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Bayesian Ensembles for Exploration in Deep Q-Learning

(Extended Abstract)

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ABSTRACT

Exploration in reinforcement learning remains a difficult challenge. In order to drive exploration, ensembles with randomized prior functions have recently been popularized to quantify uncertainty in the value model. There is no theoretical reason for these ensembles to resemble the actual posterior, however. In this work, we view training ensembles from the perspective of Sequential Monte Carlo, a Monte Carlo method that approximates a sequence of distributions with a set of particles. In particular, we propose an algorithm that exploits both the practical flexibility of ensembles and theory of the Bayesian paradigm. We incorporate this method into a standard Deep Q-learning agent (DQN) and experimentally show qualitatively good uncertainty quantification and improved exploration capabilities over a regular ensemble.

KEYWORDS

Reinforcement Learning, Exploration, Bayesian, Uncertainty

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1 INTRODUCTION

Reinforcement learning (RL) algorithms are still notoriously sample inefficient. One pressing reason is the difficulty of exploring an environment efficiently while assuming little prior knowledge [32]. A promising approach that is currently studied is to quantify uncertainty in the value models learned by the agent, and then either provide intrinsic reward or use Thompson sampling to explore [1–4, 7, 14, 15, 21, 26, 27, 29]. However, quantifying uncertainty for deep neural networks is in itself a difficult task [18, 23].

Ensembles of neural networks have been shown to provide better predictive accuracy over a single model in supervised learning tasks [11, 20], as well as suitable methods for uncertainty quantification for exploration in reinforcement learning [13, 26, 27]. While ensembles with independent models of identical architecture tend to collapse to the same predictive model [17], several techniques have been developed to prevent this, such as adversarial learning [20], bootstrapping the data [27], and adding additive priors [26]. Furthermore, some techniques such as Stein Variational Gradient Descent [8, 22] alleviate this issue by interpreting the ensemble as an approximation to the Bayesian posterior and training it as such. The method that we propose falls into this last category and aims to be closer to the posterior for more accurate uncertainty quantification, while retaining the flexibility of ensembles.

Bayesian neural networks have been applied to RL through Variational Inference [14, 15, 30], as well as MCMC [1, 12, 19]. Due to the complex nature of Neural Networks, however, it is unclear how the model class in Variational inference biases uncertainty quantification. On the other hand, MCMC is in theory unbiased and also shows strong results in large networks in supervised learning [6, 16, 31]. However, MCMC methods such as Hamiltonian Monte Carlo [25] can struggle to find every mode for complex multimodal distributions [10]. This is an important drawback in deep learning, where the posterior distribution is likely very ill behaved, and especially in RL where under-approximation of the posterior complexity might lead to underestimating the uncertainty and therefore failure of exploration. Sequential Monte Carlo (SMC), which uses a set of particles to approximate the posterior, can be a remedy to these issues in non-deep learning applications [10].

In this work, we forego Variational Inference to avoid a decision in model class, and instead alleviate the issues in MCMC by using SMC. Noting the success of ensembles in deep learning, we unify ensembles and MCMC methods by using SMC algorithms to train an ensemble in a Bayesian manner, to benefit from both the practical effectiveness of ensembles and theoretical foundations of MCMC. Specifically, we adapt existing SMC algorithms to a mini-batch setting, and show that they are feasible methods to train ensembles as approximations to the Bayesian posterior. Furthermore, as our main contribution, we introduce Sequential Monte Carlo DQN (SMC-DQN), a RL-algorithm which uses SMC to track a posterior over the Q-values and uses this posterior to explore efficiently. We experimentally test our agent's exploration capabilities on several environments, observing significantly stronger performance compared with regular ensembles, and results that are competitive with a strong baseline.

2 BACKGROUND

We consider standard Markov Decision Process with discounted rewards in the infinite horizon setting. Ensembles of Q-networks $Q_{\theta_1}(s,a),\dots,Q_{\theta_n}(s,a)$ are a widespread method to improve exploration in an unknown environments. For example, the BootDQN algorithm [27] achieves deep exploration through Thompson sampling, sampling uniformly $i \in \{1,\dots,n\}$ and acting greedily with respect to the network Q_{θ_i} for a full episode. In BootDQN each

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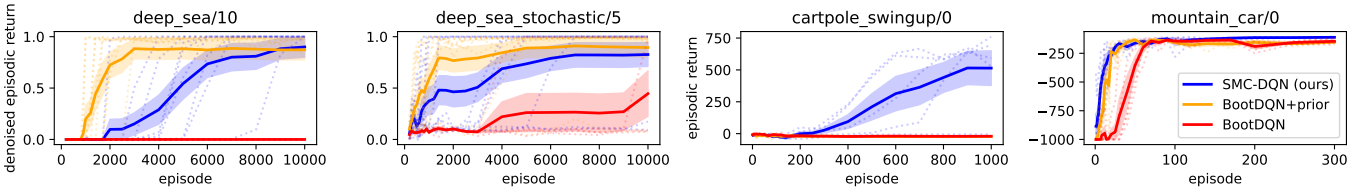

Figure 1: Learning curves over the BSuite environments. The solid line is the mean of 10 seeds for the Deep Sea environments, and 5 seeds for Cartpole Swingup and Mountain Car. The shaded area denotes the standard error of the mean.

network Q_{θ_i} is equipped with its own target network $Q_{\theta'_i}$, and gets updated using transitions (s, a, r, s') from a replay buffer:

$$\theta_i \leftarrow \theta_i - \nabla_{\theta_i} \left[Q_{\theta_i}(s,a) - r - \max_{a'} Q_{\theta'_i}(s', a') \right]^2. \tag{1}$$

To ensure diversity in the ensemble, independently initialized prior functions are added to each ensemble member's outputs. However, while effective, this technique lacks theoretical motivation when considered as Bayesian priors for neural networks. In problems with well-defined likelihoods and priors, the Bayesian posterior can therefore be expected to outperform prior functions.

Sequential Monte Carlo algorithms sample a sequence of distributions $p_0(\theta), \ldots, p_m(\theta)$. Leveraging this fact, we can set the target distributions to a sequence interpolating between the prior and posterior distribution over the parameters of a Q-learner: $p_t(\theta) \propto p(\mathcal{D}|\theta)^{\lambda_t} p(\theta)$, where λ_t is a sequence of temperatures $0 = \lambda_0 < \lambda_1 < \cdots < \lambda_m = 1$, which can be dynamically optimised for [5, 9].

3 SEQUENTIAL MONTE CARLO DQN

To improve exploration, we construct an agent that quantifies uncertainty in its Q-values by approximating the posterior distribution over its parameters using SMC. Specifically, we extend a standard DQN agent [24] by replacing its point-wise estimator $Q_\theta(s, a)$ with an ensemble $Q_{\theta_1}(s, a), \ldots, Q_{\theta_n}(s, a)$ and sampling weights $w_1, \ldots w_n$ to maintain an approximation of the posterior $p(\theta|\mathcal{D}, \boldsymbol{\theta'})$, conditioned on the replay buffer $\mathcal{D} = ((s_t, a_t, r_t, s_{t+1}))_{t=1\ldots N}$ and target parameters $\boldsymbol{\theta'} = (\theta'_1, \ldots, \theta'_n)$. In line with Schmitt et al. [30], a normal distribution

$$Q_\theta(s,a) - r(s,a) - \gamma \max_{a'} Q_{\theta'}(s', a') \sim \mathcal{N}(0, \sigma)$$

is used as a probabilistic interpretation of the squared temporal difference error, and to represent the uncertainty in the targets we define the likelihood to be a mixture distribution

$$\log p(s, a, r, s'|\theta, \boldsymbol{\theta'}) = \log \sum_{i=1}^{n} \frac{1}{n} \exp\left(-\frac{1}{2\sigma^2} [Q_\theta(s,a) - r(s,a) - \gamma \max_{a'} Q_{\theta'_i}(s', a')]^2 \right), \tag{2}$$

contrasting BootDQN which shares no target values between ensemble members. After collecting a new batch of trajectories $\mathcal{B}$ by acting in the environment, the posterior distribution can be updated efficiently by interpolating between the previous posterior $p(\theta|\boldsymbol{\theta'}, \mathcal{D})$ and the new posterior $p(\theta|\boldsymbol{\theta'}, \mathcal{D} \cup \mathcal{B})$ with SMC.

Updating the target networks $\boldsymbol{\theta'}$ changes the target distribution, meaning that the sample $(\theta_1, \ldots, \theta_n, \quad w_1, \ldots, w_n)$ is no longer a sample of the posterior with respect to the updated targets, i.e., $p(\theta|\boldsymbol{\theta'}_{\text{new}}, \mathcal{D})$. Therefore, the typical target update $\theta'_i \leftarrow \theta_i$ is now accompanied by another SMC step, which interpolates between $p(\theta|\boldsymbol{\theta'}_{\text{old}}, \mathcal{D})$ and $p(\theta|\boldsymbol{\theta'}_{\text{new}}, \mathcal{D})$.

4 EXPERIMENTAL STUDY

We test our agent in the exploration environments as well as Mountain Car in BSuite [28], against BSuite's baseline BootDQN agent with and without prior. Figure 1 shows the performance of the agents on each task. It can be seen that SMC-DQN outperforms BootDQN without priors on all our benchmarks. On Deep Sea it achieves comparable performance to BootDQN with priors, and significantly outperforms BootDQN with priors on Cartpole Swingup, where BootDQN at this ensemble size fails to learn a meaningful policy even with prior functions. Further, on Mountain Car SMC-DQN learns at the same speed as BootDQN with priors in the beginning, but converges to a slightly better policy.

Our results show a gap between Deep Sea and the continuous environments in the performance relative to the baselines. We hypothesize that this is due to the fact that the likelihood does not explain the one-hot encoded environment Deep Sea very well. In the continuous environments, agents can exploit the generalization capabilities of neural networks, allowing the posterior to model sensible generalization behaviours. However, this generalization can lead to errors in one-hot encoded environments where unconnected states are independent.

5 CONCLUSION

We introduced the novel idea of using SMC to train an ensemble in order to approximate the Bayesian posterior distribution. Specifically, we modified the BootDQN algorithm to use SMC, thus keeping track of a posterior over the Q-values in a theoretically sound manner. We found that such an approach is able to maintain a diverse set of models that can drive exploration in difficult-to-explore environments such as Deep Sea and Cartpole Swingup. Especially in continuous state environments, the uncertainty quantification provided by the posterior distribution leads to better exploration compared to our baselines. In the future, we intend to investigate the influence of the choice of likelihood and derive methods to synthesize meaningful likelihoods.

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