Safe Model-Based Reinforcement Learning With an Uncertainty-Aware Reachability Certificate

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Abstract—Safe reinforcement learning (RL) that solves constraint-satisfactory policies provides a promising way to the broader safety-critical applications of RL in real-world problems such as robotics. Among all safe RL approaches, model-based methods reduce training time violations further due to their high sample efficiency. However, lacking safety robustness against the model uncertainties remains an issue in safe model-based RL, especially in training time safety. In this paper, we propose a distributional reachability certificate (DRC) and its Bellman equation to address model uncertainties and characterize robust persistently safe states. Furthermore, we build a safe RL framework to resolve constraints required by the DRC and its corresponding shield policy. We also devise a line search method to maintain safety and reach higher returns simultaneously while leveraging the shield policy. Comprehensive experiments on classical benchmarks such as constrained tracking and navigation indicate that the proposed algorithm achieves comparable returns with much fewer constraint violations during training. Our code is available at https://github.com/ManUtdMoon/Distributional-Reachability-Policy-Optimization.

Note to Practitioners—Although it has been proven that RL can be applied in complex robotics control tasks, the training process of an RL control policy induces frequent failures because the agent needs to learn safety through constraint violations. This issue hinders the promotion of RL because a large amount of failure of robots is too expensive to afford. This paper aims to reduce the training-time violations of RL-based control methods, enabling RL to be leveraged in a broader application area. To achieve the goal, we first introduce a safety quantity describing the distribution of potential constraint violations in the long term. By imposing constraints on the quantile of the safety distribution, we can realize safety robust to the model uncertainty, which is necessary for real-world robot learning with environment uncertainty. Second, we further devise a shield policy aiming to minimize the constraint violation. The policy will intervene when the agent is about to violate state constraints, further enhancing exploration safety. Third, we implement a line search method to find an action pursuing near-optimal performance when fulfilling safety requirements strictly. Our experimental results indicate that the proposed algorithm reduces training-time violations significantly while maintaining competitive task performance. We make a step towards applying RL safely in real-world tasks. Our future work includes conducting physical verification on real robots to evaluate the algorithm and improving safety further by starting from an initially safe control policy that comes from domain knowledge.

Index Terms—Safe reinforcement learning (RL), reachability analysis, model-based RL, robot learning.

I. INTRODUCTION

Reinforcement learning (RL) has achieved success across different automated control tasks such as robotics locomotion [1], navigation [2] and transportation management [3], [4]. However, the trial-and-error process of RL hinders its application in more real-world tasks due to the large number of failures brought by unconstrained policies, threatening the safety of users and systems. Therefore, safe RL [5] is proposed to impose constraints on agents and enhance the safety of policies both after convergence and during the training process. The training time safety issue, also called safe exploration (i.e., reducing the number of constraint violations during learning), is thought to be challenging and significant, especially when the dynamics of the environment are unknown. In this paper, we not only focus on the safe RL problem subject to certain constraints after convergence, but also take a step towards safe exploration.

Previous work formulates safe RL problems as constrained Markov decision process (CMDP) [5]. CMDP augments MDP with an additional cost signal indicating state-action pairs that violate constraints. By setting thresholds on the costs,
one gets policies with a low probability of failure. Common approaches to solve CMDPs include penalty function methods [6], Lagrange multiplier methods [7], [8], [9] and projection methods [10]. These work takes the expected cumulative costs (cost value in short) as the constrained quantity to realize safety in expectation. In contrast, another line of work replaces the cost value with safety certificates such as energy function [11] or reachability certificate [12] to equip algorithms with persistent safety constraint satisfaction in each state. However, all these methods utilize model-free RL (MFRL) algorithms whose low sample efficiency leads to significantly more interactions with environments, and more violations inevitably happen during learning.

An alternative way to improve training time safety is to use model-based RL (MBRL), i.e., performing policy updates with model-generated virtual data [1], [13], [14]. Recent studies combine CMDP with MBRL to reduce training violations and accelerate learning [15], [16], [17]. Despite their progress, MBRL is confronted with the uncertainty of the learned model. Because of the insufficient learning of dynamics, the model may predict transitions deviating from true dynamics, which makes the agent potentially take unsafe states as safe ones.

To address the uncertainty in safe MBRL, we propose Distributional Reachability Policy Optimization (DRPO), a Lagrangian-based MBRL approach with an uncertainty-aware reachability certificate to realize robust but non-conservative (training time) safety. Moreover, the certificate produces a shield policy, which we leverage from the perspective of the optimization problem and the perspective of policy execution, to alleviate conservativeness or potential danger caused by approximation error and insufficient learning. A detailed illustration of our DRPO framework is shown in Fig 1. Our main contributions are as follows:

- We propose a distributional reachability certificate (DRC) quantifying the safety of RL policies, whose variance explicitly represents the epistemic uncertainty of the agent in terms of its potential constraint violation in the future. To this end, the pessimism for uncertainty can be considered during learning. Existing safe MBRL approaches either ignore the model uncertainty or consider the uncertain effects of the learned model on safety implicitly (e.g., sampling and estimation). Therefore, our work gives direct intuition about to which degree the distributional reachability certificate is confident about safety.
- We leverage the shield policy produced by the DRC in different schemes to reduce conservativeness and maintain safety. Restricting the main policy subject to the certificate of the shield policy provides a looser constraint in the optimization problem, enabling the main policy to explore freely for higher return. Furthermore, the shield serves as a backup policy during interaction because it is safety-oriented. We also propose a line search method for efficient and safe action during evaluation, achieving a trade-off between performance and conservativeness.
- Comprehensive empirical results on robotics tasks such as constrained stabilization, tracking and navigation indicate the efficacy of the proposed DRC and DRPO algorithm. DRPO reaches comparable performance w.r.t. model-free and model-based baselines while reducing training time violations significantly and converging to a safe policy.

II. RELATED WORK

A. Safe Model-Free RL

Many safe model-free RL algorithms are designed under CMDP [5]. They constrain the cost value of the policy below a given threshold. Penalty function methods augment the original policy objective function by an additional term, which is the cost value multiplied by a penalty coefficient [6]. Lagrange multiplier methods convert the constrained policy optimization problem into an unconstrained problem by constructing a Lagrangian as the policy objective [7], [8], [9]. The policy parameters and the Lagrange multiplier are updated in an iterative manner using dual ascent. Projection methods update the policy in a two-step process [10]. The first step only considers the improvement of the rewards, while the second step ensures constraint satisfaction of the policy by projecting it back onto the constraint set.

Other algorithms use safety certificates instead of cost values to constrain the policy optimization. Safety certificates theoretically guarantee that the state trajectory always stays in a subset of the state space where the safety constraint is satisfied. Energy function methods synthesize a safety index with a pre-defined functional form that assigns low energy to safe states and guarantees persistent safety of energy-dissipating policies [11]. Reachability certificate methods use a safety value function to describe the worst-case constraint value and constrain it below zero in policy optimization [12].

There is also safe RL work adopting distributional RL to handle the stochasticity of the dynamics and enhance safety [18] but they also suffer from conservativeness. Moreover, a common problem of these model-free algorithms is that they cannot guarantee safety during training. It is because the cost value functions and safety certificates are learned totally from interaction data, which inevitably leads to a large number of safety violations during the learning process. Moreover, the low sample efficiency of model-free RL algorithms further increases training-time violations.

B. Safe Model-Based RL

Safe model-based RL algorithms aim at minimizing safety constraint violations during training. They learn policies on virtual data generated by environment models to improve sample efficiency and decrease the number of training-time violations in the actual environment. Thomas et al. [15] avoid unsafe states by planning ahead a short time into the future. They learn an ensemble of probabilistic dynamics models for planning and heavily penalize unsafe trajectories to ensure constraint satisfaction. Bayesian world models are leveraged in [16] to approximate the true dynamics. Then estimation of optimistic upper bounds on the task objective and pessimistic upper bounds on the safety constraints are made by posterior sampling. The augmented Lagrangian method solves the constrained policy optimization problem based on the estimated bounds. Zanger et al. [17] address the problem of accumulative model errors by adaptive resampling from
an ensemble of probabilistic environment models and using dynamically limited rollout horizons. Our method differs from these work in that we explicitly model the uncertainty of the safety value caused by the learned probabilistic model and learn a robust safe policy to address the uncertainty.

III. PRELIMINARY

A. Reinforcement Learning Formulations

**Constrained Markov decision process** is the common formulation of safe RL problems. We consider an infinite-horizon CMDP defined by the tuple \( \langle S, A, P, r, c, \gamma \rangle \), where (1) the state space \( S \) and the action space \( A \) are bounded and possibly continuous, (2) the unknown transition dynamics \( P : S \times A \mapsto \Delta(S) \) gives the distribution of the next state \( P(\cdot \mid s_t, a_t) \), where \( \Delta(S) \) is a distribution on the space \( S \). (3) \( r : S \times A \mapsto \mathbb{R} \) is the reward function. (4) \( c \) is called the cost signal where \( c(s, a) = \mathbb{I}_{h(s,a)=0} \), indicating we get 1 and the episode is terminated once the desired state constraint \( h(s, a) \leq 0 \) is violated and otherwise 0. The state constraint \( h(s, a) \) can be interpreted as signed distance towards the safe states boundary as illustrated in Fig 2 and we aim to keep the system states inside the desired safe states. (5) \( \gamma \in [0, 1) \) is the discounted factor. At each time step \( t \in \mathbb{N} \), the agent observes state \( s_t \) and chooses action \( a_t \) according to the policy \( \pi(\cdot | s_t) \in \Pi \), where \( \Pi \) is the set of all Markovian stationary policies. Then the dynamics transit to state \( s_{t+1} \) and send reward \( r_t \), cost \( c_t \), constraint violation \( h_t \) to the agent. Note that for simplicity we sometimes denote \( s_t, a_t \) as \( s, a \) and denote \( s_{t+1}, a_{t+1} \) as \( s', a' \), respectively. Given the initial state distribution \( d_0(s) \), we have \( d_t(s,a) := \sum_{s'} \gamma^t P(s_t = s; d_0, \pi, \gamma) \pi(a | s) \) as the state-action marginals following \( \pi \). We also denote the initial state set as \( S_0 := \{ s \mid d_0(s) > 0 \} \). The purpose of safe RL is to solve the following problem:

\[
\begin{align*}
\max_{\pi \in \Pi} & \quad \mathbb{E}_{s \sim d_0(s), a \sim \pi(\cdot | s)}[Q^\pi(s,a)] \\
\text{s.t.} & \quad \mathbb{E}_{s \sim d_0(s), a \sim \pi(\cdot | s)}[Q^\pi(s,a)] \leq \eta, \quad (1)
\end{align*}
\]

where the state-action value \( Q^\pi(s,a) := \mathbb{E}_{(s,a) \sim d_t} [\sum_{i} \gamma^i r_i] \) is the expected discounted cumulative rewards starting from \( (s,a) \) following \( \pi \); the cost value \( Q^\pi_c(s,a) := \mathbb{E}_{(s,a) \sim d_t} [\sum_{i} \gamma^i c_i] \) is the expected discounted violation probability and \( \eta \in [0, 1] \) is the cost threshold.

**Remark 1:** Although several approaches have been proposed to solve problem (1) and made achievements, the problem formulation is still a chance-constrained problem which is not safe enough for safety-critical systems. According to the property of the expectation of indicator functions, we have

\[
\begin{align*}
\mathbb{E}_{s \sim d_0(s), a \sim \pi(\cdot | s)}[Q^\pi(s,a)] &= \mathbb{E}_{s \sim d_0(s), a \sim \pi(\cdot | s)} \sum_t \mathbb{I}_{h(s,a)>0} \\
&= \sum_t \mathbb{E}_{s \sim d_0(s), a \sim \pi(\cdot | s)} \mathbb{I}_{h(s,a)>0} \\
&= \sum_t \Pr(h(s_t, a_t) > 0) \\
&\geq \Pr\left( \bigcup_t h(s_t, a_t) > 0 \right) \\
&= \Pr(\text{the trajectory is unsafe})
\end{align*}
\]

based on Boole’s inequality when \( \gamma = 1 \) and the episode is terminated when the constraint is violated. Therefore, the constraint imposed on the cost value is actually imposed on the probability of emergence of unsafe trajectories where \( \eta \in [0, 1) \) is the threshold. The probability of danger is low but not 0 when \( \eta \neq 0 \). However, setting \( \eta = 0 \) will bring challenges to reinforcement learning due to approximation error and the constraint may never be satisfied. Hence, a more appropriate quantity to describe safety is needed and we will introduce it in the following sections.

**Model-based RL** \([1], [13], [14], [19]\) replaces the unknown transition dynamics with a learned model \( \hat{P} \) which is trained by minimizing \( \mathbb{E}_{(s,a) \sim \mathcal{B}(D(P, \hat{P}))} \), where \( D \) is a certain
distance metric and B is either an offline dataset of state-action pairs or a replay buffer storing historical interactions. That is, the samples \((s, a, s')\) are generated by the learned model rather than the true dynamics. If the learned model is accurate enough, the virtual data are similar to the ones from interaction with the real environment, which guarantees the performance of MBRL and reduces exploration and potential violation in the real environment [20]. Another line of MBRL is to utilize the learned model to perform planning instead of policy learning, which is also known as model predictive control (MPC) [19], [21].

B. Reachability Certificate

Besides the cost value, researchers are working on advanced quantities describing the costliness of policies, including control barrier function (CBF) [22] or barrier certificate, safe index (SI) [11] and reachability certificate [12], [23]. These functions emphasize a vital property of safety-critical systems, the forward invariance property, i.e., satisfying constraints persistently. Therefore, replacing the constraints in (1) with certificates mentioned above enables the system to avoid violation at each time step instead of in expectation, and then brings stricter safety. Among all these certificates, the reachability certificate aims to locate as many persistently safe states as possible [24] and characterize the potentially safe states without handcrafted thresholds. In safe RL, more accessible safe states lead to a larger workspace for the agent to explore safely and hence possibly higher returns. Thus, we adopt reachability certificate in this work as well.

Rather than cumulative costs in the cost value, reachability certificate focuses on the worst-case constraint violation starting from the state-action pair \((s, a)\). We first discuss about a deterministic \(P\) and \(\pi\) here for simplicity and the stochastic case is illustrated in detail in Section IV-A:

\[
\bar{Q}^\pi_B(s, a) := \max_{\pi \in \Pi} h(s, a) \mid s_0 = s, a_0 = a, \pi, P, \tag{2}
\]

which means after taking action \(a\) at state \(s\), the agent follows the policy \(\pi\) and observes the worst-case constraint value. If (1) \(\min_{s \in A} Q^\pi_B(s, a) \leq 0\), there must exist an action \(a^*\) guaranteeing the safety of the agent in the infinite horizon starting from \(s\); (2) \(\min_{s \in A} Q^\pi_B(s, a) > 0\), the agent is doomed to violate the constraint \(h(s, a) \leq 0\) in the future following \(\pi\). We define the persistently safe states in the former case as feasible states:

**Definition 1 (Persistently safe states):** All states starting from which the constraint will not be violated if following a given policy \(\pi\) are defined as persistently safe feasible states. They are included in the feasible set of \(\pi\):

\[
S^\pi_f := \{s \in S : \min_{a \in A} Q^\pi_B(s, a) \leq 0\}. \tag{3}
\]

Now we can characterize the persistently safe states in safe RL by computing the reachability certificate, which follows a Bellman equation like \(Q^\pi\) in conventional RL [12], [23]:

\[
Q^\pi_B(s, a) = \max \{h(s, a), Q^\pi_B(s', \pi(s'))\}. \tag{4}
\]

Similar to [12] and [23], we introduce a discounted factor \(\gamma\) for the convergence convenience. Moreover, As \(\gamma \rightarrow 1\), the discounted version of reachability certificate approaches the original undiscounted value. Thus, the Bellman equation of \(Q^\pi_B(s, a)\) becomes:

\[
Q^\pi_B(s, a) = (1 - \gamma)h(s) + \gamma \max\{h(s, a), Q^\pi_B(s', \pi(s'))\}. \tag{5}
\]

Till now, we can perform dynamic programming or temporal-difference learning with (5) to calculate the reachability certificate like the computation of the \(Q\) function in conventional RL.

**Remark 2:** The two violation indicators \(h\) and \(c\) may share the similar functions because the super zero-level sets of \(Q^\pi_B(s, a)\) and \(Q^\pi_I(s, a)\) both contains states are doomed to be unsafe. We introduce two notations here to bridge the RL community which leverages \(c\) more often [5], [25] and the control community which prefers \(h\) [23]. More importantly, we choose \(h\) finally because \(h\) has a substantial physical interpretation such as the signed distance towards the unsafe region. Therefore, it offers more information from the environment. The negative gradients of \(h\) (\(Q^h_B\) further) implies the direction along which the system should be driven. In other words, \(h\) tells the agent to decrease the value to avoid danger as its states evolve. In contrast, the step property of \(c\) cannot offer this gradient-style information in the neighborhood of a point \((s, a)\). Therefore, leveraging \(Q^h_B\) will accelerate the learning of agents.

C. Problem Statement

Leveraging the aforementioned reachability certificate in safe RL problems (1) to replace the constraint imposed on cost value functions, we can get a more appropriate formulation characterizing the persistently safe states rather than the safe ones in expectation [12], [23]:

\[
\max_{\pi \in \Pi} \mathbb{E}_{s \sim d_0} [Q^\pi_B(s, a) \cdot \mathbb{1}_{s \in S^f} - Q^\pi_B(s, a) \cdot \mathbb{1}_{s \notin S^f}] \quad \text{s.t.} \quad Q^\pi_B(s, a) \leq 0, \forall s \in S_0 \cap S^f, \tag{6}
\]

where \(a\) is the action taken at state \(s\) without exploration noise given by policy \(\pi\) (thus a deterministic action); \(\mathbb{1}_A = 1\) holds when the event \(A\) is true and otherwise \(\mathbb{1}_A = 0\).

Note that this safe RL formulation in (6) is different from the conventional one (1) in two ways: (1) the objective function is separated into two parts where for states inside \(S^f\), it is possible to realize persistent safety so we can maximize return and guarantee safety simultaneously. However, for initial states outside \(S^f\), the desired constraint \(h(s, a) \leq 0\) will be violated sooner or later so it is meaningless to optimize the return. We only try to minimize the worst violation; (2) the constraint is imposed on every initial state inside the feasible set \(S^f\). Therefore, there are multiple (maybe infinite in continuous cases) constraints in the formulation rather than an expected one in (1). Prior work [11], [26] call this type constraints state-wise constraints and this formulation aims at safety at each time step and each possible state. The merits of reachability certificate in RL are discussed in [12] and we utilize it directly in this paper.
Fig. 3: We illustrate the core idea of distributional reachability certificate. Due to the probabilistic model (either posterior sampling in [16] or gaussian ensembles in [14]), the state trajectories vary a lot, leading to a distribution of $Q_h^\pi(s,a)$. Therefore, we approximate $Q_h^\pi(s,a)$ with a distribution rather than only focusing its expectation. Our goal is to optimize the policy to shift the distribution and make its $\beta$-quantile to be below zero. Then the possible trajectory will be (i.e., a robust safety).

IV. SAFE MBRL VIA UNCERTAINTY-AWARE REACHABILITY CERTIFICATE

Besides solving the constrained optimization problem (6), we aim to reduce the training violation. To achieve this, we extend the reachability certificate to an uncertainty-aware formulation (i.e., a distributional certificate) as well as a shield policy considering the model uncertainty in Section IV-A and IV-B. Section IV-C shows the practical algorithm. Specifically, we show how we learn and leverage the model in Section IV-C1. We implement the distributional reachability certificate (DRC) in a Gaussian form and impose constraints on its quantile in Section IV-C2. Section IV-C3 gives the objective functions of each parameterized model while Algorithm 1 illustrates DRPO further.

A. Distributional Reachability Certificate: Uncertainty-Aware Safety Critic

One key issue that arises in MBRL is the model error [13], which results in discrepancies between the predicted return under the learned model and the true dynamics. Probabilistic model ensembles and clipped rollouts are proposed to cover the true dynamics within the support of the ensembles and mitigate the error [13], [14]. However, the stochasticity of the subsequent states $s'$ generated by the uncertain model $\hat{P}$ will still lead to a deviated or even wrong estimation about the cost value or reachability certificate in safe RL if not addressed properly. In the context of safety-critical problems, it is not enough to only care about the expected safety quantities of the predicted trajectories because an unsafe state misunderstood as safe will bring catastrophic failure to the system.

Furthermore, the reachability certificate value $Q_h^\pi(s,a)$ of a given state-action pair $(s,a)$ under the learned model is inevitably a random variable rather than a fixed quantity. This is because the subsequent states and the subsequent state trajectories may be totally different during the model rollouts due to the probabilistic transition, as shown in Fig 3.

Hence, we need a reachability certificate robust to the potential model error and aware of the uncertainty of the learned model. Inspired by recent progress in distributional RL (i.e., modeling the value functions in RL as distributions instead of focusing on its expected value) [27], [28], we propose distributional reachability certificate. By imposing constraints on its $\beta$-quantile (a.k.a. value-at-risk, VaR), we are able to get a safety quantity robust to the model error and uncertainty with a high confidence level. Furthermore, the robust reachability certificate is not conservative because the model accuracy is improved and the uncertainty is decreased as learning proceeds.

We consider to model the distribution of the reachability certificate instead of its expected value. We define $\mathcal{Z}(Q_h^\pi(s,a)|s,a) : S \times A \mapsto P(Q_h^\pi(s,a))$ as the mapping from $(s,a)$ to a distribution over the reachability certificate value and call it the distributional reachability certificate (DRC). Similar to [27], we define the distributional Bellman operator of reachability certificate as

$$T^\pi Q_h(s,a) := \mathbb{E}[(1-\gamma)h(s,a) + \gamma \max \{h(s,a), Q_h(s',a')\}]$$

$$s' \sim \hat{P}(\cdot|s,a), a' \sim \pi(\cdot|s')$$ \hspace{1cm} (7)

where $A \overset{D}= B$ denotes that two random variables $A$ and $B$ shares the same probability density function. The uncertainty of $T^\pi Q_h(s,a) \sim T^\pi \mathcal{Z}(\cdot|s,a)$ consists of two parts under settings in this paper: (1) the probabilistic transition model $s' \sim \hat{P}(\cdot|s,a)$ and (2) the distributional next-state-action certificate $Q_h(s',a')$. Similar to [27], we can prove that $T^\pi$ is $\gamma$-contraction as the following corollary states.

**Corollary 1 (contraction):** $T^\pi : \mathcal{Z} \mapsto \mathcal{Z}$ is a $\gamma$-contraction in $\tilde{d}_p$, where $\tilde{d}_p$ is a maximal form of the Wasserstein metric and $1 \leq p \leq \infty$:

$$\tilde{d}_p(\mathcal{Z}_1, \mathcal{Z}_2) = \sup_{s,a} d_p(\mathbb{E}[Q_h(s,a)], \mathbb{E}[Q_h(s,a)])$$

$$= \sup_{s,a} \inf_{\mathcal{Z}_1, \mathcal{Z}_2} \| \mathbb{E}[Q_h(s,a)] - \mathbb{E}[Q_h(s,a)] \|_p$$.

**Proof:** Consider $\mathcal{Z}_1$ and $\mathcal{Z}_2 \in \mathcal{Z}$. By definition,

$$\tilde{d}_p(T^\pi \mathcal{Z}_1, T^\pi \mathcal{Z}_2) = \sup_{s,a} d_p(T^\pi Z_1(Q_h(s,a)), T^\pi Z_2(Q_h(s,a))).$$

By the properties of $d_p$, we have

$$d_p(T^\pi Z_1(Q_h(s,a)), T^\pi Z_2(Q_h(s,a)))$$

$$= d_p((1-\gamma)h(s) + \gamma \max\{h(s), Q_h^1(s',a')\})$$

$$= (1-\gamma)h(s) + \gamma \max\{h(s), Q_h^1(s',a')\}$$

$$\leq d_p(\gamma \max\{h(s), Q_h^1(s',a')\}, \gamma \max\{h(s), Q_h^2(s',a')\})$$

$$\leq \gamma d_p(\max\{h(s), Q_h^1(s',a')\}, \max\{h(s), Q_h^2(s',a')\})$$

$$\leq \gamma \inf_{Q_h^1, Q_h^2} \| \max\{h(s), Q_h^1(s',a')\} - \max\{h(s), Q_h^2(s',a')\} \|_p$$

$$\leq \gamma \inf_{Q_h^1, Q_h^2} \| Q_h^1(s',a') - Q_h^2(s',a') \|_p$$

$$\leq \gamma \sup_{s',a'} \inf_{Q_h^1, Q_h^2} \| Q_h^1(s',a') - Q_h^2(s',a') \|_p$$

$$\leq \gamma \sup_{s',a'} d_p(\mathcal{Z}_1(Q_h(s',a')), \mathcal{Z}_2(Q_h(s',a')))$$

$$\leq \gamma \tilde{d}_p(\mathcal{Z}_1, \mathcal{Z}_2).$$

□
Therefore, $T^π$ has a fixed point $\mathcal{Z}(Q^n_π(s, a))$ by checking the conditions of Banach’s fixed point theorem. The sequence $\{Z_k(\cdot, s, a)\}$ produced by solving the following optimization problem iteratively converges to $\mathcal{Z}(Q^n_π(s, a))$:

$$Z_{\text{new}} = \arg \min_z \mathbb{E}_{(s, a) \sim d_s} [D(T^n Z_{\text{old}}(\cdot, s, a), Z(\cdot, s, a))],$$  

(8)

where $D$ is the Wasserstein metric between two distributions. However, the Kullback-Leibler (KL) divergence $D_{\text{KL}}$ is commonly adopted in distributional RL instead [27], [28].

Suppose that the distribution $Z(\cdot, s, a)$ covers the true reachability certificate value of the $(s, a)$ pair. In order to realize safety robust to the model uncertainty, we need to guarantee that most samples of $Z(\cdot, s, a)$ adhere to the constraints (i.e., less than or equal to zero). Given a user-specified quantile fraction (a.k.a. confidence level) $\beta \in (0, 1]$ (ideally, $\beta$ is close to one), the $\beta$-quantile function (or VaR of $(1 - \beta)$) of the DRC is defined as $F_{Q^n_π(\cdot, s, a)}^{-1}(\beta) := \inf \{q^n_π \in \mathbb{R} : F_{Q^n_π}(q^n_π) \geq \beta\}$, where $F_{Q^n_π}(q^n_π)$ is the cumulative distribution function (CDF) of the distribution $Z(\cdot, s, a)$ and $F^{-1}$ is its inverse; $Q^n_π$ is the random variable and $q^n_π$ is a specific value. The meaning of the $\beta$-quantile function of DRC lies in that once we guarantee $F_{Q^n_π(\cdot, s, a)}^{-1}(\beta) \leq 0$, the trajectory starting from $(s, a)$ remains safe with at least the probability of $\beta$ as long as following $\pi$ because the true value $q^n_π(\cdot, s, a)$ (the worst-case violation in the long term) is covered by $(\infty, F_{Q^n_π(\cdot, s, a)}^{-1}(\beta))$ with at least the probability of $\beta$. Thus, we get $\mathbb{P}[Q^n_π(\cdot, s, a) \leq 0] \geq \beta$ if $F_{Q^n_π(\cdot, s, a)}^{-1}(\beta) \leq 0$. We denote $Z_{\beta}(s, a; \pi) := F_{Q^n_π(\cdot, s, a)}^{-1}(\beta)$ for simplicity from now on. Finally, all we need to do to realize a robust safety w.r.t. the model uncertainty is to replace the terms $Q^n_π(s, a)$ in (6) with $Z_{\beta}(s, a; \pi)$:

$$\max_{\pi \in \Pi} \mathbb{E}_{s \sim d(s)} \left[ Q^n(s, a) \cdot 1_{s \in S^β_{\pi}} - Z_{\beta}(s, a; \pi) \cdot 1_{s \notin S^β_{\pi}} \right]$$

s.t. $Z_{\beta}(s, a; \pi) \leq 0, \forall s \in S_0 \cap S^β_{\pi}$,  

(9)

where $S^β_{\pi} := \{ s : \min_{a \in A} Z_{\beta}(s, a; \pi) \leq 0 \}$. 

**B. Shield Policies and Safety Framework**

In practice, an intermediate solution policy of (9) may trade-off between safety and performance inappropriately and tend to violate constraints for more rewards because of insufficient updates, which we want to mitigate in this work. Hence, we propose a shield policy minimizing the $\beta$-quantile of long-term constraint violation (reachability certificate). The action $a$ proposed by the original policy will be overwritten by the shield policy when the predicted $\beta$-quantile DRC of $(s, a)$ is possibly dangerous (i.e., beyond zero). We first give formal definitions of the shield policy.

**Definition 2 ($\beta$-shield policy):** An $\beta$-shield policy $\pi$ for $Z(\cdot, s, a)$ minimizes the $\beta$-quantile of $Q^n_π$. The set of $\beta$-shield policies is

$$\Pi_\beta := \{ \pi \in \Pi : \sum_a \pi(a|s)Z_{\beta}(s, a; \pi) = \min_{a \in A} Z_{\beta}(s, a; \pi) \}.$$  

(10)

Analogous to the value iteration architecture in conventional RL [29], [30], a $\beta$-shield policy $\pi_\beta \in \Pi_\beta$ and its corresponding DRC can be computed by alternating between solving $\min_{\pi \in \Pi} \mathbb{E}[Z(s, a; \pi)]$ and solving $\min_{\pi} \mathbb{E}[D_{\text{KL}}(TZ, Z)]$, where $T$ is the distributional Bellman optimality operator of reachability certificate.

$$T Q_\pi = T^n Q_\pi$$

for some $\pi \in \Pi_\beta$.

Once we get an intermediate $\pi_\beta$ and its DRC $\mathcal{Z}(\cdot, s, a)$, we will leverage it in exploration to reduce training time violations by invoking $\mathcal{Z}$ before taking action $a$.

If $Z_{\beta}(s, a; \pi_\beta) > 0$, following a safety-oriented policy $\pi_\beta$ will still violate constraints with a high probability after taking $a$ at $s$, so $a$ should be overwritten by a safer action, e.g. $\pi_\beta(s)$.

One possible issue arises from the overwriting action is the conservativeness because the action given by $\pi_\beta$ is safety-oriented and it will hinder the reward acquisition temporarily. We address this issue in two ways, one from the perspective of optimization problem and the other from policy execution, forming our safe RL framework illustrated in Fig 1.

From the optimization problem: We replace the constraint $Z_{\beta}(s, a; \pi) \leq 0$ in (9) with the constraints on the DRC of the shield policy, leading to the final problem formulation of this work.

$$\max_{\pi \in \Pi} \mathbb{E}_{s \sim d(s)} \left[ Q^n(s, a) \cdot 1_{s \in S_0} - Z_{\beta}(s, a; \pi) \cdot 1_{s \notin S_β} \right]$$

s.t. $Z_{\beta}(s, a; \pi) \leq 0, \forall s \in S_0 \cap S_β$, for some $\pi_β \in \Pi_β$,  

(11)

where $S_{\beta} := \{ s : \min_{a \in A} Z_{\beta}(s, a; \pi_\beta) \leq 0 \}$ and the main difference is that all constraint parts are related to the shield policy. The merit of taking $Z_{\beta}(s, a; \pi_\beta)$ as the constraint lies in that $Z_{\beta}(s, a; \pi_\beta) \leq Z_{\beta}(s, a; \pi), \forall s \in \Pi$. Therefore, it is easy to obtain $S_{\beta}^β \subseteq S_{\beta}$, which means the agent is allowed to work in a larger subspace of $S$. This is because the long-term violation of $(s, a)$ will be decreased by taking $\pi_\beta$, a safety-only policy, as the future policy. This approach is also similar with the least-restrictive method [31] due to a larger workspace.

From the policy execution: As shown in Fig 1(b), there may be a margin between the safe action $a_\delta$ and the action $a$ given by $\pi$. Therefore, applying $a_\delta$ directly will lose the optimality. We propose a line search method between $a_\delta$ and $a$ in the action space, i.e., finding the nearest coarse action $a := ka + (1 - k)a_\delta$ whose DRC is below zero, where the optimal $k^*$ is given by

$$k^* = \min \{ k \in \{0, \frac{1}{N}, \ldots, \frac{N - 1}{N}, \ldots, 1\} : Z_{\beta}(s, a + (1 - k)a_\delta; \pi_\beta) \leq 0 \}.$$  

(12)

We find $N = 10$ is sufficient for tasks in this work. This simple approach resembles the projection method in [10] but the line search trick is simpler and we find it effective during execution. Note that we adopt the line search method only when evaluating the intermediate policy, and we still overwrite $a$ with $a_\delta$ if unsafe (i.e., $Z_{\beta}(s, a; \pi_\beta; \psi) > 0$) during training. The whole process of DRPO is illustrated in Fig 1(b), including an RL problem constraining the distributional reachability certificate, a $\beta$-shield policy and the line search method, forming a complete safe RL framework.
Algorithm 1: Distributional Reachability Policy Optimization

Require: Rollout length $H$, episode length $T_{ep}$, gradient descent steps $N_{grad}$

1: Initialize main policy $\pi_\theta$, critic $Q^T_{\theta}$, DRC $Z_\psi$, shield policy $\pi_{\theta_h}$, multiplier $\lambda_\xi$; and empty buffer $D_{real}$ and $D_{virt}$; the ensemble of learned models $\{\hat{P}_i\}_{i=1}^B$.

2: for episode 1, 2, ... do

3: for $T_{ep}$ times do

4: Interact with $\pi_\theta$ and $\pi_{\theta_h}$ by checking the $\beta$-quantile $Z_\beta(s, a; \pi_{\theta}; \psi) \leq 0$; add samples to $D_{real}$  \rightarrow Interaction

5: Fit models $\{\hat{P}_i\}_{i=1}^B$ by performing mini-batch GD on (13) with $D_{real}$  \rightarrow Model Learning

6: Sample $s \sim D_{real}$

7: Rollout from $s$ for $H$ steps with $\pi_\theta$ and $\{\hat{P}_i\}_{i=1}^B$; add the samples to $D_{virt}$  \rightarrow Model rollout

8: for $N_{grad}$ times do

9: Sample mini-batch from $D_{virt}$ for successive updates

10: Update $Q_\theta$ by mini-batch GD on (20); Update $Z_\psi$ by mini-batch GD on (14)  \rightarrow Critics learning

11: Update $\pi_\theta$ by mini-batch GD on (21); Update $\pi_{\theta_h}$ by mini-batch GD on (19)  \rightarrow Actors learning

12: Update $\lambda_\xi$ by mini-batch GD on (21)  \rightarrow Multiplier learning

C. Practical Implementation

1) Model Learning and Usage: Same as prior MBRL work [13], [14], [15], we adopt an ensemble of diagonal Gaussian dynamics model parameterized by $\phi$ as the world model approximators, denoted as $\{\hat{P}_i\}_{i=1}^B$, where $\hat{P}_i = \mathcal{N}(\mu_i(s, a), \sigma_i^2(s, a))$ is one diagonal Gaussian and $B$ is the number of independent Gaussian models in the ensemble. We choose $B = 5$ as previous papers [14], [15] do. The models are updated via maximum likelihood on all historical transitions $(s, a, r, s', h)$ from the replay buffer $D_{real}$:

$$\mathcal{J}_\mu(\phi_i) = - \mathbb{E}_{(s, a, r, s') \sim D_{real}} \log \hat{P}_i(s', r | s, a). \quad (13)$$

Note that the constraint function can either be known a priori or be learned similarly as the reward function. We test both cases in Section V. Each model in the ensemble is initialized randomly and updated with the same mini-batch selected from the buffer $D_{real}$, resulting in totally different models and rollouts given the same starting point $(s, a)$. The models are utilized to generate virtual transitions for learning the critics and policies. At each time step, we sample a mini-batch from the buffer as the starting point and perform one-step prediction by choosing one model $\hat{P}_i$ randomly from the ensemble. After repeating the rollout for $H$ times, where $H$ is a hyper-parameter, we add the transitions to a virtual buffer $D_{virt}$ for updating the critics and policies. This type of truncated rollout method leads to a smaller error in terms of the value function [14]. But its probabilistic nature still brings distributional predictions that need to be addressed, especially under safety-critical circumstances.

2) Gaussian Approximated DRC Learning: Despite the shape of the true reachability certificate, we can approximate it with parameterized and tractable distribution, e.g., a diagonal Gaussian. As long as the mean of the approximated Gaussian is close to the true certificate value, the $\beta$-quantile of the Gaussian will cover the true value with high-probability, leading to a safety guarantee. This can be achieved by model learning, which brings a decreasing discrepancy between the certificate of the learned model and the one under the true dynamics. However, a Gaussian may still be a coarse approximation of a complicated distribution as mentioned in [18] and interested readers are referred to [18] for advanced approaches.

We denote the parameterized Gaussian approximation of DRC as $Z_\psi(\cdot | s, a) := \mathcal{N}(\mu_\psi(s, a), \sigma_\psi^2(s, a))$ with parameter $\psi$. For example, the mean and the variance can be approximated by two neural networks parameterized by $\psi$. Then the model-based KL-divergence version of (8) is

$$J_Z(\psi) = \mathbb{E}_{(s, a) \sim D_{real}} \left[ D_{KL}(T \mathcal{Z}_\psi(\cdot | s, a), Z_\psi(\cdot | s, a)) \right]$$

$$= - \mathbb{E}_{(s, a) \sim D_{real}} \mathbb{E}_{a' \sim \pi_{\theta}} \mathbb{E}_{Q_\theta(s, a) \sim \mathcal{Z}_\psi(\cdot | s, a)} \left[ \log \mathcal{P}(T Q_\theta(s, a)|Z_\psi(\cdot | s, a)) \right], \quad (14)$$

where $c$ is a term independent of $\psi$ and detailed derivation can be found in [28]. By minimizing (14), we obtain a Gaussian approximation of $\mathcal{Z}(\cdot | s, a)$ and its $\beta$-quantile is

$$Z_\beta(s, a) = \mu_\psi(s, a) + \Phi^{-1}(\beta)\sigma_\psi(s, a), \quad (15)$$

where $\Phi^{-1}(\beta) \in (0, 1)$ is the inverse function of CDF of standard normal distribution. Common $(\beta, \Phi^{-1}(\beta))$ pairs include $(0.841, 1), (0.977, 2)$ and $(0.999, 3)$ and we compare their corresponding efficacy in the ablation study.

3) Model-Based Lagrangian Optimization: We leverage the widely used Lagrange multiplier method to solve the constrained optimization problem (11). The problem is transformed into solving the saddle point of Lagrangian $L(\pi, \lambda)$. Similar to [12] and [26], the statewise constraints are imposed on each state in $S_\beta \cap S_{\theta}$, so the Lagrangian is formulated as

$$L(\pi, \lambda) = \mathbb{E}_{s \sim d_{\theta}(s)} [-Q^T(s, a) \cdot 1_{s \in S_\beta} + Z_\beta(s, a; \pi_{\theta}) \cdot 1_{\lambda > 0} \cdot 1_{s \in S_{\theta}}] + \int_{S_\beta \cap S_{\theta}} \lambda(s) Z_\beta(s, a; \pi_{\theta})ds, \quad (16)$$

where $\lambda : S \mapsto [0, \lambda_{max}]$ is the statewise multiplier function. We do not optimize (16) directly due to the intractability of $S_\beta$ in advance but a surrogate version that is easier to handle. The surrogate shares the same optimal solution with (16) according to [12]:

$$\hat{L}(\pi, \lambda) = \mathbb{E}_{s \sim d_{\theta}(s)} \lim_{\lambda \to \lambda_{max}} \mathbb{E}_{a \sim \pi(\cdot | s)} [-Q^T(s, a) + \lambda(s) Z_\beta(s, a; \pi_{\theta})]. \quad (17)$$
Therefore, (11) can be solved by finding the saddle point of the surrogate Lagrangian (17) by gradient descent (GD):

$$\min_{\pi} \max_{\lambda} \hat{J}(\pi, \lambda).$$  \hspace{1cm} (18)

For the overall structure of DRPO, we adopt the popular actor-critic framework with deep neural networks as the approximators. In particular, we have two actor-critic structures, one for solving the $\beta$-shield policy $\pi_\beta(\cdot\mid s; v)$ and its corresponding DRC $\mathcal{Z}(\cdot\mid s, a; \pi_\beta; \psi)$, and the other for solving the main policy $\pi(\cdot\mid s; \theta)$, the Q-value function $Q(s, a; \omega)$ and the multiplier $\lambda(s; \xi)$. The DRC is updated by taking SGD on (14) while the $\beta$-shield policy $\pi_\beta(\cdot\mid s; v)$ tries to minimize the $\beta$-quantile of DRC

$$\mathcal{J}_\beta(v) = \mathbb{E}_{s \sim \mathcal{D}_{\text{train}}[\cdot\mid x,v]} \left[ Z_\beta(s, a; \pi_\beta; \psi) \right].$$ \hspace{1cm} (19)

The Q-value function is updated by minimizing the mean squared error between the current and target value:

$$\mathcal{J}_Q(\omega) = \mathbb{E}_{(s,a,r,s') \sim \mathcal{D}_{\text{train}}[\cdot\mid x]} \left[ Q(s, a; \omega) - (r + \gamma Q(s', a'; \omega)) \right]^2.$$ \hspace{1cm} (20)

As mentioned earlier, the main policy $\pi(\cdot\mid s; \theta)$ is updated by descending the surrogate Lagrangian while the multiplier $\lambda_\xi$ tries to ascend it:

$$\mathcal{J}_\pi(\theta) = -\mathcal{J}_\xi(\xi) = \mathbb{E}_{s \sim \mathcal{D}_{\text{train}}[\cdot\mid x,\theta]} \left[ -Q(s, a; \omega) + \lambda(s; \xi) Z_\beta(s, a; \pi_\beta; \psi) \right].$$ \hspace{1cm} (21)

We adopt soft-actor-critic (SAC) [32], a popular off-policy RL algorithm, as the policy optimizer. Thus, a regularization term related to the policy entropy is added to $\mathcal{J}_\pi(\theta)$. A complete version of DRPO is summarized in Algorithm 1. Note that sometimes we take the parameters $(\theta, \nu, \omega, \psi, \phi, \xi)$ as the subscript of the notation for simplicity.

V. EXPERIMENTS

We evaluate our methods DRPO on classical robotics tasks such as constrained stabilization, tracking and sensorimotor navigation. Our goal is to validate: (1) whether DRPO is able to learn a safe policy with non-trivial performance; (2) whether the proposed DRC and the corresponding shield policy help to reduce training time violations.

A. Environments

We test all algorithms on four environments in three benchmarks. Note that each episode will be terminated if the constraint is violated during training unless further explained.

**Cartpole-Move** is a task based on cartpole in OpenAI-Gym [33], [34] and MuJoCo [35], borrowed from [36]. The goal is to move the cart (yellow part in Fig 4a) to control the pole (blue part in Fig 4a). Starting from $(\theta, x) = (0, 0)$, the system is constrained in the space $\{(\theta, x) : |x| \leq 0.9, |\theta| \leq 0.2\}$, i.e., $h(s) = [x - 0.9, -0.9 - x, \theta - 0.2, -0.2 - \theta]^T$ (here we temporarily use $\theta$ to denote the deviation angle of the pole). The reward function is $r(s, a) = x^2$. Therefore, there is a conflict between obtaining rewards and staying safe. The cart should move slowly towards one direction and then stay still around $x < 0.9$. The length of an episode $T_{ep}$ is 1000.

**Quadrotor** is a 2D quadrotor tracking task in safe-controlgym [37]. The policy needs to output normalized torque to control the quadrotor to track the circle trajectory (red line in Fig 4b) as accurately as possible. However, the quadrotor is constrained w.r.t. its height $z$ where $h(s) = [z - 1.5, 0.5 - z]^T$ (black straight line). Therefore, the constraint contradicts the reward as well. The length of an episode $T_{ep}$ is 360.

**CarGoal** and **PointGoal** come from Safety-Gym [9], a constrained robot navigation benchmark. The robot (red in Fig 4c) should reach the goal region while avoiding entering the blue hazards. The dynamics of car is more complex than one of point. The layout of the environment is initialized randomly before each episode begins or after the robot reaches the goal. There are five hazards in the layout so the constraint is $h(s) = \max_{1 \leq i \leq 5} \{-\text{dist}(\text{robot, hazard}_i)\}$, where dist is the signed distance between two objects. The reward is the difference of the distance between the robot and the goal of two time steps. These two tasks are more complicated than the other two because besides sensor readings and goal position, the robot have only access to lidar point clouds of the hazards instead of their exact position. Therefore, the constraint function and the state of the robot should be learned. The length of an episode $T_{ep}$ is 1000.

B. Baselines

The baselines for comparison include both model-free and model-based (safe) RL algorithms. We choose five model-free algorithms: **Constrained Policy Optimization** (CPO) [25] approximates the objective function and the constraint using trust region methods, and analytically solves for the policy parameters. **PPO-Lagrangian** (PPO-L) [9] combines PPO with the Lagrangian method, which takes a weighted sum of the value and cost value function as the policy objective, and updates the multiplier using dual ascent. **SAC-Lagrangian** (SAC-L, a.k.a. Reward Constrained Policy Optimization, RCPO) combines SAC with the Lagrangian method similarly with PPO-L. **Conservative Safety Critic** (CSC) [38] learns a safety critic that overestimates the probability of failure and uses it to constrain the policy improvement through primal-dual gradient descent. **Reachable Actor Critic** (RAC) [12] leverages the self-consistency condition to learn the expected reachability certificate, which characterizes the largest feasible set, and uses it to constrain the policy.

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**Fig. 4.** Snapshots of the three tasks, including agents and constraints.
optimization. We also choose two model-based algorithms. Model-Based Policy Optimization (MBPO) [14] uses short model-generated rollouts branched from real data to update the policy, and does not consider safety constraints. Safe MBPO (SMBPO) [15] builds on MBPO and heavily penalizes unsafe trajectories to avoid safety violations. Our DRPO relies on MBPO as well but leverages DRC and the shield policy to reduce violations. We set $\Phi^{-1}(\beta)$ to 2 in Cartpole-Move and Quadrotor and to 1 in Safety-Gym tasks.

There are also safe RL approaches we do not compare with since they assume additional knowledge or other reasons. Recovery RL [39] utilizes an offline dataset to pre-train a recovery policy and a recovery zone to guard the training process. Zhao et al. [40] assume access to an accurate black-box model during planning, which is difficult to get in real-world. Luo et al. [36] and Berkenkamp et al. [41] start from an initially safe policy to guarantee safe learning, which is hard to obtain in complex tasks. Distributional functions in safe RL have been investigated recently in [18] but they focus on the stochasticity of model-free settings, which may cause more violations during interaction. In contrast, we propose DRC to address the model-uncertainty in model-based algorithms which leads to fewer violations in nature so we do not list their results in this work. Furthermore, DRC and the learned model in this work can be adopted in broader approaches such as model-based planning (MPC).

C. Results

We evaluate all algorithms with three metrics: (1) episode return (ER) $\sum_{t=0}^{T-1} r_t$ indicates the performance of different intermediate agents; (2) episode constraint violation (ECV) $\sum_{t=0}^{T-1} c_t$ shows the constraint satisfaction of intermediate policies and we do not terminate an episode upon violation during evaluation (different from training); and (3) cumulative training violations (CTV) $\sum_{t=0}^{T-1} c_t$ indicates the exploration safety of algorithms, where $T$ is the total interactions since the training begins. CTV is the main criterion we focus on for safety-critical RL tasks. Note that all baselines except CPO and PPO-L are off-policy ones. Therefore, several transitions of a random policy are added to the buffer before the updates. That is why the training violation curves in some tasks and the total env interactions (x-axis) do not start from zero. Each run of one algorithm per task is repeated with 5 random seeds and we record the mean and the 95% confidence interval.

The results are shown in Fig 5. As expected, the proposed DRPO converges to a policy with comparable even better performance and nearly perfect constraint satisfaction across all tasks. Furthermore, DRPO outperforms all baselines w.r.t. CTV in all tasks, showing its safety during the whole training process. Among all tasks, model-based algorithms (DRPO, MBPO and SMBPO) have fewer CTVs due to their high sample efficiency. Besides the model rollouts, DRPO reduces violations further with the proposed DRC and the shield policy and we investigate the specific effects of each component in the ablation study. Therefore, the ECV of DRPO decreases faster than other baselines in most of the tasks and reaches a zero-violation policy earlier except in Cartpole-Move. We hypothesize that cartpole has simple dynamics so modeling the uncertainty may not be that significant for efficient learning. Moreover, due to the instability of the system, little deviation of the policy outputs will cause the state to be unsafe because of high-risk-high-reward property of this case. One may note that sometimes EVs of DRPO are slightly lower than other baselines. This is because we terminate the episode during training when constraints are violated and the one-step reward for optimal policies are above zero. Therefore, collecting rewards does not compromise on safety (i.e., a low-risk-high-return (LRHR) setting) and baselines perform closely in terms of ER. The inferior performance of DRPO in ER arises from the shield policy considering uncertainty and the coarse line search. However, we believe it is acceptable with the presence of significantly fewer training violations.

D. Ablation Study

Ablating sub-modules: To dig further about the effectiveness of the proposed modules, we ablate the DRC and shield policy respectively and conduct tests on Quadrotor and CarGoal. We denote DRPO-vanilla as the one removing both DRC and shield policy, DRPO-uncertainty only as the one removing shield policy, DRPO-shield only as the one removing DRC and DRPO as the proposed algorithm. Although DRPO-vanilla is strong enough, results shown in Fig 6 validate the advantages of both DRC and shield policy in terms of safety during training and evaluation at the cost of little loss in ER. Adding either DRC or the shield policy reduces CTVs, leading to better safety when they are combined in DRPO. However, the evaluation safety of DRPO-uncertainty only (mid row, orange curves) is not stable because it will violate constraints at times. We attribute this to the limited multipliers. Theoretically, $\lambda(s)$ should be $+\infty$ when $Z_{\beta}(s, a; \pi_h) > 0$ but if $Z_{\beta}(s, a; \pi_h) \rightarrow 0_+$ and $\lambda_{\text{max}} Z_{\beta}(s, a; \pi_h) \approx 0$, the policy will pay little attention to the constraint term in the Lagrangian, leading to unsafe actions. Fortunately, this can be rectified by the shield policy because it overwrites the action when $Z_{\beta}(s, a; \pi_h) > 0$. One may question that DRPO is a simple combination of two methods (DRC and shield policy) but it is not the case. The $\beta$-shield policy comes exactly from minimization of the DRC and the formulation in (11) bridges the certificate and the shield policy (mid part in Fig 1). Moreover, the shield policy serves as a supplement for insufficient updates of the approximators of its source, i.e., the DRC and the corresponding constrained optimization problem.

Choosing varying $\Phi^{-1}(\beta)$: To study the effects of considering different levels of uncertainty, we compare DRPO with varying $\Phi^{-1}(\beta)$ from $-1$ to 3 on CarGoal. Note that we disable the safety shield to focus on the uncertainty confidence level. In order to focus on the impacts of different levels of uncertainty consideration, we also adopt a high-risk-high-return (HRHR) setting where the trajectory will continue upon constraint violation. The differences between HRHR and the normal low-risk-high-return (LRHR) setting are illustrated in Fig 7. The safety requirement and high return are in conflict in HRHR setting so the safety level gaps among RL agents can be distinguished clearly. We here count the number of unsafe

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trajectories rather than cumulative violations. Results in Fig 8a show that as $\Phi^{-1}(\beta)$ increases (more uncertainty is considered by the agent), the violations during training become fewer and the final policy tends to be totally safe even without a shield. However, the ER only changes slightly when $\Phi^{-1}(\beta)$ changes and we attribute this to the decreasing model uncertainty. As the model learning proceeds, the variance of the predicted trajectory is getting lower and considering different levels of uncertainty has similar impacts. To summarize, choosing $\Phi^{-1}(\beta) = 2$ (i.e., covering safety of 97% of the possible subsequent cases) is enough for tasks in this work.

Although the ideal value of $\beta$ is one, ensuring safety in spite of uncertain transitions within the true dynamics. However, we then have to consider all samples in the distribution,
which is intractable in the Gaussian case because the RC and different constraint formulations on CarGoal.

**VI. Discussion**

Conservativeness: Considering safety w.r.t. uncertainty may lead to conservativeness to some degree but it is necessary for the crucial safety. The approaches proposed in this work will not bring significantly decreasing cumulative rewards. Two levels of worst-case are considered in this work: (1) the first level lies in focusing on the worst violation in future time horizon. This is because we want to guarantee that the state constraint is always satisfied rather than satisfied in expectation, where the latter case is broadly studied in conventional safe RL but the former case is more significant in safety-critical systems. (2) The second level is the robust safety in terms of stochastic transition and model uncertainty. This is inevitable because the true state transition can possibly appear within the whole distribution so the safety measure should cover the worst case in the distribution. We adopt several methods to improve returns while maintaining safe: (1) truncated uncertainty: we impose constraints on the $\beta$-quantile instead of the entire distribution; (2) modification of the optimization problem: constraints are imposed on $Z_\beta(s, a; \pi_h)$ instead of $Z_\beta(s, a; \pi)$ to realize a larger feasible region. The second and third ablation studies indicate improvements on returns. Consequently, although DRPO exhibits marginally reduced returns compared to baselines, it remains the only algorithm achieving zero-violation upon convergence, accompanied by the fewest cumulative training violations.

Convergence: Regarding the convergence of the vanilla version of DRPO (i.e., without shield, model-free), the proof follows the one presented in [12], as the only difference lies in the reachability certificate now being a distribution, the convergence of which has been proven in Corollary 1. Consequently, we choose not to duplicate the process in this work, as theoretical convergence is not the primary focus of this paper. Moreover, the assumptions required may be overly strict to provide practical guidance, particularly when the algorithm is combined with function approximators, such as deep neural networks. After introducing model-based rollouts and DRC of the shield policy, the convergence cannot be guaranteed theoretically because the operator $T$ (different from $T^s$) may not converge to a well-behaved fixed point according to [27]. However, the practical algorithm exhibits convergence empirically when setting lower and upper bounds to variance to avoid divergence. Future work may include exploring tabular and discrete cases and categorical distribution to have insights about the convergence.

Developments: The starting problem statement and the approach addressing constrained optimization problems resemble our previous work [12] but developments have been made to enhance the algorithm. While [12] provides a formulation characterizing persistently safe states in RL, the designed algorithm engenders more constraint violations during training. In this work, we want to follow the formulation but render approach safe states with possibly more rewards. Even if the danger is going to happen, the shield policy will intervene and override the unsafe actions, pulling the agent back to safe states. Thus, DRPO reaches higher return while maintaining safe during training and evaluation.
TABLE I
OFF-POLICY ALGORITHMS HYPERPARAMETERS

| Parameter                  | Value                          |
|----------------------------|--------------------------------|
| **Shared**                 |                                |
| Optimizer                  | Adam ($\beta_1 = 0.99, \beta_2 = 0.999$) |
| Approximation function     | Multi-layer Perceptron (MLP)   |
| # of hidden layers         | 2                              |
| # of neurons per layer     | 256                            |
| Nonlinearity of hidden layer | ReLU                         |
| Critics learning rate (lr) | cos anneal (c.a.) 3e-4 → 8e-5 |
| Cartpole                   | c.a. 1e-4 → 4e-5               |
| Actor lr                   | Quadrotor: c.a. 1e-4 → 4e-5    |
| Safety-Gym: c.a. 8e-5 → 4e-5 |                                |
| Temperature factor $\alpha$ lr | same as initial lr of actors    |
| Discount factor ($\gamma$) | 0.99                           |
| # of total episodes        | Cartpole: 50                   |
| # of critic updates per step | Quadrotor, Safety-Gym: 100   |
| # of actors updates per step | 10                            |
| # of actor updates per step | 5                              |
| Target smoothing coefficient ($\tau$) | 0.005                       |
| Expected entropy ($\mathbb{H}$) | -lim(A)                     |
| Replay buffer size         | Cartpole: Safety-Gym: 500k     |
| Quadrator                  | Safety-Gym: 500k               |
| Replay batch size          | Cartpole: 1,000                |
| Buffer warm-up size        | Safety-Gym: 5,000              |
| Mix-up ratio               | 10% real data, 90% virtual data|
| Model approximator         | 5 MLPs                         |
| # of model hidden layers   | 2 trunk, 1 for $\mu_a$ and $\sigma_a$ head |
| # of neurons per model layer | 200                          |
| Model lr                   | 1e-3                           |
| # of model initial updates | 10,000                         |
| # of model updates interval | $T_{ep}/4$                    |
| # of GD steps per model update | 1,000                      |
| Nonlinearity of model hidden layer | swish                      |
| Rollout batch size         | 100                            |
| Rollout length             | 10                             |
| **DRPO, RAC**              | c.a. 3e-4 → 1e-5               |
| **CSC, SAC-L**             |                                |
| Multiplier lr              | 3e-4                           |
| Critic conservative coefficient | 0.05                        |
| **SMBPO**                  | Look-ahead horizon: 10         |

TABLE II
ON-POLICY ALGORITHMS HYPERPARAMETERS

| Parameter                  | Value                          |
|----------------------------|--------------------------------|
| **Shared**                 |                                |
| Optimizer                  | Adam ($\beta_1 = 0.9, \beta_2 = 0.999$) |
| Approximation function     | MLP                            |
| # of hidden layers         | 2                              |
| # of neurons per layer     | 256                            |
| Nonlinearity of hidden layer | Tanh                        |
| Critics learning rate (lr) | 1e-3                           |
| Actor lr                   | 3e-4                           |
| Discount factor ($\gamma$) | 0.99                           |
| GAE parameter ($\lambda$)  | 0.97                           |
| Batch size                 | 4000                           |
| # of actors                | 4                              |
| # of critic updates per iteration | 80              |
| Target KL                  | 0.01                           |
| Cost threshold             | 0                              |
| **PPO-Lagrange**           |                                |
| Clip ratio                 | 0.2                            |
| Max # of actor updates per iteration | 80                        |
| KL margin                  | 1.2                            |
| Initial multiplier         | 1.0                            |
| Multiplier lr              | 5e-2                           |
| # of multiplier updates per iteration | 1                          |
| **CPO**                    |                                |
| Backtrack coefficient      | 0.8                            |
| Max # of backtrack iterations | 10                           |

the method more practical. Therefore, we introduce distributional RC to address the uncertainty of stochastic systems and the corresponding shield policy to reduce training time violations, which are both novel and effective. Experiments show that DRPO outperforms RAC (Reachable Actor Critic proposed in [12]) in terms of cumulative training violations and converges to a safe policy more quickly, aligning with our motivation.

VII. CONCLUSION

In this paper, we propose DRPO, a safe RL algorithm, to address the model-uncertainty in model-based safe RL, thereby improving training time and evaluation safety. We first extend the reachability certificate to a distributional setting, realizing safety robust to model discrepancy or probabilistic prediction. The shield policy obtained from the DRC serves as the constraint in the problem formulation to further improve performance. The shield is leveraged in a switch-based scheme during training and a line search method during evaluation to maintain safety and reduce conservativeness. DRPO solves the constrained optimization problem with primal-dual method and deep neural network approximators. We evaluate DRPO and seven baselines on MuJoCo, safe-control-gym and safety-gym. Results show that DRPO outperforms all other algorithms in terms of policy safety while reaching competitive return performance. We also validate the effectiveness of the proposed DRC and the shield policy as well as the constraint formulation. Future work may include deploying DRPO on real-world robots to evaluate its practical ability. Moreover, if starting from a trivial but safe policy and a well-calibrated model, whether DRPO can be improved to realize provably safe learning remains an interesting question.

APPENDIX

A. Detailed Hyperparameters

The hyperparameters of implemented algorithms are listed in Table I and Table II respectively.

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