A Study of Off-policy Learning in Computational Sustainability

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Abstract

Off-policy evaluation is the problem of evaluating a decision-making policy using data collected under a different behavior policy. While several methods are available for addressing off-policy problems, the existing literature does not offer much in terms of identifying the best-performing ones. In this paper, we conduct an in-depth comparative study of off-policy evaluation methods in non-bandit, finite-horizon MDPs, using a well-known Mallard population dynamics model (Anderson, 1975). We find that un-normalized importance sampling can exhibit prohibitively large variance in problems involving look-ahead longer than a few time steps, and that dynamic programming methods perform better than Monte-Carlo style methods.

1. Introduction

One of the core competencies of most intelligent decision-making agents is the ability to properly evaluate their decision-making strategy. In a reinforcement learning context, this is the policy evaluation problem, which involves the estimation of the expected return associated with a policy. The ideal method for evaluating policies is to apply them in practice, observe the return, and estimate the expected return (and its uncertainty) using this data. However, if data is expensive (or rare), or the number of policies to evaluate is large, this may be infeasible. A popular alternative is to evaluate the decision-making policy of interest (called the *target policy*) using data collected under a different, *behavior policy*. This method is known as *off-policy policy evaluation*. Off-policy learning has been used in a range of applications, such as energy systems (Hannah and Dunson, 2011), robotics (Riedmiller, 2005), clinical studies (Pineau et al., 2009), and tax collection (Abe et al., 2010).

Existing off-policy estimators for discrete MDPs take two forms: model-based (Sutton and Barto, 1998; Mannor et al., 2007), and importance sampling weighting of the returns (Precup et al., 2000; Robins et al., 2000; Murphy, 2005). Methods for continuous MDPs that would fall in neither category, such as LSTD, can be shown to reduce to a model-based estimator in the discrete setting (Boyan, 2002). In this paper, we study the empirical bias and variance of existing model-based and importance sampling estimators. We also propose two new estimators, per-step importance sampling and normalized per-step importance sampling, which are extensions of existing importance sampling methods that aim to reduce variance by taking advantage of the Markov property.

Previous comparative studies for off-policy estimators considered single-step contextual bandit problems (Kang and Schafer, 2007; Dudik et al., 2011). We present an empirical study for finite-horizon discrete MDPs with arbitrary horizon length (thus avoiding problems generated by a non-Markovian state representation). We study the performance of the different off-policy estimators on a natural resource management problem. Running controlled experiments in the real world

for such problems ranges from difficult to downright unfeasible, so we use a simulated model of the Mallard population dynamics first proposed by Anderson (1975) and subsequently used by Fonnesbeck (2005). In order to mimic the type of situation that would arise in practice, we use the model to generate the data, but do not provide any knowledge of the model to the estimation methods. This setup is sufficient to highlight key differences between the various methods.

2. Finite-horizon MDPs

We adopt the framework of finite-horizon MDPs, defined as a tuple $\langle S, A, P, R \rangle$, where S is a set of states; A is a set of actions; $P : S \times A \times S \to [0, 1]$ is the transition model, with $P_{sa}^{s'}$ denoting the conditional probability of a transition to state s' given current state s and action a; $R : S \times A \to [0, 1]$ is the reward function, with R_{sa} denoting the immediate expected reward for state s and action a. A policy $\pi : S \times A \to [0, 1]$ specifies how decisions are made. In a finite MDP, the model can be represented using matrices $P \in \mathbb{R}^{|S\times A|\times|S|}$ and $R \in \mathbb{R}^{|S\times A|}$. Similarly, policies can also be represented as block-diagonal matrices $\pi \in \mathbb{R}^{|S|\times|S\times A|}$.

The value of a policy π for a decision horizon of length K is defined as:

$$V_K^\pi(s) = E[r_0 + r_1 + \cdots + r_K | s_0 = s] = \sum_a \pi_{sa} \left(R_{sa} + \sum_{s'} P_{sa}^{s'} V_{K-1}(s') \right).$$

or, if we consider V_K^π to be the vector of all state values,

$$V_K^\pi = \pi(R + PV_{K-1}^\pi) = \cdots = \sum_{k=0}^{K} (\pi P)^k \pi R. \tag{1}$$

3. Off-policy value function estimation

In practice, the model of the MDP is usually unknown, so Eq. (1) cannot be applied directly. Furthermore, the user might not be able to obtain trajectories using policy π. In natural resource management, in particular, implementing a policy is not only expensive but also potentially unrealistic, given that we are often interested in time horizons that may span decades. Instead, the user may have access to data gathered under some existing policy b (or possibly, under several known policies from different geographic regions or different periods). Off-policy value function estimation methods are designed to deal with this case.

All estimators used in this paper are summarized in Table 3. We will now describe the notation and context for each of them.

Importance sampling (Rubinstein, 1981) is a technique for sampling from one distribution by weighting the samples generated from another distribution. It has been proposed as an off-policy estimator for MDPs both in reinforcement learning (Precup et al., 2000) and in the clinical trial literature (Robins et al., 2000), where it is called inverse probability weighting. Importance sampling methods typically assume that the behavior policy used to collect the data, denoted b, is known, and that $\pi_{sa} > 0 \implies b_{sa} > 0$. The naive implementation of importance sampling for off-policy evaluation weights entire trajectories. This existing estimator is the (un-normalized) *per-trajectory importance sampling* (PTIS) in Table 3. It is computed based on n_s trajectory fragments of length K that start from state s in the batch, where the i^{th} trajectory is denoted by:

$$(s_{i:0} = s, a_{i:0}, r_{i:0}, s_{i:1}, a_{i:1}, r_{i:1}, ..., s_{i:K}, a_{i:K}, r_{i:K}),$$

	Un-normalized	Normalized
Per-trajectory importance sampling	$\hat{V}_K^{PTIS}(s) = \frac{1}{n_s}\sum_{i=1}^{n_s}\left(\prod_{j=1}^{K}\frac{\pi(s_{i:j},a_{i:j})}{b(s_{i:j},a_{i:j})}\right)\sum_{l=1}^{K} r_{i:l}$	Instead of n_s, divide by $\sum_{i=1}^{n_s}\left(\prod_{j=1}^{K}\frac{\pi(s_{i:j},a_{i:j})}{b(s_{i:j},a_{i:j})}\right)$
Per-step importance sampling	$\hat{V}_k^{PSIS}(s) = \frac{1}{n_s}\sum_a \frac{\pi_{sa}}{b_{sa}} \sum_{i\in B(s,a)} [r_i + \hat{V}_{k-1}^{PSIS}(s'_i)]$	Instead of n_s, divide by $\sum_{i\in B(s)}\frac{\pi(s,a_i)}{b(s,a_i)} = \sum_a n_{sa}\frac{\pi_{sa}}{b_{sa}}$
Model-based	$\hat{V}_K^{MB}(s) = \sum_a \pi_{sa}\left(\hat{R}_{sa} + \sum_{s'}\hat{P}_{sa}^{s'}\hat{V}_{K-1}^{MB}(s')\right) = \sum_{k=0}^{K}(\pi\hat{P})^k\pi\hat{R}$	

Table 1: Off-policy estimators for discrete MDPs. **All methods are consistent, but (un-normalized) per-trajectory importance sampling is the only one that is unbiased.**

The weights in the importance sampling estimator can be scaled to the $[0, 1]$ interval by normalizing over their sum. This is seen as a way to reduce estimator variance, and leads to the *normalized per-trajectory importance sampling estimator* in Table 3, which we will denote by $\hat{V}^{PTIS-N}$. This is also an existing estimator (Precup et al., 2000; Murphy, 2005).

In order to avoid the variance introduced by weighting entire trajectories, we introduce *per-step importance sampling* as an alternative. Consider the more general setting where a sample i is composed of start state s_i, action a_i generated from b at s_i, and (r_i, s'_i) the response of the model (P, R) at (s_i, a_i). The (un-normalized) *per-step importance sampling estimator*, shown in Table 3, uses n_s, n_{sa}, and $n_{sas'}$ to denote the sizes of the subsets restricted by the start state s, action a and/or next state s', and $B(s)$ and $B(s, a)$ to denote the subsets of samples for which the start state and/or action choice is s, a. If $n_s = 0$, there is no data at this state, so we have to pre-define $\hat{V}_k^{PSIS}(s)$. We also constructed a normalized version, which we will denote by $\hat{V}_K^{PSIS-N}$.

The estimators in (Precup et al., 2000) are similar to the per-step estimators proposed here, but introduce an additional weight on the trajectory *prior* to a state (rather than just weighting the next step). This initial weighting can further increase variance, and is not required in order to obtain a consistent estimator in discrete MDPs.

Model-based MDP estimators construct approximations $\hat{P}$ and $\hat{R}$ of the transition and reward model, and then use standard methods such as dynamic programming to compute the value function for the estimated model. For discrete MDPs, consistent estimators of the model are given by:

$$\hat{R}_{sa} = \frac{1}{n_{sa}}\sum_{i\in B(s,a)} r_i, \qquad \hat{P}_{sa}^{s'} = \frac{n_{sas'}}{n_{sa}}. \tag{2}$$

Similarly to per-step importance sampling, we have to use a pre-defined value if $n_s = 0$ or $n_{sa} = 0$. The finite-horizon value function can then be estimated using the approximate model $\hat{R}, \hat{P}$.

This estimator is intuitive and has a long history. However, we are only aware of one work on its statistical properties, by Mannor et al. (2007). For infinite-horizon discrete MDPs with discounting, Mannor et al. (2007) compute second-order approximations for the bias and variance of the model-based estimator, and examine its empirical performance on a discretized version of a catalog ordering problem.

Note that the MB estimator can be expressed in the same form as the per-step importance sampling estimators, but with an estimate of b as surrogate:

$$\hat{V}_k^{MB}(s) = \frac{1}{n_s} \sum_a \frac{\pi_{sa}}{n_{sa}/n_s} \sum_{i \in B(s,a)} \left(r_i + \hat{V}_{k-1}^{MB}(s_i') \right) \tag{3}$$

Results from (Rubinstein, 1981) can be used to show that both PTIS and PTIS-N are consistent estimators. PTIS is also unbiased; however, normalization can introduce bias, while typically reducing variance. The dynamic programming estimators (PSIS, PSIS-N and MB) are also consistent. This can be proven using Slutsky's theorem (Dudewicz and Mishra, 1988), by noting that all of them can be written in the form

$$\hat{V}_K = \sum_{k=0}^{K} (\pi Z \hat{P})^k \pi Z \hat{R}, \tag{4}$$

where Z is a diagonal matrix with entries

$$Z_{sa}^{PSIS} = (n_{sa}/n_s)/b_{sa} \qquad Z_{sa}^{PSIS-N} = (n_{sa}/W(s))/b_{sa} \qquad Z_{sa}^{MB} = 1,$$

with $W(s)$ denoting the normalization term for PSIS-N.

4. Empirical results

In this section we study the empirical performance of the different off-policy estimators on a natural resource management problem. In order to make sure that our error estimates are not affected by extraneous factors, we need a controlled experiment, whereby we can measure the performance of the target policy precisely, and compare this to estimates obtained using the off-policy algorithms. Hence, we use a simulated model, described below.

4.1. Mallard population model

Anderson's model is formulated as a Markov Decision Process with yearly time increments, two-dimensional state, and continuous actions. The state variables are the adult population N_t and the number of ponds P_t (both expressed in millions), while the action H_t represents the proportion of animals to be harvested in year t. The state transitions are defined by the following equations:

$$N_{t+1} = N_t(1 - 0.37e^{2.78H_t}) + \left(\frac{1}{12.48} P_t^{0.851} + \frac{0.519}{N_t} \right)^{-1} (1 - 0.49e^{0.9H_t})$$
$$P_{t+1} = -2.76 + 0.391P_t + 0.233\epsilon_t$$

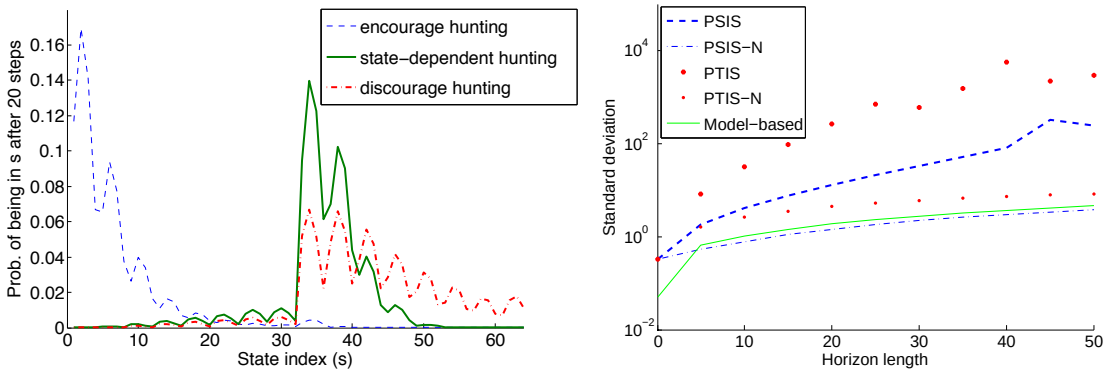
where $\epsilon_t \sim N(16.46, 4.41)$ is a normally distributed random variable describing the amount of precipitation during year t (in inches). The reward is defined as the number of birds harvested in a given year, computed as

$$R(N_t, P_t, H_t) = H_t \left(0.92 N_t + \left(\frac{1}{12.48} P_t^{0.851} + \frac{0.519}{N_t} \right)^{-1} \right).$$

Anderson constructed and validated this model based on real data about the evolution of the Mallard population. For more details, including model justification, we refer the reader to (Anderson, 1975).

For our experiments, we used a discretized version of the model. Since the states where the bird population is close to 0 are particularly important, we used a discretization with higher resolution in that region of the state space. More precisely, we divided N_t into intervals of length 2 when $N_t > 2$, and length 0.25 when $N_t \leq 2$. P_t was divided into four intervals of unit length. We also assumed that state features are bounded, so $N_t \in [0, 17]$ and $P_t \in [0, 4]$. This resulted in 64 states. We generated 10 million transitions from the original MDP by sampling starting states uniformly randomly; then, we used the data to estimate a transition matrix and reward function for the discrete MDP. The transition function was estimated using maximum likelihood estimation, whereas the reward function was defined as a Gaussian for each discretized interval, with its mean and variance estimated from the generated data. This produced the MDP that we used as "ground truth"; that is, we investigated how well our methods estimate the value function for this discretized MDP.

4.2. Experimental setup



(*a*) Probabilities of being in different states after 20 steps, under the three different policies

(*b*) Standard deviations of the three estimators based on a 500-sample trajectory with *state-dependent hunting* as the target.

Figure 1: State probabilities (left) and standard deviations of three estimators (right). Results averaged over $100,000$ runs. Note the logarithmic scale for the y axis in the right panel.

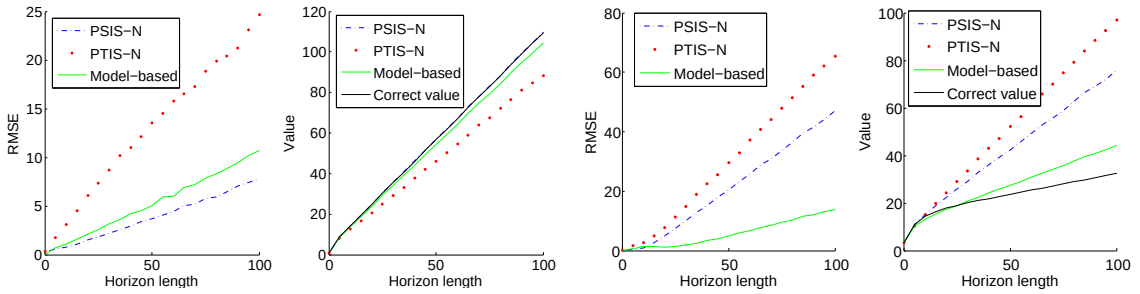
We considered three policies, all selecting from two actions: a_1 representing $H_t = 0$ and a_2 representing $H_t = 0.3$. The first policy, which we call *discourage hunting*, selects a_1 with probability 0.2 and a_2 with probability 0.8. The second policy, which we call *state-dependent hunting*, prescribes reduced hunting when the mallard population or the number of ponds is low, and larger amounts of hunting otherwise; more precisely, it selects a_1 with probability 0.8 in the

discrete states corresponding to $[0, 12] \times [0, 1]$, $[0, 8] \times [1, 2]$, $[0, 4] \times [2, 3]$, and $[0, 2] \times [3, 4]$, and a_2 with probability 0.8 for the rest of the state space. The third policy, called *encourage hunting*, selects a_2 with probability 0.8 in all states. Throughout the experiments, we used *discourage hunting* as the behavior policy, and used the discrete state corresponding to $N_t = 7$ and $P_t = 1.5$ as the starting state s_0. Each batch of training data was generated as a single, uninterrupted trajectory starting in s_0, with actions selected according to the behavior policy. Hence, the number of samples in a batch is the length of this trajectory. We present results estimating the value of the start state s_0 under all policies. Unless otherwise specified, the results are averages over 1000 batches.

As seen in Figure 1(a), the three policies tend to visit different regions of the state space. In particular, the distribution of states under *encourage hunting* leads predominantly to states corresponding to low population numbers, which is very different from the other two policies. Intuitively, this discrepancy should make estimating the value function for *encourage hunting* particularly challenging, given that *discourage hunting* is used as the behavior policy. This intuition is confirmed by our empirical results.

4.3. Bias and variance

Figure 1(*b*) contains a plot of the standard deviations of the different estimators when *state-dependent hunting* is the target policy. Even for a target policy that induces a state distribution fairly close to the one under the behavior policy, PSIS and PTIS can have very large variance for horizons longer than a few time steps.



(*a*) RMSE and bias for various horizons and batches of 500 samples each, using *state-dependent hunting* as the target policy.

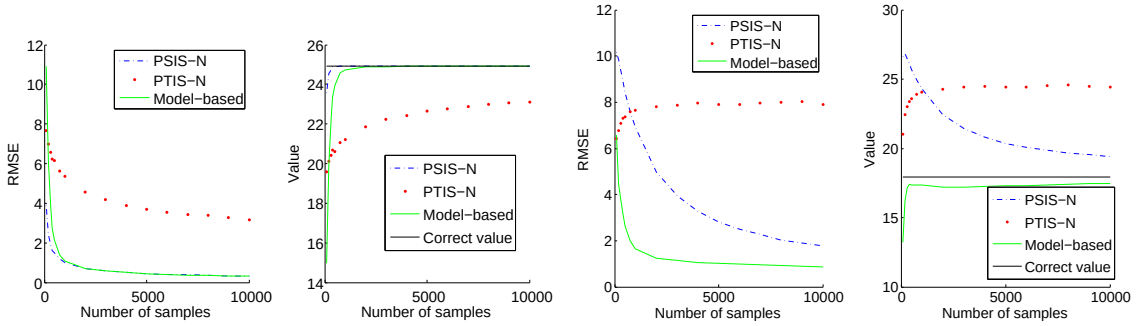
(*b*) RMSE and bias for various horizons and batches of 500 samples each, using *encourage hunting* as the target policy.

Figure 2: RMSEs and biases of different estimators as a function of the horizon.

For the remainder of this section, we further investigate the performance of PSIS-N, PTIS-N, and MB. We examine the performance of these three estimators in terms of bias and root mean squared error, when either *state-dependent hunting* or *encourage hunting* is the target policy. Figure 2 illustrates how the length of the horizon affects performance. The performance of all methods degrades as the horizon increases. This is expected, as increasing the horizon while maintaining the same number of samples means that we effectively have fewer samples per time step, which increases the variance. However, the rates at which performance degrades differ: when *state-dependent hunting* is the target policy, PSIS-N exhibits the slowest rate of degradation, whereas for *encourage hunting*, the model-based method is best. These results suggest that PSIS-N performs better when the behavior and target policies are relatively close, whereas MB deals better

with very different behavior and target policies. Given that MB can be viewed as estimating b, these results are intuitive from the point of view of existing statistical work on single-stage inverse probability weighting (Tsiatis, 2006).

PTIS-N exhibits the poorest performance in all settings. This is interesting, because PTIS-N is commonly used as an evaluation method in medical applications (Robins et al., 2000; Murphy, 2005). One reason for its use in such settings may be that sequential clinical trials typically have very short horizon lengths (two and three stage trials are common), and for such short horizons the difference between the methods' performance is not as large.



(*a*) RMSE and bias of the 20-step value function estimate for various sample sizes, using *state-dependent hunting* as the target policy.

(*b*) RMSE and bias of the 20-step value function estimate for various sample sizes, using *encourage hunting* as the target policy.

Figure 3: RMSEs and biases of different estimators as a function of the sample size. The RMSE and bias of PTIS-N also decreases eventually, but after orders-of-magnitude more samples.

For a particular horizon, we can get more insight into the methods' behavior if we examine the dependence of their performance on the amount of data available, as illustrated in Figure 3. As expected, the performance of both methods improves when increasing the size of the batch, although much slower if the target policy is very different from the behavior policy.

5. Discussion

We studied several off-policy learning algorithms, including two new estimators, PSIS and PSIS-N, that are per-step versions of importance sampling which take advantage of Markov assumptions about the model. We briefly discussed the estimators' bias and consistency, and presented a detailed empirical analysis of their performance in a case study pertaining to the management of an animal species. We found that the model-based estimator and the normalized per-step estimator (PSIS-N) performed particularly well.

We emphasize that the importance sampling estimators require a fixed and known behavior policy. If the behavior policy is instead estimated from data, we obtain the model-based estimator (as shown). Cases in which the data is gathered according to multiple behavior policies (e.g. gathered from different geographic locations), could also be easily incorporated in the estimators by appropriate weighting of the different data batches.

The bias and variance of the off-policy estimators were illustrated through the empirical results. From a theoretical standpoint, there are challenges in providing a formal analysis of the weighted estimators in the sequential case (horizon > 1). This is an interesting area for future work, though we expect it may be difficult to obtain closed-form expressions for these quantities.

As shown in our experiments, it is crucial to assess values for longer time horizons, as the horizon impacts the value of a policy, as well as the ordering of policies. Our results suggest that the horizon length should also be an important factor when choosing an estimator. Some decision-making domains, notably in medicine, deal with relatively short horizons, and in those cases estimators such as PTIS, which have large variance over long horizons but are unbiased, may be preferable. In domains with longer decision horizons, estimators such as PSIS-N tend to have lower error (though the error increases with horizon length).

We focused on discrete MDPs because such models are easier to interpret, hence often used in practice. In continuous MDPs, off-policy learning can also be applied, but generates further complications. In particular, the discrepancy between the probability of a trajectory under the behavior and the target policy cannot be ignored for estimators whose values are guaranteed to converge. Several algorithms have been proposed in order to account for trajectory distribution discrepancies. Precup et al. (2001) use importance sampling weights to correct for the probability of reaching a specific point in a trajectory. The resulting estimators are consistent (in the space of representable value functions) but tend to have high variance. Sutton et al. (2009) address the problem of off-policy learning from on-line data. The main idea is to estimate a secondary set of parameters (in addition to those describing the value function), which are used to stabilize the value function weights and prevent divergence. In discrete MDPs, however, all these estimators are more conservative and hence less sample-efficient than those we propose.

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