Statistical Bootstrapping for Uncertainty Estimation in Off-Policy Evaluation

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Abstract

In reinforcement learning, it is typical to use the empirically observed transitions and rewards to estimate the value of a policy via either model-based or $Q$-fitting approaches. Although straightforward, these techniques in general yield biased estimates of the true value of the policy. In this work, we investigate the potential for statistical bootstrapping to be used as a way to take these biased estimates and produce calibrated confidence intervals for the true value of the policy. We identify conditions – specifically, sufficient data size and sufficient coverage – under which statistical bootstrapping in this setting is guaranteed to yield correct confidence intervals. In practical situations, these conditions often do not hold, and so we discuss and propose mechanisms that can be employed to mitigate their effects. We evaluate our proposed method and show that it can yield accurate confidence intervals in a variety of conditions, including challenging continuous control environments and small data regimes.

1 Introduction

Providing accurate and trustworthy estimates of a policy’s long term value in a decision-making environment is an important problem in reinforcement learning (RL). Typically, due to cost or safety constraints, one must perform this estimation without actually running the policy in the live environment. Instead, one must predict the value of the policy using only a limited set of experience of some other logging (or behavior) policies acting in the sequential environment. This problem is generally referred to as off-policy evaluation (OPE) [30]. The OPE problem is especially relevant to many practical domains, such as health [22, 18], education [21], and recommendation systems [34], where accurate evaluation of a new policy is critical to maximize safety and minimize risks associated with deployment of a new policy [38].

Perhaps the most straightforward approach to OPE is to use the given finite dataset of experience to determine the environment’s empirically observed initialization, transition, and reward probabilities, and then to evaluate the expected value of the target policy in this empirical environment. This straightforward approach is known as the direct method (DM) [6, 39]. In addition to encompassing model-based (MB) methods [35, 11], this general paradigm is also implicitly implemented by $Q$-evaluation (QE), or its parametric counterpart fitted $Q$-evaluation (FQE) [28, 39, 2]. Indeed, the mathematical equivalence of QE and MB, even under certain function approximation schemes, has been recently demonstrated [5].

Although the DM paradigm is a straightforward and intuitive approach, it is traditionally seen as undesirable due to it yielding biased estimates. That is, the estimates returned by QE or MB over multiple experiments on randomly sampled finite datasets are not centered around the true value of the target policy. This fact has led much of the OPE literature to focus on a variety of importance

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We consider the standard Markov Decision Process (MDP) setting \[31\], in which the environment where we only have access to a finite empirical dataset of experience samples from these distributions. Where the OPE estimate is a complex function of the input data, it is not immediately clear whether Efron’s bootstrap is a well-known method in statistics for deriving confidence intervals from biased estimates, and so it may be a promising technique for use in conjunction with DM \[11\]. Still, while bootstrapping is a simple approach widely used in statistics, it is not always guaranteed to yield accurate confidence intervals \[32, 1\], and in the case of MB or QE, where the OPE estimate is a complex function of the input data, it is not immediately clear whether Efron’s bootstrap would be valid.

In this paper, we investigate the validity of Efron’s bootstrap applied to DM. We derive theoretical guarantees that show that, if certain conditions are satisfied, Efron’s bootstrap applied to DM yields asymptotically accurate confidence intervals. The conditions we identify – namely, sufficient sample size and sufficient coverage of the underlying experience data distribution – may not hold in many practical scenarios. Therefore, we use insights from our derivations to suggest mechanisms – noisy rewards and regularization – for mitigating the effect of these in practice. We present empirical results in tabular settings that show the validity of our theory and the benefit of our heuristic mechanisms. Extending our methods to more complex environments with function approximation, we present state-of-the-art results, showing that MB and QE with Efron’s bootstrap can yield accurate and useful confidence intervals on challenging continuous control benchmarks.

2 Background

We consider the standard Markov Decision Process (MDP) setting \[31\], in which the environment is specified by a tuple \(M = (S, A, R, T, \mu_0, \gamma)\), consisting of a state space \(S\), an action space \(A\), a reward distribution function \(R\), a transition probability function \(T\), an initial state distribution \(\mu_0\), and a discount \(0 \leq \gamma < 1\). A policy \(\pi\) interacts with the environment iteratively, starting with an initial state \(s_0 \sim \mu_0\). For simplicity, we will restrict the text to consider the infinite-horizon setting, although all results apply in the finite horizon setting as well.

In this work, we largely focus on estimation of the value of a given target policy \(\pi\), defined as the expected accumulated reward of \(\pi\) in \(M\), averaged over time via \(\gamma\)-discounting:

\[
\rho(\pi) := (1 - \gamma) \cdot \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t \cdot r_t \middle| s_0 \sim \mu_0, a_t \sim \pi(s_t), r_t \sim R(s_t, a_t), s_{t+1} \sim T(s_t, a_t) \right].
\]

We consider the off-policy setting, in which we do not have explicit knowledge of \(R\), \(T\), \(\mu_0\). Rather, we only have access to a finite empirical dataset of experience samples from these distributions. More concretely, we have a dataset \(D_n := \{(s^{(j)}_0, s^{(j)}, a^{(j)}, r^{(j)}, s^{(j)}_t)\}_{j=1}^n\) consisting of \(n\) tuples \((s_0, s, a, r, s')\) independently sampled via

\[
s_0 \sim \mu_0; \quad (s, a) \sim d^D; \quad r \sim R(s, a); \quad s' \sim T(s, a),
\]

where \(d^D\) is some unknown distribution over state-action pairs. We will abuse notation at times and use \(d^D(s_0, s, a, r, s')\) to denote the joint distribution on tuples and \(d^D(s_0), d^D(r, s'|s, a)\) the appropriately marginalized and conditioned distributions. The finite dataset \(D_n\) induces its own empirical distribution over tuples, which we denote

\[
d_n^D := \frac{1}{n} \sum_{j=1}^n \delta((s^{(j)}_0, s^{(j)}, a^{(j)}, r^{(j)}, s^{(j)}_t)),
\]

where \(\delta\) is the Dirac delta distribution centered at \(\chi\). The empirical distribution over tuples \(d^D_n\) in turn determines an empirical initial state distribution \(\mu_0^D(s_0) := d^D_n(s_0)\), an empirical reward distribution function \(R_{D_n}(r|s, a) := d^D_n(r|s, a)\), and an empirical transition probability function \(T_{D_n}(s'|s, a) := d^D_n(s'|s, a)\). To appropriately define \(R_{D_n}, T_{D_n}\) when \(d^D_n\) has poor coverage of the state or action space, we define \(R_{D_n}(r|s, a) := \mathcal{R}_{prior}(r|s, a), T_{D_n}(s'|s, a) := \mathcal{T}_{prior}(s'|s, a)\) for all \(s, a\) such that \(d^D_n(s, a) = 0\), for some fixed prior distribution functions \(\mathcal{R}_{prior}, \mathcal{T}_{prior}\).
The direct method (DM) uses the empirically observed $\mu_n^D, R_n, T_n$ to estimate $\rho(\pi)$ as
\[
\rho_{DM}(\pi|D_n) := (1 - \gamma) \cdot E\left[ \sum_{t=0}^{\infty} \gamma^t \cdot r_t \mid s_0 \sim \mu_n^D, a_t \sim \pi(s_t), r_t \sim R_n(s_t, a_t), s_{t+1} \sim T_n(s_t, a_t) \right].
\]

The direct method may be implemented explicitly through a model-based (MB) procedure, where $\mu_n^D, R_n, T_n$ are either determined analytically or approximated by parametric models via maximum likelihood. Then, $\rho_{DM}(\pi|D_n)$ is approximated by Monte Carlo trajectories of $\pi$ rolled out using these models. Alternatively, DM can also be implemented in a model-free fashion via Q-evaluation (QE). In this approach, a Q-value function $Q: S \times A \rightarrow \mathbb{R}$ is iteratively learned via the Bellman backup procedure,
\[
Q^{(i+1)}(s, a) \leftarrow E_{d^{\pi_n}}(r, r'|s, a', \pi(s')) \left[ r + \gamma Q^{(i)}(s', a') \right].
\]

Ignoring issues of function approximation, this procedure converges to a fixed point $\hat{Q}^\pi = \lim_{i \to \infty} Q^{(i)}$, which is the Q-value function of $\pi$ under the empirical MDP. Once this fixed point is determined, the value of $\pi$ may be approximated as $\rho_{DM}(\pi|D_n) = (1 - \gamma) \cdot E_{d^{\pi_n}}(s_0, a_0 \sim 0) \left[ \hat{Q}^\pi(s_0, a_0) \right]$. When the iterative procedure in (4) is performed via a regression over parameterized $Q$, this procedure is known as fitted Q-evaluation (FQE). The reader may look to [39] for a review of a variety of instantiations of the direct method.

Although DM via either MB or QE is straightforward, it generally yields biased estimates of $\rho(\pi)$:
\[
\rho(\pi) \neq E_{D_n}[\rho_{DM}(\pi|D_n)].
\]

Still, unbiased estimates are not completely necessary in practical risk-sensitive applications, where one would rather have access to accurate confidence intervals, and the bias of a single point estimate is irrelevant. In the statistics literature, Efron’s bootstrap (Algorithm 1) is widely used to provide asymptotically accurate confidence intervals, even when point estimates of the statistic are biased, and doing the same for DM methods has been proposed in the past [11]. However, Efron’s bootstrap is not always guaranteed to yield accurate confidence intervals [32, 11]. In this paper, we will investigate conditions under which Efron’s bootstrap applied to DM is guaranteed to yield accurate confidence intervals, and suggest mechanisms to improve the validity of the confidence intervals when these conditions do not hold.

Before getting into our main contributions, we list a few useful assumptions. For ease of exposition, we state these assumptions and our theoretical results with respect to countable sets $S$ and $A$; this allows us to avoid technical details from measure theory.

**Assumption 1** (Bounded rewards). *The rewards of the MDP are bounded by some finite constant $R_{\text{max}}$: $\|r\|_\infty \leq R_{\text{max}}$.***

For the next assumption, we make use of the discounted on-policy distribution $d^\pi$, which measures the likelihood of the policy $\pi$ encountering state-action pair $(s, a)$ when interacting with $M$ [24]:
\[
d^\pi(s, a) := (1 - \gamma) \cdot \sum_{t=0}^{\infty} \gamma^t \cdot \Pr[s_t = s, a_t = a \mid \pi_0, \pi, R, T].
\]

**Assumption 2** (Sufficient data coverage). *There exists $\epsilon > 0$ such that for any $(s, a)$, $d^\pi(s, a) > 0$ implies $d^D(s, a) > \epsilon$.***

As we will discuss later, Assumption [2] is very strong and often not satisfied in practice (e.g., in infinite state or action spaces).

### 3 Investigating the Validity of Efron’s Bootstrap

We begin by presenting a theoretical result showing the validity of using Efron’s bootstrap based on estimates $\rho_{DM}(\pi|D_n)$ prescribed by the direct method.

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[2] When $d^D_n$ has poor coverage, the fixed point $\hat{Q}^\pi$ depends on the initial Q-values $Q^{(0)}$. The fixed point $\hat{Q}^\pi$ is still the Q-value function of $\pi$ under the empirical MDP, where the prior reward and transition functions $R_{\text{prior}}, T_{\text{prior}}$ are implicitly defined by the initialization of $Q^{(0)}$. 

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We encapsulate this in the following theorem.

Although necessary conditions for the validity of Efron’s bootstrap are not known in general, where $d$ where $d$ where $d$

**Algorithm 1** Efron’s non-parameteric, bias-corrected bootstrap [7].

| **Inputs:** A functional $F$, a desired confidence $1 - \alpha$, a finite sample dataset $D_n := \{(s_0^{(j)}, s^{(j)}, a^{(j)}, r^{(j)}, s'^{(j)})\}_{j=1}^n$, number of bootstraps $b$ to use for percentile calculation. |
| **Note:** $F$ is a function from distributions over $(s_0,s,a,r,s')$ to $\mathbb{R}$. When applied to a finite dataset $\mathcal{D}$, it is understood to be applied to the empirical distribution $d^\mathcal{D}$ determined by $\mathcal{D}$. |
| **Compute empirical estimate** $\hat{y} := F(D_n)$. |
| **Create** $b$ bootstrapped datasets $\{D_n^{(k)}\}_{k=1}^b$, each of $n$ elements sampled uniformly from $D_n$.
| **Compute** bootstrapped estimates $\hat{y}_1 := F(D_n^{(1)}), \ldots, \hat{y}_b := F(D_n^{(b)})$.
| **Compute** $\alpha/2$ and $1 - \alpha/2$ quantiles $z_{\alpha/2}, z_{1-\alpha/2} / \{\hat{y}_k - \hat{y}\}_{k=1}^b$.
| **Return** $C := [\hat{y} - z_{1-\alpha/2}, \hat{y} - z_{\alpha/2}]$. |

**Theorem 1** (Correctness of DM with bootstrapping). Under Assumptions [12] and use of Algorithm 1 with $F(d^{\mathcal{D}_n}) := \rho_{DM}(\pi|D_n)$ yields confidence intervals $C(d^{\mathcal{D}_n})$ which are asymptotically correct, in the sense that

$$\Pr[\rho(\pi) \in C(d^{\mathcal{D}_n})] = 1 - \alpha - O_p(n^{-1/2}),$$

where $O_p$ is used to denote order in probability. Additionally, the one-sided confidence intervals are asymptotically correct at rate $O_p(n^{-1/2})$. These asymptotic rates may be improved by using more sophisticated bootstrapping methods in place of Algorithm 1 such as BCa or ABC [4].

**Proof.** (Sketch) First, it is clear by the definition of $d^\mathcal{D}$ in [2] and Assumption 2 that $F(d^\mathcal{D}) = \rho(\pi)$. Thus it is left to show that bootstrap yields correct intervals around $F(d^\mathcal{D})$. Sufficient conditions for correctness of Efron’s bias-corrected bootstrap are known, and they are given by smoothness (specifically, Hadamard differentiability) of the functional $F$ evaluated in a neighborhood (i.e., a sufficiently small $L_\infty$ ball) around the true distribution $d^{\mathcal{D}}$ [40,29,9]. In the appendix, we show that under the assumption of bounded rewards (Assumption 1) and the derivative $F'(d^\mathcal{D})$ for general distribution $d^\mathcal{D}$ satisfies

$$||F'(d^\mathcal{D})||_{\infty} = O \left(||d^\mathcal{D}_{\mathcal{D}} / d^\mathcal{D}||_{\infty}\right),$$

where $d^\mathcal{D}_{\mathcal{D}}$ is the discounted-on-policy distribution of $\pi$ under $\mu^\mathcal{D}, \mathcal{R}, T^\mathcal{D}$. When $d^\mathcal{D} = d^\mathcal{D}$, we have $||F'(d^\mathcal{D})||_{\infty} = O (||d^\mathcal{D} / d^\mathcal{D}||_{\infty})$. In the appendix, we show that $||d^\mathcal{D}_{\mathcal{D}} / d^\mathcal{D}||_{\infty}$ is bounded within a sufficiently small neighborhood of $d^\mathcal{D}$, given sufficient coverage of $d^\mathcal{D}$ (Assumption 2), and this completes the proof.

Although necessary conditions for the validity of Efron’s bootstrap are not known in general, Hadamard differentiability is the key property typically used to prove validity. Our derivations make it clear that Assumption 2 is necessary to ensure Hadamard differentiability of $F$; otherwise, a small change in $d^\mathcal{D}$ may take $d^\mathcal{D}$ out of the support of $d^\mathcal{D}$, causing divergence in the derivative [8]. In contrast, a weaker variant of this assumption, $||d^\mathcal{D} / d^\mathcal{D}||_{\infty} = W_{\text{max}} < \infty$, which appears in previous OPE literature [23], is not sufficiently strong to guarantee differentiability in the neighborhood of $d^\mathcal{D}$. We encapsulate this in the following theorem.

**Theorem 2** (Necessity of Assumption 2). Suppose Assumption 1 holds and define functional $F(d^{\mathcal{D}_n}) := \rho_{DM}(\pi|D_n)$. There exists $d^{\mathcal{D}_n}$ with uniformly bounded ratios $||d^\mathcal{D} / d^\mathcal{D}||_{\infty} = W_{\text{max}} < \infty$ such that $F$ is not Hadamard differentiable within any neighborhood of $d^{\mathcal{D}_n}$.

**Proof.** See the appendix.

**Note:** Theorem 2 is somewhat disappointing, as Assumption 2 is strong and often not satisfied in practice; in continuous state or action settings, it is almost never satisfied.

In addition to the need for Assumption 2, the other major lacking of Theorem 1 is that it only guarantees correct intervals asymptotically. For any finite $n$, the confidence intervals yielded by

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3. See the appendix for a definition of Hadamard differentiability.
Efron’s bootstrap will generally exhibit under-coverage, and in practice this can lead to overly confident confidence intervals. Indeed, in the extreme case of \( n = 1 \), there will be no variation in the boostrapped estimates of \( \rho \) leading to confidence intervals \( C(d^{D_n}) \) that are single points.

In the following subsections, we elaborate on our suggested mechanisms for appropriately compensating for these two main theoretical shortcomings of Efron’s bootstrap applied to DM.

### 3.1 Regularizations for Insufficient Coverage

To better understand the need for sufficient coverage, we can look at a simple scenario illustrated in Figure 1. If the data distribution includes \( s_2 \) but does not cover the action \( \pi(s_2) \) chosen by the policy, then the estimates \( R_{D_n}(s_2, \pi(s_2)) \), \( T_{D_n}(s_2, \pi(s_2)) \) will be set to the priors \( R_{\text{prior}}(s_2, \pi(s_2)), T_{\text{prior}}(s_2, \pi(s_2)) \). However, if the data distribution includes state action pair \((s_2, \pi(s_2))\) with even a tiny probability, the estimates \( R_{D_n}(s_2, \pi(s_2)), T_{D_n}(s_2, \pi(s_2)) \) are changed to their empirical estimates. In general, this change is not smooth (i.e., not Hadamard differentiable) with respect to the underlying data distribution, and this leads to issues with the validity of Efron’s bootstrap applied to \( \rho_{DM} \).

It is thus clear that to ensure validity of Efron’s bootstrap, we require estimates \( R_{D_n}, T_{D_n} \) that are smoother around \( d^{D_n}(s, a) \approx 0 \). For example, smoother empirical reward and transition functions may be found by defining biased reward and transitions in terms of some fixed \( \kappa > 0 \),

\[
R^\kappa_{D_n}(r|s, a) := \frac{d^{D_n}(s, a, r) + \kappa \cdot R_{\text{prior}}(r|s, a)}{d^{D_n}(s, a) + \kappa}, \tag{9}
\]

\[
T^\kappa_{D_n}(s'|s, a) := \frac{d^{D_n}(s, a, s') + \kappa \cdot T_{\text{prior}}(s'|s, a)}{d^{D_n}(s, a) + \kappa}. \tag{10}
\]

These biased functions would yield a regularized DM estimate:

\[
\rho^\kappa_{DM}(\pi|D_n) := (1 - \gamma) \cdot \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t \cdot r_t \middle| \mu_{0}^{D_n}, \pi, R^\kappa_{D_n}, T^\kappa_{D_n} \right]. \tag{11}
\]

This estimator is provably amenable to statistical bootstrapping regardless of data coverage, although at the cost of providing intervals for a biased estimate of \( \rho(\pi) \), as stated by the following theorem.

**Theorem 3** (Correctness of regularized DM with bootstrapping). Under Assumption \[7\] the use of Algorithm \[7\], with \( F(d^{D_n}) := \rho^\kappa_{DM}(\pi|D_n) \) yields confidence intervals \( C(d^{D_n}) \) which are asymptotically correct, in the sense that

\[
\Pr[\rho^\kappa_{DM}(\pi|d^\cdot) \in C(d^{D_n})] = 1 - \alpha - O_p(n^{-1/2}). \tag{12}
\]

As for Theorem \[7\], the one-sided intervals converge at a rate \( O_p(n^{-1/2}) \) and these rates may be improved by using more sophisticated bootstrapping methods.

**Proof.** See the appendix.

For succinctness, we have expressed Theorem 3 in terms of the specific \( R^\kappa_{D_n}, T^\kappa_{D_n} \) defined above. In general, the guarantees of the theorem hold for any suitably smooth \( R^\kappa_{D_n}, T^\kappa_{D_n} \), i.e., reward and transition functions that are locally differentiable around \( d^\cdot \); see the appendix for details. This more general result is promising for function approximation settings. In such settings, when using model-based evaluation or fitted \( Q \)-evaluation, it is straightforward to smooth out the estimated reward and transition functions via a number of standard regularizations. For example, in our experiments with neural network function approximators, we utilize standard weight decay, which acts as a regularization towards prior reward and transition functions implicitly defined by the network structure.

### 3.2 Noisy Rewards

Even with sufficient coverage or appropriate regularization, the computed confidence intervals will generally be over-confident and under-cover the true value, especially in low-data regimes. This
is due to the fact that for finite \( n \), the empirical variance of the functional \( F \) over the bootstrapped datasets is in general an underestimate of the true variance.

To incorporate additional variance, we propose to augment the dataset \( \mathcal{D}_n \) via perturbations applied to observed rewards,

\[
\tilde{\mathcal{D}}_n \leftarrow \mathcal{D}_n \cup \{(s_0, s, a, r + R_{\text{noise}}, s') \mid (s_0, s, a, r, s') \in \mathcal{D}_n\} \cup \{(s_0, s, a, r - R_{\text{noise}}, s') \mid (s_0, s, a, r, s') \in \mathcal{D}_n\}. \tag{13}
\]

Note that the variance of the empirical dataset is increased to \( \text{Var}_{\tilde{\mathcal{D}}_n}[r] = \frac{3}{2} R_{\text{noise}}^2 + \text{Var}_{\mathcal{D}_n}[r] \). Given the augmented dataset \( \tilde{\mathcal{D}}_n \), one may perform Algorithm 1 as-is, sampling \( b \) bootstrapped datasets each of \( n \) elements. This same technique of augmenting a dataset with noisy rewards has been used in the bandit literature as a way to perform better exploration [15, 16]. As in this previous literature, a large enough \( R_{\text{noise}} \geq \sqrt{\frac{3}{2} \cdot (1 - \gamma)^{-1} \cdot R_{\text{max}}} \) would be sufficient to compensate for the inherent under-coverage in bootstrapping, although in practice a much smaller \( R_{\text{noise}} \) can still yield good coverage.

With noisy rewards, we are able to compensate for the under-coverage of Theorems 1 and 3. However, this generally comes at the cost of over-coverage. In practice, the parameter \( R_{\text{noise}} \) provides a way to trade-off between safety in small data regimes and looseness of the confidence intervals. In our experiments, we found that setting \( R_{\text{noise}} = 0.25 \cdot \sqrt{\text{Var}_{\mathcal{D}_n}[r]} \) provides a reasonable trade-off for our considered environments.

4 Related Work

Our paper focuses on producing confidence bounds for off-policy evaluation and therefore follows a long line of work on high-confidence policy evaluation (HCOPE) [26]. Many of the existing methods for HCOPE focus on importance sampling (IS) based estimators, in which the rewards of a trajectory are re-weighted according to an inverse propensity ratio to yield an unbiased estimate of \( \rho(\pi) \) [30]. Given a dataset with several trajectories, one may derive several unbiased estimates and then use concentration inequalities to derive high-confidence lower and upper bounds on the true average [36]. Since these concentration inequalities typically require unbiased estimates, they are not applicable to the direct method.

In terms of statistical bootstrapping, there have been several instances of its use for off-policy evaluation. Specifically, [27] combined statistical bootstrapping with IS to derive OPE confidence intervals. Unlike for DM, the validity of Efron’s bootstrap with IS is straightforward, since the functional \( F \) in this case is the standard mean. We are aware of one previous instance in which statistical bootstrapping was used for high-confidence policy evaluation with DM; specifically, [11] proposes to use Efron’s bootstrap in conjunction with model-based learning, similar to the present work. However, the validity of using Efron’s bootstrap is not addressed in this previous work. The theoretical investigation we presented is a key contribution of our paper. Notably, we found that the use of Efron’s bootstrap directly is misguided without the use of strong assumptions, or alternatively, as we suggest, the use of mechanisms like regularization and noisy rewards. Furthermore, our experimental work presents strong results on continuous control benchmarks, while previous work mostly focuses on tabular domains.

Outside of the narrow scope of HCOPE, the ideas behind Efron’s bootstrap have inspired a number of existing RL algorithms. Specifically, statistical bootstrapping has been proposed as a mechanism for exploration; e.g., bootstrapped DQN [26, 27]. However, in practice, the type of bootstrapping performed in these algorithms is far from that prescribed by Efron’s bootstrap. Usually, an ensemble of models is learned over the whole dataset, without any re-sampling or bias correction, and thus the theory behind bootstrap does not readily apply. Although this simple paradigm has achieved impressive results on hard exploration environments [25], in our initial experiments for off-policy evaluation we found the naive ensembling approach to yield poor confidence intervals. In the bandits literature, ideas from statistical bootstrapping have also been investigated as an exploration mechanism [16, 12]. While we have focused on policy evaluation, extending the insights and derivations of the present paper to propose better algorithms for exploratory policy learning (or, conversely, safe policy learning) is an interesting avenue for future work.
5 Experiments

We evaluate our methods first in a discrete tabular domain, where we investigate how well the coverage of the estimated bootstrap intervals matches the intended coverage and show how reward noise can assist in low-data regimes. Sufficient coverage is not much of an issue in finite domains and so we continue to a more difficult set of continuous control tasks from OpenAI Gym, where we evaluate the use of appropriately regularized function approximators in conjunction with bootstrapping and noisy rewards.

5.1 Tabular Tasks

We use Frozen Lake as a discrete domain for tabular experiments. In this environment, the agent navigates in a discrete world from a start state to a goal state. The environment dynamics are stochastic and some actions lead to episode terminations. We use $\gamma = 0.999$. We use a target policy that is near-optimal in this domain. We collect an experience dataset using a behavior policy derived as the target policy injected with $0.2\epsilon$-greedy noise (this reduces the value of the policy $\rho(\pi)$ from about 0.0007 to about 0.0002). For this task, policy evaluation with DM with either MB or QE can be equivalently solved using the exact tabular method, so we plot a single variant labelled DM.

We present empirical results in Figure 2. We plot the results of using Efron’s bootstrap with DM to construct confidence intervals with confidence $1 - \alpha$ across a number of dataset sizes. The results here show empirical coverage of the estimated confidence intervals, as measured over 200 randomly sampled datasets (each dataset is then resampled repeatedly for computing bootstrap estimates). We find that DM with bootstrapping is able to achieve near-correct empirical coverage as the dataset size grows. As suggested by the theory, the bootstrap typically underestimates the desired coverage, and this is severe in low-data regimes (when the number of episodes is less than 50).

We show the results of using noisy rewards to combat this low-data issue. We perturb the rewards with $R_{\text{noise}} = 0.25 \cdot \sqrt{\text{Var}_D [r]}$. The resulting difference in performance in the low-data regime is striking; DM with noisy bootstrap is able to yield near-optimal coverage, although, as expected, it typically slightly overestimates the desired coverage.

As a point of comparison, we plot a number of other high-confidence policy evaluation methods: IS with bootstrapping, IS with empirical Bernstein’s, IS with Student’s $t$, IS with Hoeffding’s, and doubly robust (DR) IS with bootstrapping (see [36, 37, 11]). We find that all of these previous methods mostly either severely underestimate or severely overestimate the desired coverage. There is a potential for our proposed noisy rewards to be beneficial for some of these baselines as well (e.g., DR bootstrap), and this is a promising avenue for future work.

5.2 Continuous Control Tasks

We now evaluate the use of bootstrapping on continuous control tasks from OpenAI gym. Due to high computational demands, we focus on Reacher, HalfCheetah, and Hopper. We follow a protocol

\[^4\text{In finite domains, Assumption 2 reduces to } d^n(s, a) > 0 \Rightarrow d^P(s, a) > 0.\]
We have investigated the validity of Efron’s bootstrap for computing confidence intervals with respect to the direct method (DM) for off-policy evaluation. Our theoretical results show that Efron’s bootstrap is valid given that specific conditions – sufficient data size and sufficient coverage – are satisfied. While these conditions are often not satisfied in practice, there are a number of heuristic mechanisms that can be employed to mitigate their effects, although at a cost of overly conservative or biased intervals. Still, empirically we find that these mechanisms can be used to yield impressive performance for OPE in challenging environments. In the future, we hope to use the ideas and

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3DR with bootstrap produces even worse intervals, and so we do not plot it.
techniques presented here and apply them to policy optimization problems, where safety is also a key concern.

**Broader Impact**

Our work focuses on the practically relevant problem of off-policy evaluation. Interestingly, our work reveals the potential issues with applying a well-known technique – Efron’s bootstrap – without considering its validity. Our work shows that Efron’s bootstrap may often not be valid. Although we propose mechanisms to remedy this, our solutions are not fool-proof. In a practical setting, where many of our assumptions may not hold, one must take special care when applying our method to mitigate risks of failure.

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A Proofs

A.1 Hadamard Differentiability

We provide a definition of Hadamard differentiability, which is a key property for showing validity of Efron’s bootstrap. The following is paraphrased from [40].

Definition 1. Suppose \( F \) is a functional mapping distributions over \( \mathcal{P} := \mathcal{S} \times \mathcal{S} \times \mathcal{A} \times \mathbb{R} \times \mathcal{S} \) (i.e., distributions of tuples \((s_0,s,a,r,s')\)) to \( \mathbb{R} \). Denote \( \mathcal{P}_L \) as the the linear space generated by \( \mathcal{P} \). The functional \( F \) is said to be **Hadamard differentiable** at \( d^D \in \mathcal{P} \) if there exists a linear functional \( L_{d^D} \) on \( \mathcal{P}_L \) such that for any \( \epsilon_n \) and \( P, P_1, P_2, P_3, \ldots \in \mathcal{P}_L \) such that \( \|P_n - P\|_\infty \to 0 \) and \( d^D + \epsilon_n P_n \in \mathcal{P}_L \),

\[
\lim_{n \to \infty} \left| \frac{F(d^D + \epsilon_n P_n) - F(d^D)}{\epsilon_n} - L_{d^D}(P) \right| = 0. \tag{14}
\]

A.2 Proof of Theorem 1

As in the main text, we use \( \bar{\mu}_0^D, \bar{\mathcal{R}}_{\bar{D}}, \bar{T}_{\bar{D}} \) to denote the initial state, conditional reward, and conditional transition distributions observed in \( d^D \). Furthermore, let \( \bar{\mathcal{R}}_{\bar{D}} = \mathbb{E}_{\bar{R}_{\bar{D}}}[r] \). For ease of notation, we will use matrix notation and assume finite state and action spaces (an extension to Hilbert spaces with linear operators is straightforward). The functional \( F \) may be expressed as,

\[
F(d^D) := (1 - \gamma) \cdot \bar{\mathcal{R}}_{\bar{D}}^T (I - \gamma \bar{T}_{\bar{D}})^{-1} \bar{\Pi} \mu_0^D, \tag{15}
\]

where we use \( \bar{\Pi} \) to denote the matrix mapping distributions over states to distributions over state actions, where actions as sampled by \( \pi \).

Note that, assuming \( d^\pi(s,a) > 0 \Rightarrow d^D(s,a) > 0 \), the components of this expression for \( F \) at \( d^D = d^D \) yield the \( Q^\pi \)-values and on-policy distribution \( d^\pi \). Specifically,

\[
d^\pi = (1 - \gamma)(I - \gamma \bar{\Pi} \bar{T})^{-1} \bar{\Pi} \mu_0, \tag{16}
\]

\[
Q^\pi = \bar{\mathcal{R}}_{\bar{D}}^T (I - \gamma \bar{T})^{-1}. \tag{17}
\]

For general \( d^D \), these expressions will yield \( d^\pi_{\bar{D}} \), the on-policy distribution in the empirical MDP, and \( Q^\pi_{\bar{D}} \), the \( Q^\pi \) values in the empirical MDP, respectively.

As mentioned in the proof sketch, the validity of Theorem 1 rests on the Hadamard differentiability of \( F(d^D) \) for all \( d^D \) in a neighborhood around \( d^D \). In addition to local Hadamard differentiability, one must also have that the derivative linear functional \( L_{d^D} \) satisfy

\[
0 < \mathbb{E}_{(s_0,s,a,r,s') \sim d^D} [L_{d^D}(\delta_{(s_0,s,a,r,s')} - d^D)^2] < \infty. \tag{18}
\]

See Theorems 3.19 and 3.21 in [40] for more information. In the text below, we will show that \( F \) is indeed Hadamard differentiable with derivative satisfying

\[
L_{d^D}(\delta_{(s_0,s,a,r,s')} - d^D) = O(d^\pi(s,a)/d^D(s,a)). \tag{19}
\]

The result 19 in conjunction with Assumption 2 will immediately make it clear that \( \mathbb{E}_{(s_0,s,a,r,s') \sim d^D} [L_{d^D}(\delta_{(s_0,s,a,r,s')} - d^D)^2] < \infty \). Moreover, the linear nature of the functional \( F \) with respect to \( \mathcal{R}_{\bar{D}} \) makes it clear that \( 0 < \mathbb{E}_{(s_0,s,a,r,s') \sim d^D} [L_{d^D}(\delta_{(s_0,s,a,r,s')} - d^D)^2] \), thus showing the validity of the bootstrap.

We now continue to characterize the linear functional \( L_{d^D} \). We will first derive, via standard Frechet differentiation, the derivatives of \( F(d^D) \) with respect to \( \mathcal{R}_{\bar{D}}, \mu_0^D \), and \( T_{\bar{D}} \), for \( d^D \) that satisfy Assumption 1. We will later use these results in conjunction with Assumption 2 to show the Hadamard differentiability of \( F \) with respect to \( d^D \) in a ball around \( d^D \).

- \( \mathcal{R}_{\bar{D}} \): It is clear from (16) that \( \partial F/\partial \mathcal{R}_{\bar{D}} = d^\pi_{\bar{D}} \).
- \( \mu_0^D \): It is clear from (17) that \( \partial F/\partial \mu_0^D = (1 - \gamma)Q^\pi_{\bar{D}} \bar{\Pi} \). 

...
We may see that each of these influences on $F$ with respect to $\Pi$, we may apply it here, interpreting $T_{\tilde{D}}$ as the stationary "policy" whose gradient we wish to calculate ("transitions" are now between state-action pairs and the "actions" are choices of next states). Specifically, we may re-write (15) as

$$K + (1 - \gamma) \cdot (R^T_{\tilde{D}} \Pi)(I - \gamma T_{\tilde{D}} \Pi)^{-1} T_{\tilde{D}} (\Pi \mu_{\tilde{D}}),$$

(20)

where $K$ is constant with respect to $T_{\tilde{D}}$. This way, we deduce that $\frac{dF}{dT_{\tilde{D}}(s|s,a)} = d\pi_{\tilde{D}}(s, a) \cdot \mathbb{E}_{\alpha' \sim \pi(s')} [Q^\pi_{\tilde{D}}(s', a')]$ for all $s, a, s'$. With these three partial derivatives calculated, we may continue to show differentiability of $F$ in a neighborhood around $d\tilde{D}$. Without loss of generality, we assume that $d\tilde{D}$ has full support; if not, we may simply ignore all tuples outside of the support, since they do not affect $\rho(\pi)$ or $\rho_{DM}(\pi)$ (note that by Assumption 2, this means $d\tilde{D}$ also has full support).

Now we continue to characterize the derivative of $F$. Denote the derivative of $F$ by $F'$, where $F'(d\tilde{D})$ is defined to be the linear functional satisfying,

$$\left\langle F'(d\tilde{D}), \delta(s_0, s_0', a_0, r_0, s_0') - d\tilde{D} \right\rangle = \lim_{t \to 0} \frac{1}{t} \left( F((1 - t) \cdot d\tilde{D} + t \cdot \delta(s_0, s_0', a_0, r_0, s_0')) - F(d\tilde{D}) \right),$$

(21)

for all tuples $(s_0, s_0', a_0, r_0, s_0')$. We analyze the behavior of these directional limits. We again split our analysis into three parts:

- **Influence of $r^*$.** The influence of $r^*$ is in the empirical average reward function at $s^*, a^*$: $R_{\tilde{D}}(s^*, a^*)$. At a change of $t$, this value is updated to

$$\frac{(1 - t)d\tilde{D}(s^*, a^*)R_{\tilde{D}}(s^*, a^*) + tr^*}{(1 - t)d\tilde{D}(s^*, a^*) + t}.$$  

(22)

The derivative of this expression at $t = 0$ is $-\frac{R_{\tilde{D}}(s^*, a^*) + r^*}{d\tilde{D}(s^*, a^*)}$. Combined with the partial derivative computed earlier, we find the total influence on $F$ is $\frac{d\pi_{\tilde{D}}(s^*, a^*)}{d\tilde{D}(s^*, a^*)} (\frac{R_{\tilde{D}}(s^*, a^*) + r^*}{d\tilde{D}(s^*, a^*)}) \cdot t$ as $t \to 0$.

- **Influence of $s_0$.** The influence of $s_0$ is in the empirical initial state distribution $\mu_{\tilde{D}}(s_0)$, which is updated to $(1 - t)\mu_{\tilde{D}} + t\delta_{s_0}$. To deduce the influence on $F$, we combine with the partial derivative computed earlier, and find the change in $F$ to be

$$\left( -\rho_{DM}(\pi|d\tilde{D}) + (1 - \gamma)\mathbb{E}_{a_0 \sim \pi(s_0)} [Q^\pi_{\tilde{D}}(s_0, a_0)] \right) \cdot t.$$  

- **Influence of $s^*$.** As for the reward, the influence here is in the empirical transition probabilities $T_{\tilde{D}}(s'|s^*, a^*)$, which is updated to

$$\frac{(1 - t)d\tilde{D}(s^*, a^*)T_{\tilde{D}}(s'|s^*, a^*) + t\delta_{s^*}(s')}{(1 - t)d\tilde{D}(s^*, a^*) + t}.$$  

(23)

The derivative of this expression at $t = 0$ is $-\frac{T_{\tilde{D}}(s'|s^*, a^*) + \delta_{s^*}(s')}{d\tilde{D}(s^*, a^*)}$. Combining this with the known partials of $F$ with respect to $T_{\tilde{D}}$, we find that the total influence on $F$ is $\frac{d\pi_{\tilde{D}}(s^*, a^*)}{d\tilde{D}(s^*, a^*)} \left( -\mathbb{E}_{s' \sim T_{\tilde{D}}(s^*, a^*)} [Q^\pi_{\tilde{D}}(s', a')] + \mathbb{E}_{a' \sim \pi(s')} [Q^\pi_{\tilde{D}}(s', a')] \right) \cdot t$ as $t \to 0$.

We may see that each of these influences on $F$ are linear in $t$. By Assumption 1, $r^*$ is uniformly bounded, as are $R_{\tilde{D}}$ and $Q^\pi_{\tilde{D}}$. Thus, in conjunction with the Riesz representation theorem, we deduce that the derivative $F'$ satisfies

$$\|F'(d\tilde{D})\|_\infty = O \left( \left\| \frac{d\pi_{\tilde{D}}}{d\tilde{D}} \right\|_\infty \right).$$  

(24)
Now consider an arbitrary distribution $d\tilde{\pi}$ and the directional limit
\[ \lim_{t \to 0} \frac{1}{t} \left( F((1 - t) \cdot d\tilde{\pi} + t \cdot d\tilde{\pi}) - F(d\tilde{\pi}) \right). \tag{25} \]

Analogous to the derivations above, we may find,

- The empirical average reward $R_{d\tilde{\pi}}(s, a)$ at a change of $t$ is updated to
  \[ \frac{(1 - t)d\tilde{\pi}(s, a)R_{d\tilde{\pi}}(s, a) + td\tilde{\pi}(s, a)\tilde{R}(s, a)}{(1 - t)d\tilde{\pi}(s, a) + td\tilde{\pi}(s, a)}. \tag{26} \]

- The empirical initial state distribution at a change of $t$ is updated to
  \[ (1 - t)\mu_0^D + t\mu_0^\tilde{\pi}. \tag{27} \]

- The empirical transition probabilities $T_{d\tilde{\pi}}(s'|s, a)$ at a change of $t$ are updated to
  \[ \frac{(1 - t)d\tilde{\pi}(s, a)T_{d\tilde{\pi}}(s'|s, a) + td\tilde{\pi}(s, a)\tilde{T}(s'|s, a)}{(1 - t)d\tilde{\pi}(s, a) + td\tilde{\pi}(s, a)}. \tag{28} \]

By considering the limits of (26), (27), (28) as $t \to 0$, it is clear that
\[ \langle F'(d\tilde{\pi}), d\tilde{\pi} - d\tilde{\pi} \rangle = \lim_{t \to 0} \frac{1}{t} \left( F((1 - t) \cdot d\tilde{\pi} + t \cdot d\tilde{\pi}) - F(d\tilde{\pi}) \right). \tag{29} \]

To show Hadamard differentiability, we invoke Assumption 2, which implies that there exists a sufficiently small $\zeta = \epsilon/2$ such that the $L_\infty$ ball centered at $d\tilde{\pi}$ with radius $\zeta$ has uniformly bounded $\|d\pi/d\tilde{\pi}\|_\infty$. Since the support of $d\tilde{\pi}$ is contained within the support of $d\pi$, this means that the same ball has uniformly bounded $\|d\pi/d\tilde{\pi}\|_\infty$. Moreover, it is clear that within this ball $d\tilde{\pi} > \epsilon/2$ uniformly, and so the directional derivatives of (26), (27), and (28) converge uniformly with $t \cdot \|d\tilde{\pi}\|_\infty$. Thus, there exists a sufficiently small ball around $d\pi$ within which $F$ is Hadamard differentiable. This completes our proof.

### A.3 Proof of Theorem 2

First, a brief sketch: If Assumption 3 does not hold, then for any $L_\infty$ ball, one may find a distribution near $d\tilde{\pi}$ outside of the support of $\pi$, and this will cause discontinuities in $F$.

Now more concretely: Consider an MDP with state space $\{s_{\text{start}}, s_{\text{term}}, s_1, s_2, \ldots\}$. The MDP’s initial state distribution is $\mu_0 := \delta_{s_{\text{start}}}$. The MDP has a single action $a$ and the transition function is defined as,
\[ T(s_n|s_{\text{start}}, a) = \frac{6}{\pi^2 + \pi^2}, \tag{30} \]
\[ T(s_{\text{start}}|s_{\text{start}}, a) = 0, \tag{31} \]
\[ T(s_{\text{term}}|s_{\text{start}}, a) = 0, \tag{32} \]
\[ T(s_n, a) = \delta_{s_{\text{term}}}, \tag{33} \]
\[ T(s_{\text{term}}, a) = \delta_{s_{\text{term}}}. \tag{34} \]

The reward function is defined as
\[ R(s_{\text{start}}, a) = \delta_0, \tag{35} \]
\[ R(s_n, a) = \delta_0, \tag{36} \]
\[ R(s_{\text{term}}, a) = \delta_1. \tag{37} \]

Define prior reward and transition functions
\[ T_{\text{prior}}(s, a) := \delta_{s_{\text{term}}}, \tag{38} \]
\[ R_{\text{prior}}(s, a) := \delta_1. \tag{39} \]
Let policy $\pi$ be a policy on this MDP (there exists only one). Consider $\gamma = 0.5$. Thus we have

$$\rho(\pi) = \frac{1}{4},$$  \hspace{1cm} (40)$$

$$d^{\pi}(s, a) = \frac{3}{2\pi^2n^2}.$$  \hspace{1cm} (41)$$

Let $d^D$ be defined as $d^D := d^{\pi}$. It is clear that $d^D$ satisfies $||d^{\pi}/d^D||_\infty = 1 < \infty$ but that Assumption 2 does not hold.

Now consider any $L_\infty$ ball around $d^D$. Suppose this ball has radius $\zeta > 0$ and let $N$ be such that $\frac{3}{2\pi^2N^2} < \zeta$. We may define the distribution

$$d^\hat{D} := d^D - \frac{3}{2\pi^2N^2} \delta(s_{start}, s_N, a, 0, s_{term}) + \frac{3}{2\pi^2N^2} \delta(s_{start}, s_{term}, a, 1, s_{term}).$$  \hspace{1cm} (42)$$

It is clear that $d^\hat{D}$ is within the $L_\infty$ ball and $d^\hat{D}(s, a) = 0$. Thus, $R_{D}^\hat{D}(s, a) = R_{\text{prior}}$ and so

$$F(d^\hat{D}) = \frac{1}{4} + \frac{3}{2\pi^2N^2}.$$  \hspace{1cm} (43)$$

Now we define

$$P := \delta(s_{start}, s_1, a, 0, s_{term}) - d^\hat{D},$$  \hspace{1cm} (44)$$

$$\epsilon_n := \frac{1}{n}.$$  \hspace{1cm} (45)$$

It is clear that a change $d^\hat{D} \rightarrow d^\hat{D} + \epsilon_n \cdot P$ would not change the empirical reward or transition functions, and so we have,

$$\lim_{n \to \infty} \frac{1}{\epsilon_n} (F(d^\hat{D} + \epsilon_n \cdot P) - F(d^\hat{D})) = 0.$$  \hspace{1cm} (46)$$

We may also consider a sequence $\{P_n\}_{n=1}^\infty$ defined as

$$P_n := \frac{1}{n} \cdot \delta(s_{start}, s_N, a, 0, s_{term}) + \left(1 - \frac{1}{n}\right) \delta(s_{start}, s_{term}, a, 1, s_{term}) - d^\hat{D}.$$  \hspace{1cm} (47)$$

Clearly $\lim_{n \to \infty} P_n = P$. However, $P_n$ changes the empirical reward distribution at $(s_N, a)$, and this causes

$$\lim_{n \to \infty} \frac{1}{\epsilon_n} (F(d^\hat{D} + \epsilon_n \cdot P_n) - F(d^\hat{D})) = \lim_{n \to \infty} \frac{1}{\epsilon_n} \cdot \frac{3}{2\pi^2N^2} = \infty.$$  \hspace{1cm} (48)$$

Thus, $F$ is not Hadamard differentiable at $d^\hat{D}$.

### A.4 Proof of Theorem 3

We prove a more useful generalization of this theorem, stated below:

**Generalized Theorem** Suppose $R_{D}^\pi$, $T_{D}^\pi$ are reward and transition probability functions defined with respect to general distributions $d^D$ and that these functions are differentiable with respect to $d^D$ in a neighborhood around $d^D$ with uniformly bounded derivatives. Under Assumption 1, the use of Algorithm 1 with $F(d^D) := \rho_{\text{DM}}^\pi(D_n)$ yields confidence intervals $C(d^D)$ which are asymptotically correct, since in the sense that

$$\Pr[\rho_{\text{DM}}^\pi(D_n) \in C(d^D)] = 1 - \alpha - O_{p}(n^{-1/2}).$$  \hspace{1cm} (49)$$

As for Theorem 1, the one-sided intervals converge at a rate $O_{p}(n^{-1/2})$ and these rates may be improved by using more sophisticated bootstrapping methods.

**Proof** The proof is straightforward given the derivations in Section A.2. Specifically, analogous to Section A.2 one may readily show that

$$\frac{\partial F}{\partial R_{D}^\pi} = d^D_{\pi},$$  \hspace{1cm} (50)$$

$$\frac{\partial F}{\partial T_{D}^\pi(s,a)} = d^D_{\pi}(s, a) \cdot \mathbb{E}^\pi_{s \sim \pi} [Q^\pi_{D}(s', a')] \mathbb{E}^\pi_{s \sim \pi} [Q^\pi_{D}(s', a')].$$  \hspace{1cm} (51)$$

Using chain rule with the assumption of differentiability of $R_{D}^\pi$, $T_{D}^\pi$ then immediately shows that $F'$ is well-defined and thus $F$ is appropriately differentiable around $d^D$.

15
A.5 Additional Experiments

In this section we provide additional experiments for Model Based Policy Evaluation. In particular, we demonstrate that the scale of the noise has a similar effect for MB policy evaluation as for Fitted Q-Evaluation (see Figure 4).

![Figure 4: Additional results for MB. We plot different the confidence interval for different values of the noise scale.](image)

A.6 Experimental Details

For the ease of reproducibility we provide details of our experimental setup. For all methods we normalize the states and rewards to have mean of 0 and standard deviation of 1. We normalize the terminating rewards accordingly. For all neural networks we use orthogonal initialization.

**Fitted Q-Evaluation** We use 2 layer MLP with 256 hidden units and perform standard TD-0 policy evaluation. In order to compute the target value for FQE, we use target networks that are updated using Polyak averaging with $\tau = 0.005$ as in [19]. For the results we plot predictions from the target network.

**Model based policy evaluation** We perform model based policy evaluation as described in [10]. We found that to make the algorithm stable in low data regime, it is crucial to apply L2 regularization and clip states and rewards generated by the models to the limits observed in the training data. The forward model predicts offset from the current state: $f_\theta(s, a) \rightarrow s' - s$ and trained by optimizing a mean squared error $\frac{1}{N} \sum_{i=1}^{N} (f_\theta(s_i, a_i) + (s_i - s'_i))^2$, while for rewards we train a model that regresses rewards directly $\frac{1}{N} \sum_{i=1}^{N} (g_\theta(s_i, a_i) - r_i)^2$. We also train a model that predicts terminating condition via binary classification.