# Scalable Safety-Critical Policy Evaluation with Accelerated Rare Event Sampling

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Abstract-Evaluating rare but high-stakes events is one of the main challenges in obtaining reliable reinforcement learning policies, especially in large or infinite state/action spaces where limited scalability dictates a prohibitively large number of testing iterations. On the other hand, a biased or inaccurate policy evaluation in a safety-critical system could potentially cause unexpected catastrophic failures during deployment. This paper proposes the Accelerated Policy Evaluation (APE) method, which simultaneously uncovers rare events and estimates the rare event probability in Markov decision processes. The APE method treats the environment nature as an adversarial agent and learns towards, through adaptive importance sampling, the zero-variance sampling distribution for the policy evaluation. Moreover, APE is scalable to large discrete or continuous spaces by incorporating function approximators. We investigate the convergence property of APE in the tabular setting. Our empirical studies show that APE can estimate the rare event probability with a smaller bias while only using orders of magnitude fewer samples than baselines in multi-agent and single-agent environments.

## I. INTRODUCTION

There has been a growing interest in applying reinforcement learning (RL) to complex high-stakes robotics problems, including controlling autonomous vehicles and healthcare assistant robots [1], [2]. As one can expect, before deployment of any RL policy, such safety-critical applications often require an accurate policy evaluation because inaccurate estimations could lead to false optimism or even catastrophic consequences. However, a main difficulty for policy evaluation in these settings is that we are crucially interested in assessing certain rare but high-stake events in safety-critical systems. The *de facto* standard evaluation method is the vanilla Monte Carlo (MC) which, in a multitude of practical settings of interest, requires a prohibitively large number of testing before the evaluation can be deemed statistically valid [3]. For example, [1] shows that, in order to demonstrate the safety of self-driving cars, the number of miles that needs to be clocked in is technically in the hundreds of billions. Consequently, when such large-volume testing is high-stakes, costly, or time-consuming, a growing



Fig. 1: The interactions among the environment transition model, the agent and the environment adversary introduced by our proposed accelerated policy evaluation method. The reward signal r is for updating the adversary policy  $\pi_E$ . The subscript n denotes the time step.

number of studies have been developed to accelerate the estimation of rare event probability as the policy evaluation metric [4], [5]. However, existing literature typically either fails to exploit the sequential, interactive nature of tasks by confining to specific failure-causing initial conditions [6], [7] or only focuses on small state/action spaces due to the curse of dimensionality [8], [9].

In this paper, we develop an efficient and scalable policy evaluation method for estimating rare event probabilities in sequential decision-making tasks, which expedites the policy evaluation in large or continuous state/action spaces. In particular, we specify a rare event set and estimate the probability of entering the set under a given RL policy in an environment of interest. We focus on episodic settings with an adjustable grey-box testing ground that simulates the environment (i.e., a simulator with adjustable disturbances or vehicle policies), which is the common practice in third-party evaluations or in curriculum design [6], [10]. We summarize our major contributions as follows:

- We propose the Accelerated Policy Evaluation (APE) method, suitable for Markov decision processes (MDPs) and motivated by adaptive importance sampling [9]. In a novel way, APE introduces an adversary that controls the environment transition at each step and gradually exploits sequential interactions that cause rare events. We further theoretically establish the convergence property of APE in the tabular setting.
- We propose a scalable implementation of APE and denote it as *APE\_scalable*. *APE\_scalable* incorporates two function approximators: a Gaussian Process (GP) [11] to estimate rare event probability with high data efficiency, and a conditional normalizing flow model [12] to expressively represent the adversary's policy. We further design a two-timescale gradient-based updating

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rule for GP to adapt to the rare event setting.

• We empirically show that APE\_scalable estimates the rare event probability with a smaller bias and orders of magnitude fewer samples than baselines, in driving scenarios [13] and in a LunarLander control task [14].

### II. RELATED WORK

Motivated by the inherent difficulty of assessing rare, safety-critical events in lab or field tests, there has been a growing literature to maximize the sampling efficiency of rare event probability estimation. Two powerhouses are the importance sampling method [4], [15], [16] and the multilevel splitting method [17]. However, little literature focuses on MDP settings. Recent developments in [6], [18] adjust the environment setting at the beginning of each episode while ignoring the intermediate interactive steps. However, our proposed APE method is designed to leverage the sequential nature of tasks and hence is more suitable in the RL settings. The APE is similar to the adaptive stochastic approximation (ASA) for Markov chains [9]. Nonetheless, ASA restricts to discrete state space and is not incorporated with the decision process, thus handicapping its applicability for sophisticated decision-making agents such as continuous-space RL. Our setting is similar to [5] because both utilize a dynamic programming paradigm. However, [5] relies on discretizing and decomposing the simulation scene to make it scalable.

APE is within the regime of safe validation [19] and specifically focuses on finding the distribution of failurecausing disturbances and estimating the failure rate. Adversarial evaluation [6], [20], mainly motivated by attacks on RL agents, also aims to find failure cases but in a distributionfree manner. Instead of searching for worst-case scenarios as in adversarial attacks [21], APE aims to directly find those rare but possible (failure) cases when the agent interacts with the original environment of interest.

APE utilizes updating rules involving dynamic programming and importance weights over changing policies. The rules share a similar form with off-policy evaluation [22] methods including Retrace [23], V-trace [24], and importance resampling [25]. Concretely, the environment's ground truth policy  $\pi_{E,gt}$  and the proposed adversary policy  $\pi_E$  in APE are analogous to the evaluation policy and behavior policy in off-policy evaluation [26], respectively.

# III. RARE EVENT PROBABILITY AS POLICY VALUE

A general MDP consists of a tuple (S, A, p, r). S and A denote the state and action space. s' denotes the proceeding state of s. The stochastic transition model is  $p(s'|s, a) : s, s' \in S, a \in A$  and the one-step reward is  $r(s, s'), s, s' \in S$ . In the rare event setting, we consider the state space  $S = T \cup I$  is a partition of terminal states T and interior states  $I, T \cap I = \emptyset$ . We assume T is reachable from any states in I for all policies under consideration and the episode length  $\tau$  is finite almost surely. The rare event set is denoted by  $\mathcal{R}$  and  $\mathcal{R} \subset T$ .

We formulate the rare event probability (or the probability of hitting  $\mathcal{R}$  before  $\mathcal{T} \setminus \mathcal{R}$ ) starting from an initial state  $s_0 \in \mathcal{I}$  in an environment of interest, as the expected undiscounted total reward until termination. With  $v^*$  as the true value, we have the following Bellman equation holds:

$$v^{\star}(s_{0}) \coloneqq \mathbb{E}_{p_{E,gt},\pi_{A}} \Big[ \sum_{n=0}^{\tau-1} r(s_{n}, s_{n+1}) \Big] =$$
(1)  
$$\sum_{n=0}^{\tau} \pi_{A}(a_{A}|s_{0}) \sum_{n=0}^{\tau} n_{E,st}(s_{1}|s_{0}, a_{A}) \Big[ r(s_{0}, s_{1}) + v^{\star}(s_{1}) \Big]$$

$$\sum_{a_A \in \mathcal{A}_A} \pi_A(a_A|s_0) \sum_{s_1 \in \mathcal{S}} p_{E,gt}(s_1|s_0, a_A) \left[ r(s_0, s_1) + v^*(s_1) \right]$$

where  $\pi_A$  is the given Markov policy (typically obtained through training).  $p_{E,gt}$  is the ground truth transition probability of the environment of interest. n is the timestep. Furthermore,  $a_A \sim \pi_A$  is the agent action, and  $\mathcal{A}_A$  is the agent action space. The one-step reward is an indicator function with r(s, s') = 1 if  $s' \in \mathcal{R}$  and 0 otherwise. We set  $v^*(s) = 0$  for  $s \in \mathcal{T}$ . The goal is to estimate  $v^*(s), s \in \mathcal{I}$ .

In settings with large/continuous state space, approximating values in (1) is expensive or infeasible. Moreover, it is hard to guarantee a satisfactory level of estimation error because the considered rare event region  $\mathcal{R}$  is not visited frequently enough. In order to frequently visit  $\mathcal{R}$  in these high or infinite-dimensional situations, one is motivated to consider the importance sampling [27] to modify the environment transition probability, which achieves variance reduction by approaching a target (zero-variance) distribution and learns to generate rare events efficiently.

## IV. ACCELERATED POLICY EVALUATION (APE)

In this section, we introduce the proposed APE paradigm. In MDPs, the environment transition probability relates to both agent A's policy  $\pi_A$  and the environment's transition probability  $p_E(s'|a_A, s)$ ,  $p_{s,s'} = \sum_{a_A \in \mathcal{A}_A} \pi_A(a_A|s) p_E(s'|a_A, s)$ . Therefore,  $v^*(s_0)$  can be reformulated by rolling out trajectories with the newly proposed environment transition probability  $p_E^{(n)}$  and agent policy  $\pi_A^{(n)}$  at step n as follows:

$$v^{\star}(s_{0}) = \mathbb{E}_{p_{E}^{(n)}, \pi_{A}^{(n)}} \Big[ \sum_{n=0} \rho_{n}(s_{n}, s_{n+1}, a_{A}) \cdot r(s_{n}, s_{n+1}) \Big]$$
$$= \sum_{a_{A} \in \mathcal{A}_{A}} \pi_{A}^{(0)}(a_{A}|s_{0}) \sum_{s_{1} \in \mathcal{S}} p_{E}^{(0)}(s_{1}|s_{0}, s_{A}) \cdot \rho_{0}(s_{0}, s_{1}, a_{A}) \Big[ r(s_{0}, s_{1}) + v^{\star}(s_{1}) \Big],$$
(2)

where  $\rho_n(s_n, s_{n+1}, a_A)$  is the importance weight at step n,

$$\rho_n(s_n, s_{n+1}, a_A) = \frac{\pi_A(a_A|s_n) \cdot p_{E,gt}(s_{n+1}|a_A, s_n)}{\pi_A^{(n)}(a_A|s_n) \cdot p_E^{(n)}(s_{n+1}|a_A, s_n)}.$$
 (3)

a) Environment Nature as an Adversary. One key idea in APE is to treat uncertainties in environment transition probabilities  $p_E(\cdot|\cdot, \cdot)$  (e.g., the actions of surrounding vehicles on the road or sensor noises in a robotics control task), as stochastic decisions made by the environment nature E with policy  $\pi_E(\cdot) : S \times A_A \times A_E \to \mathbb{R}$ , where  $A_E$  is the environment nature's action space. Treating the environment nature as an adversary agent is widely used in robust learning and multi-agent RL [28]. It reduces the computation complexity when the selected environment agent E's action space  $A_E$  has a smaller dimension than that of the state space S, and relaxes the assumption of a known environment transition model  $f_E : S \times A_A \times A_E \to S$ . Note that we assume known and adjustable environment policy  $\pi_E$  and unknown  $f_E$  in (5) which lead to a grey-box environment setting.

Formally, at step n, we have the following equations hold

$$p(s_{n+1}|a_{A,n},s_n) = \pi_E(a_{E,n}|a_{A,n},s_n)$$
(4)

$$s_{n+1} = f_E(s_n, a_{A,n}, a_{E,n})$$
(5)

$$a_{E,n} = f_E^{-1}(s_n, a_{A,n}, s_{n+1}) \tag{6}$$

Moreover, we only focus on importance sampling over  $p_E(s_{n+1}|a_A, s_n)$  and leaves  $\pi_A^{(n)}(a_A|s_n) = \pi_A(a_A|s_n), \forall n$ . Therefore the importance weight in (3) becomes

$$\rho_n(s_n, s_{n+1}, a_{A,n}) = \frac{p_{E,gt}(s_{n+1}|a_{A,n}, s_n)}{p_E^{(n)}(s_{n+1}|a_{A,n}, s_n)} \\
= \frac{\pi_{E,gt}(a_{E,n}|a_{A,n}, s_n)}{\pi_E^{(n)}(a_{E,n}|a_{A,n}, s_n)}.$$
(7)

b) Updating Rules for v(s) and  $\pi_E(a_E|s, a_A)$ . Calculating the expectation in (2), which includes the rare event probability, is generally intractable in non-discrete settings. In APE, we use TD method [29] which combines MC simulation and dynamic programming to update the value v(s). More concretely, at the end of step n,

$$v^{(n+1)}(s_n) \leftarrow (1 - \alpha_n) v^{(n)}(s_n) + \sum_{a_A \in \mathcal{A}_A} \rho_n(s_n, s_{n+1}, a_A) \alpha_n [r(s_n, s_{n+1}) + v^{(n)}(s_{n+1})]$$
(8)  
  $\approx (1 - \alpha_n) v^{(n)}(s_n) + \alpha_n \cdot [r(s_n, s_{n+1}) + v^{(n)}(s_{n+1})] \cdot \rho_n(s_n, s_{n+1}, a_{A,n}),$ (9)

where  $\alpha_n$  is a decaying learning rate. To make APE suitable for online learning and get rid of the summation over agent actions, we approximate the importance weight over state transition probability with the one-step importance weight in (7) to get an online stochastic version as in (9). (9) is accurate if the agent policy  $\pi_A$  is deterministic.

Motivated by ASA [9], which accelerates the rare event probability estimation in Markov chains, we design the updating rule for  $\pi_E$  as follows. At the end of step *n*, the un-normalized policy around the newly sampled action  $a_{E,n}$ is derived with the updated value function  $v^{(n+1)}$  and the original environment policy  $\pi_{E,at}$ 

$$\tilde{\pi}_{E}^{(n+1)}(a_{E,n}|a_{A,n},s_{n}) \leftarrow \max\left(\delta, \\ \pi_{E,gt}(a_{E}|a_{A,n},s_{n}) \left(\frac{r(s_{n},s_{n+1}) + v^{(n+1)}(s_{n+1})}{v^{(n+1)}(s_{n})}\right)\right),$$
(10)

where  $\delta$  is a positive constant to guarantee that the one-step importance weight  $\rho_n$  is bounded.

APE accelerates the policy value estimation by learning a properly designed importance policy  $\pi_E$  to reduce the estimation variance. Different from adaptive MC [8] and cross-entropy methods (CEM) [30], APE utilizes a stochastic approximation paradigm and updates state values based on



Fig. 2: A minigrid environment with rare events.

TABLE I: Estimation results at convergence in minigrid. We obtain the ground truth rare event probabilities via vanilla MC with a sufficiently large number of episodes.

methods	M	IC	APE		
metric	mean	std	mean	std	
$v(s_1) (10^{-3})$	3.99	0.38	3.90	0.24	
$v(s_2) (10^{-3})$	3.93	0.47	3.94	0.23	
$v(s_3)$ (10 <sup>-3</sup> )	4.00	0.50	3.94	0.17	
num. of time steps	78300	10600	8884	2595	
num. of episodes	19306	2612	552	134	

each single transition without waiting for a final outcome (without entering the terminal set).

# c) Convergence in Tabular Case

Theorem 1: Assume tabular MDP settings with discrete state and action spaces and let  $\pi_E^*$  denote the zero-variance environment policy. If step size  $\alpha_n$  in Eq. 8 satisfies  $\sum_n \alpha_n = \infty$  and  $\sum_n \alpha_n^2 < \infty$ , the iterative updating rules (Eq. 8 and Eq. 10) satisfies  $v^{(n)} \to v^*$  and  $\pi_E^{(n)} \to \pi_E^*$ .

The proof of Theorem 1 directly follows the structure of Theorem 1 in [9]. By defining the value function only related to state, the difference between the APE value update rule and that in [9] lies in the definition of the importance weight. However, the importance weight-related terms are included in a sequence of random vectors with zero mean and bounded norm, which do not affect the contraction of the remaining part. Based on the Perron-Frobenius theorem, we can show that the remaining part is a contraction operator and thus has a fixed point. Then by applying Theorem 1 and Theorem 3 in [31], we have the convergence of value function v. The convergence of  $\pi_E$  results from the convergence of v and the definition of  $\pi_E$ 's updating rule.

## A. Accelerated Policy Evaluation with gym-minigrid

We first empirically show that the proposed APE method without using function approximations converges to the ground truth rare event probabilities in discrete MDP settings. We experiment in a gym-minigrid [32] environment as shown in Fig. 2. Rare events happen when the agent (the red triangle) fails to reach its destination (the green square), such as getting stuck in non-terminal states or entering the lava (the yellow block). Grids denoted as  $s_1$ ,  $s_2$  and  $s_3$ are possible initial states of lava. The agent policy  $\pi_A$  is trained with the deep Q learning [33] until convergence. The environment policy  $\pi_E$  controls the policy of the lava.

We compare the efficiency of the proposed APE with vanilla MC for estimating the rare event probability. We define convergence of an estimated value when the estimation deviation in the past 2000 steps is less than 1% of the final estimate. Tab. I shows that when the ground truth rare event

probability is around  $4 \times 10^{-3}$ , APE successfully converges to the true rare event probability. APE also demonstrates high efficiency by requiring one magnitude fewer data and achieves a smaller variance than MC at convergence.

# V. SCALABLE IMPLEMENTATION: APE\_SCALABLE

In this section, we introduce how to improve the scalability of APE to handle large discrete or continuous MDP settings. The general idea is to select proper function approximators to represent the value function v(s) and the environment policy  $\pi_E$ . Before doing that, we first establish some notations. The value function approximator  $v_{\psi}(s)$  with parameter  $\psi$ takes state s as input and outputs a probability ranging from 0 to 1. The policy approximator  $\pi_{E,\theta}$  parameterized with  $\theta$  takes the state-action concatenation  $(s, a_A)$  as input and outputs a probability density on  $a_E$ . Therefore, we have  $\rho_{n,\theta} = \pi_{E,gt}(a_{E,n}|a_{A,n},s_n)/\pi_{E,\theta}^{(n)}(a_{E,n}|a_{A,n},s_n)$ . At step n, a data pair  $d_n = (s_n, a_{A,n}, a_{E,n}, s_{n+1}, r(s_n, s_{n+1}), \rho_{n,\theta})$ is appended to a history dataset  $\mathcal{D}$ . Assume  $s \in S \subset \mathbb{R}^{d_s}$ ,  $a_A \in \mathcal{A}_A \subset \mathbb{R}^{d_a}$ , and  $a_E \in \mathcal{A}_E \subset \mathbb{R}^{d_e}$ .

# A. Value Function Approximation

We learn  $v_{\psi}(s)$  by minimizing differences between the predicted values and TD targets  $v_{\psi,TD}(s_n)$ . For data pair  $d_n$ , we have

$$\rho_{n,\theta} = \pi_{E,gt}(a_{E,n}|a_{A,n},s_n)/\pi_{E,\theta}^{(n)}(a_{E,n}|a_{A,n},s_n), \quad (11)$$

$$v_{\psi,TD}(s_n) = (r(s_n, s_{n+1}) + v_{\psi}(s_{n+1})) \cdot \rho_{n,\theta}.$$
 (12)

(...)

One approximation approach is representing v(s) with an expressive deep neural network (DNN) with low prediction complexity. However, DNNs are sensitive to imbalanced data and suffer from the catastrophic forgetting problem [34], [35], especially in online learning settings. A competitive model for DNN is the Gaussian Process (GP) regression model. The equivalence between GPs and infinitely wide DNNs is derived in [36]. GPs are data-efficient and flexible in making predictions as non-parametric models but sacrifice the prediction complexity [11]. Considering that the sampled rare events may be drowned out in  $\mathcal{D}$ , especially in the initial learning phase, we choose to use GP as the function approximator for its data efficiency.

a) Use GP to Represent  $v_{\psi}(\cdot)$ . Let the data buffer for training and prediction as  $\mathcal{D}_{GP} = \{(s_i, v_{\psi,TD}(s_i))^m\}$ . The predicted value given  $s^* \in S$  is drawn from a distribution

$$p(f|\mathcal{D}, s^{\star}) = \mathcal{N}(\mathsf{m}(f), \mathsf{cov}(f)).$$
(13)

Define  $x_i = s_i$  and  $y_i = v_{\psi,TD}(s_i)$  and aggregate them into  $X \in \mathbb{R}^{d_s \times m}$  and  $Y \in \mathbb{R}^{1 \times m}$ . The mean function is  $\mathbf{m}(f) = K(s^*, X)[K_i(X, X) + \sigma^2 I]^{-1}Y$  and the covariance matrix is  $\operatorname{cov}(f) = K(s^*, s^*) - K(s^*, X)[K(X, X) + \sigma^2 I]^{-1}K_i(X, s^*)$ .  $\sigma$  is the standard deviation of observation noise. The matrix K is fully specified by the kernel function  $k(\cdot, \cdot)$ , which defines the function smoothness. We use the scaled squared exponential kernel  $k(x, x') = w^2 \exp(-\frac{1}{2} \sum_{j=1}^{d_s} w_j (x^j - x'^j)^2)$ , where  $w_j$  is the reciprocal of the lengthscale of state dimension j, and w is the output scale.  $\psi = \{w, w_1, ..., w_{d_s}, \sigma\}$  contents kernel parameters. We update  $\psi$  with gradient descent to minimize the negative log-likelihood for  $\mathcal{D}_{GP}$  together with an  $L_1$  regularizer over lengthscale parameters:

$$\psi \leftarrow \psi - \alpha_v \nabla_{\psi} \Big[ \lambda \cdot \sum_{j}^{d_s} |w_j| \\ + \sum_{(s_i, v_{\psi, TD}(s_i)) \in \mathcal{D}_{GP}} -\log p(v_{\psi, TD}(s_i)|s_i, \mathcal{D}_{GP}) \Big], \quad (14)$$

where  $\lambda$  is the regularization penalty, and  $\alpha_v$  is the learning rate. Different from standard GP regression with a fixed number of data points and fixed targets, APE learns GP in an online learning manner via streaming collected data pairs [37] as well as in a dynamic programming paradigm with changing TD targets similar to [38].

#### B. Environment Adversary Policy Approximation

In online setting, the environment's policy updates based on the most recent data pair  $d_n$  and newly updated  $v_{\psi}(s)$ . The un-normalized target density around the newly sampled action  $a_{E,n}$  conditioned on  $C_n = [a_{A,n}, s_n]$  is

$$\tilde{\pi}_E(a_{E,n}|C_n) = \pi_E(a_{E,n}|C_n) \Big(\frac{r(s_n, s_{n+1}) + v_{\psi}(s_{n+1})}{v_{\psi}(s_n)}\Big).$$
(15)

To cope with continuous spaces, we achieve the modification by adding a normal distribution  $\mathcal{N}(a_{E,n},\sigma)$  with  $\sigma$  much smaller than that of the ground truth policy  $\pi_E(a_E|x, a_A)$ . The target probability density function conditioned on  $C_n$  is

$$p_E(a_E|C_n) = (\pi_{E,\theta}(a_E|C_n) + \beta \cdot \mathcal{N}(a_{E,n},\sigma))/(1+\beta),$$
(16)

where  $\beta = \sqrt{2\pi}\sigma(\tilde{\pi}_E(a_{E,n}|C_n) - \pi_{E,\theta}(a_{E,n}|C_n)).$ 

The function approximation  $\pi_{E,\theta}$  should have a low sample complexity to quickly sample actions at each time step.  $\pi_{E,\theta}$  is desired to have interpolation/extrapolation ability across conditions to help accelerate the evaluation process by ensuring that two conditional distributions are close if the distance between their conditioned values is close. Considering that the additive modification of the target density function in (15) results in a Gaussian mixture model with an increasing mixture size,  $\pi_{E,\theta}$  is also desired to be flexible enough to model multi-mode distributions. In practice, we use the conditional Masked Autoregressive Flow model (cMAF) model [12] to represent  $\pi_E(a_E|a_A, s)$  to meet previous desiderata.

a) Use cMAF to Represent  $\pi_{E,\theta}$ . We obtain a closed-form parametric representation of  $\pi_E(a_E|a_A, s)$  using a cMAF. A cMAF is a type conditional Normalizing Flow (cNF) [12], which is a generative model that uses invertible mappings to transform a simple probability distribution into a complex one conditioned on other random variables. Compared with sample-based representation approaches such as MCMC, cNF directly generates one sample by calling one reversible path and has the capacity to model distributions that go beyond single-mode Gaussian distributions.

#### Algorithm 1 Scalable Accelerated Policy Evaluation

**Input**: Agent policy to evaluate  $\pi_A$ , ground truth environment policy  $\pi_{E,qt}$ , warm start policy  $\hat{\pi}_E$ **Parameter**: Total evaluation steps N**Output**:  $v_{\psi}(\cdot), \pi_{E,\theta}(\cdot)$ 1: Pretrain  $\pi_{E,\theta}(\cdot|a_A, x)$  with target conditional probability  $\hat{\pi}_E(\cdot|a_A,s), \ \forall a_A \in \mathcal{A}_A, s \in \mathcal{S}$ 2: for n = 0 to N - 1 do Reset environment 3: 4: Initialize empty episode buffer  $\mathcal{D}_e$ 5: repeat Sample actions  $a_A \sim \pi_A(\cdot|s), a_E \sim \pi_{E,\theta}(\cdot|a_A, s)$ 6: Execute  $a_A$  and  $a_E$ , observe s' and r(s, s')7: Get one-step importance weight  $\rho_{n,\theta}$  with (11) 8: 9: Add  $d = (s, a_A, a_E, s', r(s, s'), \rho_{n,\theta})$  to  $\mathcal{D}$  and  $\mathcal{D}_e$ Update  $v_{\psi}(\cdot)$  with two-timescale based on Algo.2 10: Update  $\pi_{E,\theta}$  with dense rewards based on Algo.3 11:  $s \leftarrow s'$ 12:  $n \leftarrow n+1$ 13: until episode finish 14: 15: end for 16: return  $v_{\psi}(\cdot), \pi_{E,\theta}(\cdot)$ 

We denote the generative function in cNFs as  $g_{\theta}: z \to a_E$ , and the differentiable normalizing function as  $f_{\theta} = g_{\theta}^{-1}$ . The base distribution  $p_Z$  of hidden variable Z is easy to sample from, such as a normal distribution or a uniform distribution. At step n, we hope to minimize the KL divergence  $L^{(n)}_{\mu}$ between the target and the cNF distribution.

$$L_{\theta}^{(n)} = \mathbb{E}_{\pi_{E,\theta}(a_{E}|C_{n})}[\log \pi_{E,\theta}(a_{E}|C_{n}) - \log p_{E}(a_{E}|C_{n})]$$
  
$$= \mathbb{E}_{p_{Z}(z|C_{n})}[\log \pi_{E,\theta}(g_{\theta}(z)|C_{n}) - \log p_{E}(g_{\theta}(z)|C_{n})]$$
  
$$= \mathbb{E}_{p_{Z}(z|C_{n})}[\log p_{Z}(z|C_{n}) - \log |\det \partial_{z}g_{\theta}(z)|$$
  
$$- \log p_{E}(g_{\theta}(z)|C_{n})].$$
(17)

We update  $\theta$  via gradient descent. We first sample from the simple base distribution  $p_Z(z|C_n)$  and pass the sampled  $z_i, i = [M]$  to the flow to get samples in target domain  $a_{E,i} = g_{\theta}(z_i), i = [M]$ . The KL divergence  $L_{\theta}^{(n)}$  is then approximated with the sample mean. With learning rate  $\alpha_{\pi}$ ,

$$\theta \leftarrow \theta - \alpha_{\pi} \nabla_{\theta} \sum_{i=1}^{M} \Big[ \log p_Z(z_i | C_n) \\ - \log |\det \partial_z g_{\theta}(z_i)| - \log p_E(g_{\theta}(z_i) | C_n) \Big].$$
(18)

### C. Algorithm Description

We present the APE\_scalable algorithm in Algo. 1 and summarize the algorithm highlights as follows:

Warm start. We initialize the environment policy  $\pi_E$ with a warm start policy  $\hat{\pi}_E$  when the rare event probability  $v^{\star}(s_0)$  is pretty small. The design of the warm start distribution may leverage domain knowledge. One possible choice is using large variances.

GP two-timescale update rules. We develop a twotimescale updating scheme for GP dynamic programming. Algorithm 2 Update  $v_{\psi}$  with Two-timescale

**Input**: new data d, current  $\pi_{E,\theta}$ **Parameters**:  $v_{\psi}$  learning rate  $\alpha_v$ ,  $\psi$  update interval  $n_{\psi}$ **Output:**  $v_{\psi}$ 1: Calculate TD target  $v_{\psi,TD}(s)$  of d with (12) 2: Append  $(s, v_{\psi,TD}(s))$  to  $\mathcal{D}_{GP}$ 3: if  $n\%n_{\psi} = 0$  then Train value function  $v_{\psi}$  with gradient descent (14) 4: 5: end if

Algorithm	3	Update $\pi_{EA}$	with	Dense	Rewards
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**Input**: new data d, current  $v_{\psi}$ , episode buffer  $\mathcal{D}_e$ **Parameters**:  $\pi_{E,\theta}$  learning rate  $\alpha_{\pi}$ , dense reward discount factor  $\gamma_r$ , momentum coefficient  $\beta_{\theta}$ 

**Output**:  $\pi_{E,\theta}$ 

- 1: Append d to  $\mathcal{D}_e$
- 2: if r(s, s') = 1 then
- Calculate adversary policy target with (16) based on 3: episode buffer  $\mathcal{D}_e$  and dense rewards
- Get updated  $\theta'$  of  $\pi_{E,\theta}(\cdot)$  with gradient descent (18) 4:
- $\theta \leftarrow \beta_{\theta} \theta' + (1 \beta_{\theta}) \theta$ 5:

6: end if

We update data pairs more frequently than the GP kernel parameters to improve training stability as in Algo. 2. We store representative data as in sparse GP [39] and early-stop appending data when sufficient representative data points.

cMAF update with dense rewards. In practice, purely updating  $\pi_{\theta}$  in an online manner raises several issues. First, it causes that cMAF easily over-fits to the latest target distribution across conditions (diminishing the effect of conditions). Second, it may induce training instability due to a quite sparse reward signal  $r(s_{n-1}, s_n)$ . Third, it requires high computational complexity for frequently updating cMAF. Therefore, we propagate the reward signal to the whole episode  $\hat{r}(s_{n-1}, s_n) = \gamma_r^{\tau-n} r(s_{\tau-1}, s_{\tau}), n = 1, \dots, \tau,$ where  $\gamma_r$  is the reward discount factor.  $\tau$  is the episode termination step. To improve training stability, we further add momentum to the parameter  $\theta$ . We early-stop training when achieving satisfactory sampled rare event rate.

#### VI. EXPERIMENTS

In this section, We empirically show that the proposed APE\_scalable method with function approximations outperforms baselines by estimating the rare event probability with smaller biases and orders of magnitude fewer samples.

# A. Baselines

We compare the proposed APE\_scalable with three baselines: APE\_discrete, CEM\_discrete and vanilla MC. APE\_discrete and CEM\_discrete discretize each dimension of s and  $a_E$  with a small slot interval, and use dictionaries to store the rare event probability estimate and the environment policy  $\pi_E$  at each slot. Note that vanilla MC does not require  $\pi_E$  for estimation or store dictionaries. We get the ground truth rare event probability  $v^{\star}(s_0)$  via MC with



initialization

Fig. 4: The LunarLander environment with rare events.

normal event

rare event

sufficiently large number of episodes. Let  $\hat{v}(s_0)$  denote the estimation and  $\bar{v}(s_0)$  denote the sampled rare-event rate along estimation process. We evaluate the estimation error based on bias  $Bias(s_0) = \mathbb{E}[\hat{v}(s_0)] - v^*(s_0)$ , standard deviation  $Std(s_0) = \sqrt{\mathbb{E}[(\mathbb{E}[\hat{v}(s_0)] - \hat{v}(s_0))^2]}$ , and risk  $MSE = \sqrt{Bias^2(s_0) + Std^2(s_0)}$ .

# B. Environments

Intersection The agent to evaluate (the green vehicle) aims to perform a collision-free unprotected left turn in a two-lane intersection with one surrounding vehicle (the vellow vehicle). A rare event is a crash, and the adversary policy is the surrounding vehicle's policy. We hope to evaluate a fixed deterministic policy  $\pi_A$ , which follows the lane with constant velocity. Note that APE is also applicable to stochastic policies. We build two intersection scenarios based on highway-env [13]: Int-v0 with  $v^*(s_0) = 6.34 \times 10^{-2}$ , and Int-v1 with  $v^{\star}(s_0) = 1.70 \times 10^{-6}$ . APE can handle more than two agents by treating all the other agents as part of the environment [40]. In Int-v0, we initialize all methods with the  $\pi_{E,qt}$  and present experiment results in Fig. 5 (a). In Int-v1, we initialize APE\_scalable, APE\_discrete and CEM\_discrete with a slightly skewed distribution (as shown in the first column in Fig. 6) with a larger variance than the ground truth  $\pi_{E,qt}$  to sample rare events at the initial stage. We present experiment results of intersections in Fig. 5 (b).

**Lunarlander** We hope to evaluate a heuristic policy by OpenAI which aims to land a lunar lander on a fixed landing pad in LunarLander [14] with  $v^*(s_0) = 1.30 \times 10^{-3}$ . The rare event is defined as if the lander crashes, flies too far away from the landing pad or the episode exceeds the maximum length. The environment agent is an adversary that controls perturbations over actions to execute to mimic controller errors. This example provides a clue for selecting factors controlled by the environment adversary, and the experimenters may draw inspiration from robust learning and add uncertainty/noise to components of MDPs [41], [42], [43]. In LunarLander, we initialize all methods with the  $\pi_{E,qt}$  and present experiment results in Fig. 5 (c).

#### C. Discussion about Evaluation Performance

Although APE\_discrete approaches the true rare event probability in Int-v0, it has a larger estimate variance than APE\_scalable. In Int-v1 and LunarLander, APE\_scalable successfully converges to the true value while APE\_discrete does not. The smaller variance and faster convergence of APE\_scalable compared with APE\_discrete across environments indicate that the discretization of continuous tasks drops the environment or action structure information and leads to biased evaluation results.

Interestingly, CEM\_discrete achieves higher rare event sample rates than APE\_scalable in Int-v0 and Int-v1, but heavily underestimates the true rare event probability. We conjecture that CEM\_discrete fails to explore enough and its environment adversary policy  $\pi_E$  only concentrates on a subset of failure modes. While in LunarLander, CEM\_discrete increases the sampled rare event rate but is less efficient compared with APE\_scalable.

Both APE\_scalable and vanilla MC approach the true value in Int-v0 and LunarLander, since the rare event probability is relatively large. Despite of that, APE still outperforms MC in terms of the variance of probability estimation in LunarLander. But in Int-v1, APE\_scalable converges within 3,000 steps (around 1,000 episodes) while MC may require 1,762,193 =  $\log(0.05)/\log(1 - v^*(s_0))$  episodes until having 95% confidence interval. Note that we omit the evaluation curve using MC in Int-v1 since MC hardly samples even one rare event within 3,000 steps. It shows that APE\_scalable dominates MC in estimation accuracy when the rare event probability is small.

## D. Discussion about Different Metrics

From Tab. II, APE\_scalable has the smallest bias across three environments compared to baselines but not the smallest variances or MSEs. Note that although in Int-v0 and Int-v1 CEM\_discrete has near-zero variance, it heavily under-estimates the rare event probability as shown in Fig. 5. Similarly, in LunarLander, APE\_discrete underestimates the rare event probability by one magnitude but has a smaller variance than other baselines. Such under-estimation phenomena are risky and not desirable in the rare event setting since they may cause catastrophic consequences by deploying overly trusted RL agents.

# E. Discussion about Environment Adversary $\pi_E$

In Int-v0, the sampled rare event rate using APE\_scalable (0.44) is 7.5 times greater than MC (0.064), and is 3.3 times greater than APE\_discrete (0.12). In LunarLander, the final sampled rare event rate using APE\_scalable is more than 100 times greater than MC. Interestingly, in the more challenging Int-v1, APE\_scalable generates much more rare events with sampled rare event rate 0.75, which is 441,176 times greater than MC ( $1.70 \times 10^{-6}$ ) and 4.7 times greater than APE\_discrete (0.16). Together with the smaller estimation biases discussed before, the learnt policy  $\pi_E$  with APE\_scalable is closer to the zero-variance distribution, and APE\_scalable performs better with smaller  $v^*(s_0)$ .

We notice that the environment adversary policies at convergence with different random seeds hold a similar interpretable behavior mode, one example of which is visualized in Fig. 6 for Int-v1. We see that the learned adversary policy  $\pi_E$  tends to accelerate (being aggressive) at the beginning of



Fig. 5: Evaluation results in Int-v0, Int-v1 and LunarLander. Each line is run with 5 random seeds. The shaded area has lower and upper bound corresponding to 5% and 95% quantile. APE\_scalable performs well in moderate high-dimensional tasks with higher estimate accuracies and sampled rare event rates compared with baselines. The performances of all the methods are measured with estimate errors and sampled rare event rates.

TABLE II: Numerical evaluation results in Int-v0, Int-v1 and LunarLander. Each number is evaluated with 5 random seeds. The best performance (the smallest number in each column) is highlighted in bold.

Environment	Int-v0 (Unit $10^{-2}$ )			Int-v1 (Unit 10 <sup>-6</sup> )			LunarLander (Unit $10^{-3}$ )		
Metrics	Bias	Std	MSE	Bias	Std	MSE	Bias	Std	MSE
APE_scalable	-0.07	6.27	6.27	1.08	2.88	3.07	-0.02	1.28	1.28
APE_discrete	-0.75	0.47	0.88	2447.75	149.44	2452.31	-1.30	0.00	1.16
CEM_discrete	-6.34	0.00	6.34	-1.70	0.00	1.70	-1.17	0.07	1.27
MC	0.23	6.57	6.57	-1.70	0.00	1.70	0.08	0.42	0.43



Fig. 6: The evolution of  $\pi_E$  in Int-v1 conditioned at the initial state  $s_0$ , a random intermediate state  $s_m$  and a state before collision  $s_n$ . The time steps  $t_0 < t_p < t_q < t_c$ .

each episode and keep the original behavior  $\pi_{E,gt}$  (being conservative) in the remaining steps.

#### VII. CONCLUSION

Motivated by the limitations of existing policy evaluation methods facing rare events, we propose APE, which scales to complex tasks by drawing from powerful function approximators and explores rare events caused by sequential interactions via learning an adversary with adaptive importance sampling. We demonstrate the effectiveness of APE with its orders of magnitude sample savings to achieve convergence. APE provides a fundamental tool to allow the evaluation, and subsequent deployment, of intelligent agents in safety-critical systems that are otherwise computationally prohibitive. It also increases policy interpretability by uncovering agent behaviors in extreme cases (rare events).

The scalability of APE in evaluating rare events in sequential environments opens up two important future directions. First is the training of rare-event-aware intelligent agents. This requires a minimax training mechanism to optimize the agent's strategies against the avoidance of rare events, the latter captured via the environment adversary learned from adaptive importance sampling as in this paper. Second is more powerful update methods for the value function and importance distribution, such as incorporating (Bayesian) uncertainty estimates in the GP regression model and using multi-step TD.

#### ACKNOWLEDGMENT

The authors gratefully acknowledge the support from the National Science Foundation (under grants IIS-1849280 and IIS-1849304), and unrestricted research grant from the Toyota Motor North America. The ideas, opinions and conclusions presented in this paper are solely those of the authors.

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