxi becomes broken.

The input space is the actions related to the movement of the taxi (south, north, east, west) and the actions related to the passenger (pick-up or drop-off). The taxi can observe if it is a successful movement or if it hits a barrier. It can also observe when it arrives at a drop-off/pick-up location, when it does a successful or wrong pick-up/drop-off, and when the passenger is inside the taxi. It can also observe the position in the arena.

In this example, the undesired behavior can be produced by scratching the taxi, breaking the taxi, or doing wrong pick-up/drop-off, because all these actions can damage either the vehicle or the passenger.
Fig. 5: The arena of Taxi. “T” represents the taxi initial position, whereas “R”, “G”, “Y”, “B” represent possible pick-up and drop-off locations for the passenger. The taxi can cross cells separated by “:” but it is not allowed to cross “|”.

Fig. 6: The arena of CliffWalk. “S” represents the initial position, and “G” represents the target position. The cliff is denoted with “x”.

D.4 CliffWalk

CliffWalk[28] is a $3 \times 13$ grid map in which the agent needs to go from the initial position to the final position without falling into a cliff (see Fig. 6). The agent can move in four directions (south, north, east, and west), and it can only observe if it is a safe move, a fall into the cliff, or reached the goal. In this simple problem, the only source of the undesired behavior is falling into the cliff.

D.5 SelfDrivingCar

SelfDrivingCar benchmark is modified from a benchmark in [1]. The objective is to train a car in a $480 \times 480$ pixels arena to run in a clockwise direction without hitting the walls (see Fig. 7). The state of the car consists of its $xy$-position and heading angle. The car starts from $xy$-position $(100, 80)$ heading upward (heading angle = $\pi/2$).

A training step consists of 10 time steps in the simulation. At each training step, the car chooses its action to be “go-straight”, “turn-left”, or “turn-right”. Based on its action, the car moves with the speed of 3 pixels per simulation time step, either following the same heading direction (go-straight) or changing the heading angle (turn-left or turn-right) by $\pi/40$ degrees per simulation time step. For example, the car moves 30 pixels following its heading direction during a training step if it chooses “go-straight”.

As in [1], the car is trained using a Deep Q-Network (DQN) with a Boltzmann exploration policy. In each training step, the car obtains a positive reward if it moves in a clockwise direction (determined using the start and end positions of
the learning step), and a penalty otherwise. A training episode ends if the car hits a wall or reaches 45 training steps. The training is successful if the car can visit green, blue, white, and red areas in order.

The undesired behavior used in the shield construction is to hit a wall. The input to the shield contains the information of \((pos, dir, safe)\), where \(pos\) is the abstract \(xy\)-position using \(60 \times 60\) pixels grids, \(dir\) is the abstract heading angle using the intervals in \(\{[d\pi/4 - \pi/8, (d + 1)\pi/4 - \pi/8] \mid d = 0, 1, \ldots, 7\}\), and \(safe\) indicates whether the car hits a wall during the previous training step.
D.6 SideWalk

SideWalk is a variant of a benchmark in MiniWorld [9] on 3D robot simulation. Fig. 8 shows a screenshot of SideWalk. Its objective is to reach the goal area in the sidewalk without entering the roadway.

The following summarizes the modifications from the original benchmark.

– The random seed is chosen from 10 possible values.
– The domain randomization is enabled.

The propositions used for shielding are as follows.

– The position of the robot is
  1. in the roadway,
  2. in front of the wall, or
  3. the others.
– The robot observes the cone
  1. in the left of the image,
  2. in the right of the image,
  3. in both left and right of the image, or
  4. nowhere in the image.
– The robot observes the goal area or not.
– The robot observes the wall in the center of the image or not.

These propositions on the robot’s perception are determined by the colors of certain pixels of the observed image. The undesired behavior used in the shield construction is to enter the roadway.

D.7 CarRacing

CarRacing is a variant of a benchmark in OpenAI Gym [7]. Fig. 9 shows a screenshot of CarRacing. Its objective is to drive a car on a predetermined racing course. The physical dynamics are simulated by Box2D\(^9\), a 2D physics engine for games.

The following summarizes the modifications from the original benchmark.

– The input space is discretized into “NONE”, “ACCEL”, “RIGHT”, “LEFT”, and “BRAKE”.
– The course creation is determinized by fixing the seed of the random number generator.
– The parameter of the course generation is modified so that the curves are smoother.

The propositions used for shielding are as follows.

– The position of the car is
  1. on the road,

\(^9\) Box2D is available at https://box2d.org/
Table 4: Detailed learning hyperparameters used in our experiments

| Environment   | Learning rate | Gamma | Batch size | nb_steps | warmup | target model update | model_update |
|---------------|---------------|-------|------------|----------|--------|---------------------|--------------|
| WaterTank     | $1 \times 10^{-4}$ | 0.99  | 64         | N/A      | N/A    | N/A                 | N/A          |
| GridWorld     | $3 \times 10^{-4}$ | 0.99  | 64         | N/A      | N/A    | N/A                 | N/A          |
| CliffWalk     | $1 \times 10^{-3}$ | 0.99  | 64         | N/A      | N/A    | N/A                 | N/A          |
| Taxi          | $1 \times 10^{-3}$ | 0.99  | 64         | N/A      | N/A    | N/A                 | N/A          |
| SelfDrivingCar| $3 \times 10^{-4}$ | 0.99  | 32         | 1,000    | 10,000 | N/A                 | N/A          |
| Sidewalk      | $5 \times 10^{-5}$ | 0.99  | 64         | N/A      | N/A    | N/A                 | N/A          |
| CarRacing     | $3 \times 10^{-4}$ | 0.99  | 64         | N/A      | N/A    | N/A                 | N/A          |

2. on the grass area, or
3. out of the arena, i.e., crashes to the wall.

- The car observes that
  1. the road curves to the left,
  2. the road curves to the right, or
  3. the road is straight.

These propositions on the car’s perception are determined from the colors of certain pixels of the observed image. As criteria of a safety violation, we measured the number of episodes with spin behavior, i.e., where ego drives off the road and keeps rotating indefinitely. The undesired behavior used in the shield construction is to deviate from the road for any consecutive steps, which is not a safety violation but tends to be a safety violation.
E Detailed hyperparameters used in our experiments

Table 4 summarizes the detailed hyperparameter of our experiment. We tuned these hyperparameters by a grid search when the default parameters defined by the libraries do not work well for the learning without shielding. For the hyperparameters not in Table 4, we used the default parameters defined by the libraries.

F Detailed experiment results and discussion

Here, we show some detailed experiment results and discussion.

F.1 Efficiency of learning with dynamic shielding

Figs. 10 to 12 show the mean of the reward of the best controllers obtained by each testing phase and the number of episodes, the number of steps, and the total execution time before the testing phase, respectively. In Fig. 10, we observe that Shielding usually requires a similar number of episodes to obtain a controller with similar performance compared to Plain or SafePadding. We also observe that Shielding sometimes requires
Fig. 11: The mean of the number of steps before each testing phase and the reward of the best controller obtained by the testing phase.
Fig. 12: The mean of the total execution time before each testing phase and the reward of the best controller obtained by the testing phase.
fewer episodes to obtain a controller with similar performance than Plain or SafePadding (e.g., WaterTank and Taxi). This improvement is likely because Shielding successfully prevented useless exploration.

In Fig. 11, we observe that Shielding usually requires a similar number of steps to obtain a controller with similar performance compared with Plain or SafePadding. We also observe that Shielding sometimes requires more episodes to obtain a controller with similar performance than Plain or SafePadding (e.g., GridWorld and SideWalk). This is likely because Shielding tends to make each episode longer by preventing failures, and the number of steps to experience a similar number of episodes tends to be larger. We can observe this tendency also in Fig. 13, which shows the relationship between the number of training episodes and the training steps before each testing phase.

In Fig. 12, we observe that Shielding usually takes a much longer time to obtain a controller with similar performance compared with Plain or SafePadding. As we discussed in Section 4.5 this is mainly because of the overhead of shield construction.
Fig. 14: The mean of the number of undesired training episodes and the number of steps before each testing phase.
Fig. 15: The mean of the number of undesired training episodes and the number of training episodes before each testing phase
Fig. 16: The mean of the training steps before each testing phase and the safe rate of the best controller obtained by the testing phase.

**F.2 Safety of learning with dynamic shielding**

Figs. 14 and 15 show the mean of the reward of the number of undesired training episodes and the number of training steps and episodes, respectively. In Fig. 14, we observe that the number of training episodes with undesired behavior tends to be smaller when using Shielding. This confirms the experiment results we observed and discussed in Section 4.3. In Fig. 14, we also observe that the curve of Plain is steeper than Shielding in CliffWalk, Taxi, and CarRacing. This shows that when we train a controller without shielding, the learning agent keeps causing undesired behaviors while dynamic shielding prevents them at least partially. In Fig. 14d, we observe that although the curve of Plain is steeper than SafePadding, the curve of SafePadding is still steeper than Shielding. This shows that SafePadding also prevents causing some undesired explorations, Shielding prevents more undesired explorations. Fig. 15 also shows a similar tendency.

**F.3 Safety of controllers learned with dynamic shielding**

Figs. 16 to 18 show the mean safe rate of the best controller obtained by each testing phase and the number of training steps and episodes and the number of episodes with undesired behavior by the testing phase, respectively. In Figs. 16
Fig. 17: The mean of the training episodes before each testing phase and the safe rate of the best controller obtained by the testing phase.
Fig. 18: The mean of the training episodes with undesired behavior before each testing phase and the safe rate of the best controller obtained by the testing phase.
Table 5: The mean and the standard deviation of the number of the training episodes with undesired behavior out of 30 trials

|               | Plain mean | Plain std | SafePadding mean | SafePadding std | Shielding mean | Shielding std |
|---------------|------------|-----------|------------------|-----------------|----------------|---------------|
| WaterTank     | 1883.67    | 83.02     | 1892.40          | 79.93           | 177.13         | 28.04         |
| GridWorld     | 6996.40    | 1510.04   | 7322.23          | 1399.39         | 5623.43        | 1256.44       |
| CliffWalk     | 1493.20    | 1523.12   | 1528.67          | 1058.68         | 478.20         | 155.09        |
| Taxi          | 8723.13    | 5593.19   | 2057.33          | 1406.02         | 37.77          | 19.79         |
| SelfDrivingCar| 6403.07    | 678.95    | 6454.60          | 895.09          | 5662.40        | 582.88        |
| SideWalk      | 373.60     | 386.11    | 427.93           | 399.94          | 273.37         | 314.05        |
| CarRacing     | 180.13     | 136.85    | 141.17           | 132.76          | 41.73          | 66.79         |

Table 6: The mean and the standard deviation of the mean reward out of 30 trials

|               | Plain mean | Plain std | SafePadding mean | SafePadding std | Shielding mean | Shielding std |
|---------------|------------|-----------|------------------|-----------------|----------------|---------------|
| WaterTank     | 918.89     | 9.50      | 919.81           | 8.15            | 921.81         | 3.46          |
| GridWorld     | 0.37       | 0.55      | 0.46             | 0.54            | 0.07           | 0.59          |
| CliffWalk     | -69.13     | 41.93     | -66.00           | 42.36           | -65.93         | 42.14         |
| Taxi          | -147.61    | 222.32    | -139.62          | 224.60          | -92.93         | 26.90         |
| SelfDrivingCar| 28.83      | 3.04      | 28.86            | 2.18            | 29.81          | 0.55          |
| SideWalk      | 0.93       | 0.44      | 0.90             | 0.50            | 0.67           | 0.54          |
| CarRacing     | 375.53     | 419.98    | 509.25           | 450.89          | 622.07         | 346.90        |

to 18, we generally observe that in most of the benchmarks, the curve of Shielding is growing faster than those of Plain and SafePadding. This shows that Shielding successfully prevented undesired explorations.

F.4 Other experiment results

Tables 5, 6 and 7 show the mean and the standard deviation of

1. the number of the training episodes with undesired behavior,
2. the success rate, and
3. the total execution time (in seconds)

out of 30 trials, respectively. Table 8 shows the mean of the difference of the total execution time between Shielding or SafePadding, and Plain.

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Table 7: The mean and the standard deviation of the execution time (in seconds) out of 30 trials

| Game          | Plain mean | Plain std | SafePadding mean | SafePadding std | Shielding mean | Shielding std |
|---------------|------------|-----------|------------------|------------------|----------------|---------------|
| WaterTank     | 1860.46    | 59.08     | 1947.09          | 80.11            | 6080.89        | 4055.24       |
| GridWorld     | 177.18     | 13.07     | 1487.10          | 125.03           | 4548.70        | 1667.95       |
| CliffWalk     | 355.18     | 11.82     | 365.54           | 13.97            | 839.06         | 148.45        |
| Taxi          | 336.04     | 10.22     | 1349.78          | 12.07            | 611.87         | 124.57        |
| SelfDrivingCar| 865.55     | 3.47      | 4919.13          | 168.00           | 10087.18       | 707.48        |
| SideWalk      | 762.67     | 64.92     | 1734.66          | 146.83           | 6395.73        | 1460.23       |
| CarRacing     | 7650.38    | 811.20    | 16694.63         | 576.96           | 12532.04       | 667.43        |

Table 8: The difference of the mean execution time (in seconds) out of 30 trials.

| Game           | Shielding – Plain | SafePadding – Plain |
|----------------|-------------------|---------------------|
| WaterTank      | 4220.43           | 86.62               |
| GridWorld      | 4371.53           | 1309.92             |
| CliffWalk      | 483.88            | 10.37               |
| Taxi           | 275.83            | 13.74               |
| SelfDrivingCar | 9221.62           | 4053.57             |
| SideWalk       | 5633.06           | 971.99              |
| CarRacing      | 4881.66           | 9044.25             |