Efficiently Breaking the Curse of Horizon: Double Reinforcement Learning in Infinite-Horizon Processes

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Abstract

Off-policy evaluation (OPE) in reinforcement learning is notoriously difficult in long- and infinite-horizon settings due to diminishing overlap between behavior and target policies. In this paper, we study the role of Markovian, time-invariant, and ergodic structure in efficient OPE. We first derive the efficiency limits for OPE when one assumes each of these structures. This precisely characterizes the curse of horizon: in time-variant processes, OPE is only feasible in the near-on-policy setting, where behavior and target policies are sufficiently similar. But, in ergodic time-invariant Markov decision processes, our bounds show that truly-off-policy evaluation is feasible, even with only just one dependent trajectory, and provide the limits of how well we could hope to do. We develop a new estimator based on Double Reinforcement Learning (DRL) that leverages this structure for OPE. Our DRL estimator simultaneously uses estimated stationary density ratios and $q$-functions and remains efficient when both are estimated at slow, nonparametric rates and remains consistent when either is estimated consistently. We investigate these properties and the performance benefits of leveraging the problem structure for more efficient OPE.

1 Introduction

Off-policy evaluation (OPE) is the problem of estimating mean rewards of a given decision policy, known as the target policy, for a sequential decision-making problem using data generated by the log of another policy, known as the behavior policy (Jiang and Li, 2016; Li et al., 2015; Liu et al., 2018b; Mahmood et al., 2014; Munos et al., 2016; Precup et al., 2000; Thomas and Brunskill, 2016; Xie et al., 2019). Reinforcement learning in settings such as healthcare (Murphy, 2003) and education (Mandel et al., 2014) is often limited to the off-policy setting due to the inability to simulate and the costliness of exploration. OPE,
Table 1: Asymptotic order of the best-achievable MSE in each model. The variables $\nu_k$, $\mu_k$ are the cumulative and marginal density ratios, respectively, defined in Section 1.2.

| Model | Characteristics          | MSE Scaling | Assumptions                      |
|-------|--------------------------|-------------|----------------------------------|
| $\mathcal{M}_1$ (NMDP) | Non-Markov, Time-variant | $O(1/N)$   | $N \to \infty$, $T = \omega(\log^{1/2}(N))$ |
|       |                          |             | $\nu_k = o(\gamma^{-k})$        |
| $\mathcal{M}_2$ (TMDP)  | Markov, Time-variant    | $O(1/N)$   | $N \to \infty$, $T = \omega(\log^{1/2}(N))$ |
|       |                          |             | $\mu_k = o(\gamma^{-k})$        |
| $\mathcal{M}_3$ (MDP)   | Markov, Time-invariant  | $O(1/(NT))$| $T \to \infty$, $N \geq 1$       |
|       |                          |             | Ergodicity                       |

however, becomes increasingly difficult for problems with long and infinitely-long horizons \cite{Liu2018}. As the horizon grows, the overlap (i.e., inverse density ratios) between trajectories generated by the target and behavior policies diminishes exponentially. This issue has been noted as one of the key limitations for the applicability of RL in medical settings \cite{Gottesman2019}.

In this paper we study the fundamental estimation limits for OPE in infinite-horizon settings, and we develop new estimators that leverage special problem structure to achieve these limits and enable efficient and effective OPE in these problem settings. Specifically, we first derive what is the best-possible asymptotic mean squared error (MSE) that one can hope for in OPE in this setting. In order to study the effect of problem structure, we separately consider three different models: non-Markov decision processes (NMDP), time-varying Markov decision processes (TMDP), and time-invariant Markov decision processes (MDP). The differences between these bounds exactly characterizes the effect of taking into consideration additional problem structure on the feasibility of OPE.

Our bounds in the NMDP and TMDP models reveal an important phase transition: if the target and behavior policies are sufficiently similar (relative to the discount factor) then consistent estimation is feasible. Otherwise, there exist examples where it is infeasible. This can be understood as a phase transition between being sufficiently close to on-policy that OPE is feasible even in infinite horizons and being sufficiently off-policy that it is hopeless. We show that adaptations of the doubly robust (DR) estimator in NMDPs \cite{Jiang2016} and in MDPs \cite{Kallus2019} to the infinite horizon case achieve these bounds, i.e., are efficient in the near-on-policy setting.

Our bounds in the MDP models, on the other hand, give hope for OPE in the truly off-policy setting if our process is ergodic. They show that by leveraging Markovian, time-invariant, and ergodic structure in RL problems, we can overcome the curse of horizon and indicate what it would mean to do so efficiently, i.e., using all the data available optimally. The question is then how to achieve these bounds for efficient OPE. We propose an approach based on double reinforcement learning \cite{Kallus2019} and on simultaneously learning average visitation distributions and $q$-functions. And, we show that, unlike importance-sampling-based estimators \cite{Liu2018}, our DRL estimator achieves
the efficiency bound under certain mixing conditions. Thus, by carefully leveraging problem structure we show how to efficiently break the curse of horizon in RL OPE.

1.1 Organization

The organization of papers is as follows. In Section 1.2 we define the decision process models and set up the OPE problem formally. In Section 1.3 we define the efficiency bounds formally, briefly reviewing semiparametric inference as it relates to our results. In Section 1.4 we review the relevant literature on OPE.

In Section 2 we derive the efficiency bounds under each of the models under consideration, NMDP, TMDP, and MDP. In Section 3 we analyze the asymptotic properties when we extend standard DR and DRL OPE estimators to infinite horizons and provide conditions for their efficiency in the NMDP and TMDP models. We note, however, that they are not efficient under the MDP model and have the wrong MSE scaling. In Section 4 we propose for their efficiency in the NMDP and TMDP models. We note, however, that they are not extend standard DR and DRL OPE estimators to infinite horizons and provide conditions

1.2 Problem Setup and Notation

A (time-invariant) Markov decision process (MDP) is defined by a tuple \((\mathcal{S}, \mathcal{A}, \mathcal{R}, p, \gamma)\), where \(\mathcal{S}\), \(\mathcal{A}\), and \(\mathcal{R}\) are, respectively, the state, action, and reward spaces, \(p(s'|s, a)\) is the distribution of the bounded random variable \(\tau \in [0, R_{\text{max}}]\) denoting the immediate reward after taking action \(a\) in state \(s\), \(p(s'|s, a)\) is the state transition probability distribution, and \(\gamma \in (0, 1)\) is the discount factor. A policy \(\pi: \mathcal{S} \times \mathcal{A} \to [0, 1]\) assigns to each state \(s \in \mathcal{S}\) a distribution over actions with \(\pi(a|s)\) being the probability density or mass of taking action \(a\) in state \(s\). We also associate with \(\pi\) an initial state distribution, \(p^{(0)}(s_0)\). Together, an MDP and a policy define a joint distribution over trajectories \(\mathcal{J} = (s_0, a_0, r_0, s_1, a_1, r_1, \ldots)\), given by the product \(p^{(0)}(s_0)\pi(a_0 | s_0)p_0(r_0 | s_0, a_0)p_1(s_1 | s_0, a_0)\cdots\). We denote this distribution by \(P_\pi\) and expectations in this distribution by \(E_\pi\) to highlight the dependence on \(\pi\), as we will consider the MDP fixed. We denote by \(p^{(t)}(s_t)\) or \(p^{(t)}(s_t, a_t, r_t, s_{t+1})\) the marginal distribution of \(s_t\) or of \((s_t, a_t, r_t, s_{t+1})\) (etc.) under \(P_\pi\). We denote by \(\mathcal{J}_{s_{T+1}} = (s_0, a_0, r_0, \cdots, s_T, a_T, r_T, s_{T+1})\) the length-(\(T+1\)) trajectory up to \(s_{T+1}\) and by \(\mathcal{H}_{s_{T+1}} = (s_0, a_0, \cdots, s_T, a_T, s_{T+1})\) the same trajectory but excluding reward variables. We similarly denote by \(\mathcal{H}_{a_T}\) the trajectory up to \(a_T\) and including the variable \(a_T\), excluding rewards.

Our ultimate goal is to estimate the average cumulative reward of the known target evaluation policy (and known initial state distribution), \(\pi^*\):

\[
\rho^{\pi^*} = \lim_{T \to \infty} \rho_T^{\pi^*}, \quad \text{where} \quad \rho_T^{\pi} = c_T(\gamma) E_\pi \left[ \sum_{t=0}^{T} \gamma^t r_t \right], \quad c_T(\gamma) = \left( \frac{\gamma^T}{\sum_{c=0}^{\infty} \gamma^c} \right)^{-1}.
\]
The quality and value functions ($q$- and $v$-functions) are defined as the following conditional averages of the cumulative reward to go (under $\pi^e$), respectively:

$$q(s_0, a_0) = E_{e^e} \left[ \sum_{k=0}^{\infty} \gamma^k r_k \mid s_0, a_0 \right], \quad v(s_0) = E_{e^e} \left[ \sum_{k=0}^{\infty} \gamma^k r_k \mid s_0 \right] = E_{e^e} [q(a, s) \mid s_0].$$

Note that the very last expectation is taken only over $a_0 \sim \pi^e(a_0 \mid s_0)$.

The OPE problem is to estimate $\rho^{\pi^e}$ using $N$ observations of length-$(T + 1)$ trajectories independently generated by the distribution induced by using another policy, $\pi^b$, in the same decision process, $\mathcal{D} = \{ \mathcal{J}^{(1)}_{s_{T+1}}, \ldots, \mathcal{J}^{(N)}_{s_{T+1}} \}$. This latter policy, $\pi^b$, is called the behavior policy and it may be known or unknown. For brevity, we often use the subscript $e$ or $b$ to mean the subscript $\pi^e$ or $\pi^b$. Note that the distributions $P_e$ and $P_b$ differ in both the action distributions and initial state distributions.

The above MDP can be generalized in two ways: NMDP, where we remove the Markov and time-invariant structure; and TMDP, where we remove the time-invariant structure. In NMDP, the reward, transition, and policy distributions can all depend on the history of states and actions. In this case, we denote the transition, reward, and policy distributions at time $t$ by $p_t(s_{t+1} \mid \mathcal{H}_{a_t})$, $p_t(r_t \mid \mathcal{H}_{a_t})$, $\pi_t(a_t \mid \mathcal{H}_{s_t})$. In TMDP, the reward, transition, and policy distributions can change with time though the Markov assumption is still retained. In this case, we denote the transition, reward, and policy distributions at time $t$ as $p_t(s_{t+1} \mid a_t, s_t)$, $p_t(r_t \mid a_t, s_t)$, $\pi_t(a_t \mid s_t)$. In NMDP and TMDP, we also need to add $t$ subscripts to the $q$- and $v$-functions, and in NMDP, these functions also depend on the whole trajectory up to $a_t$ and $s_t$, respectively. Unless otherwise noted, we assume the underlying distribution of the data follows an MDP throughout the paper.

A model is a set of distributions for the generating process of the data. Thus, without imposing any additional structure beyond NMDP, a model for $P_{\pi^e}$, which generates $\mathcal{D}$, is given by the set of products $p_e^{(0)}(s_0) \pi_e^{(0)}(a_0 \mid s_0) p_0(r_0 \mid a_0, s_0) p_1(s_1 \mid a_0, s_0) \pi_e^{(1)}(a_1 \mid s_0, a_0, s_1) \cdots$ over some possible values for each probability distribution in the product. Assuming different structure – NMPD, TMPD, or MDP – corresponds to restricting the possible range of these distributions. Specifically, we let $\mathcal{M}_1$ denote the nonparametric model where each of these distributions is unknown, completely free, may depend on the index $t$, and may depend on all the history, corresponding to the NMDP model. We let $\mathcal{M}_2$ denote the nonparametric model where each of these distributions is unknown, completely free, may depend on the index $t$, but may only depend on the recent state and action, corresponding to the TMDP model. Finally, we let $\mathcal{M}_3$ denote the nonparametric model where each of these distributions is unknown and completely free but must be the same for each index $t$ and may only depend on the recent state and action, corresponding to the MDP model. Table 1 summarizes the three models. These models are nested as follows: $\mathcal{M}_3 \subset \mathcal{M}_2 \subset \mathcal{M}_1$.

Since $\pi^e$ and $p_e^{(0)}$ are given, the parameter of interest, $\rho^{\pi^e}$, is a function of just the part of $P_e$ that specifies the decision process (transition and reward probabilities) and does not depend on the behavior policy and its initial state distribution. We may also consider the models $\mathcal{M}_{1,b}, \mathcal{M}_{2,b}, \mathcal{M}_{3,b}$, where we restrict $\pi^b$ to be fixed and known. Our results will actually be the same with or without this restriction so we generically use $\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3$ to refer to either case.
We denote the density ratio at time $t$ and the cumulative density ratio up to time $t$, respectively, by
\[
\eta_t(s,a) = \frac{\pi^e_t(a \mid s)}{\pi^b_t(a \mid s)}, \quad \nu_t(\mathcal{H}_{a_t}) = \prod_{k=0}^{t} \eta_k(s_k, a_k).
\]
In the MDP model, we simply write $\eta = \eta_t$ without a subscript ($\nu_t$, however, is still time-dependent in an MDP). We denote the the marginal state-action and state density ratios at time $t$, respectively, by
\[
\mu_t(s_t, a_t) = \frac{p_e(t)(s_t, a_t)}{p_b(t)(s_t, a_t)}, \quad w_t(s_t) = \frac{p_e(t)(s_t)}{p_b(t)(s_t)}.
\]
For an MDP, the variables
\[
\mathcal{C}_\pi = \{(s_t, a_t, r_t) : t \geq 0\}
\]
generated by $P_\pi$ form a Markov chain. When this is a Harris ergodic chain (see Meyn and Tweedie, 2009), then we have almost surely that,
\[
\frac{1}{T+1} \sum_{t=0}^{T} r_t \to E_{p_e(\infty)}[r], \quad c_T(\gamma) \sum_{t=0}^{T} \gamma^t r_t \to E_{p_{\pi,\gamma}(\infty)}[r],
\]
where $p_\pi(\infty) = p_{\pi,1}^\infty$ and $p_{\pi,\gamma}^\infty$ is the $\gamma$-discounted average visitation distribution:
\[
p_{\pi,\gamma}^\infty(s, a, r, s') = \lim_{T \to \infty} c_T(\gamma) \sum_{t=0}^{T} \gamma^t p_e(t)(s, a, r, s').
\]
We also write $p_{\pi,\gamma}^\infty(s)$, $p_{\pi,\gamma}^\infty(s, a)$ for the state or state-action average visitation distribution. When these probabilities exist, we can define the stationary density ratio:
\[
w(s) = \frac{p_{e,\gamma}^\infty(s)}{p_b^\infty(s)}.
\]
Notice that we use the $\gamma$-discounted average visitation distribution under $P_e$ in the numerator but the usual, undiscounted stationary stationary under $P_b$ in denominator.

To streamline notation, when no subscript is denoted, all expectations $E[\cdot]$ and variances $\text{var}[\cdot]$ are taken with respect to the behavior policy, $\pi^b$. At the same time, all $v$- and $q$-functions are for the target policy, $\pi^e$. The $L^p$-norm is defined as $\|g\|_p = E[|g|^p]^{1/p}$. For any function of trajectories, we define its empirical average as
\[
\mathbb{P}_N f = \mathbb{P}_N[f(\mathcal{J})] = N^{-1} \sum_{i=1}^{N} f(\mathcal{J}^{(i)}).
\]
Similarly, we write $f$ to mean the random variable $f(\mathcal{J})$. For example, we write $\eta_t = \eta_t(\mathcal{H}_{a_t})$ and $\mu_t = \mu_t(s_t, a_t)$. For any function of $s, a, r, s'$, we define its time average up to $T$ as
\[
\mathbb{P}_T f = \mathbb{P}_T[f(s, a, r, s')] = (T + 1)^{-1} \sum_{t=0}^{T} f(s_t, a_t, r_t, s_{t+1}).
\]
Since the right-hand side is now a function of the trajectory, we can also write $\mathbb{P}_N \mathbb{P}_T f$. Table 2 in the appendix summarizes our notation.

5
1.3 Efficiency Bounds

In this section, we define formally what we mean by the best-possible asymptotic MSE. In this paper, we will consider both the settings where the observations are iid (independent and identically distribution) and when they are non-iid. In particular, much of our focus will be on the non-iid setting where we only observe a single, truncated trajectory \((N = 1, T < \infty)\). Therefore, our notion of an efficiency bound is a generalization of the unified notion in the iid case and it is based on the equivalence between the efficiency bound and the supremum of Cramér-Rao lower bounds over all regular parametric submodels [Tsiatis 2006].

Suppose we have a model \(M\) for the joint distribution of the observations \(O_1, O_2, \ldots\) (e.g., a single trajectory of an MDP, or multiple independent trajectories), that is, a set of potential distributions where the their true distribution is \(F_0 \in M\). Consider a (scalar) parameter of interest \(R : M \to \mathbb{R}\). That is, we want to estimate \(R(F_0)\). Given an estimator \(\hat{R}_N = \hat{R}_N(O_1, \ldots, O_N)\), its limiting law is the distribution limit of \(\sqrt{N}(\hat{R}_N - R(F_0))\). The asymptotic MSE is defined as the second moment of the limiting law. If the second moment is infinite, then \(\hat{R}_N\) is not \(\sqrt{N}\)-consistent for \(R(F_0)\). Throughout, we will simply use “consistent” to mean \(\sqrt{N}\)-consistent.

Let \(F_N\) denote the distribution of \(O_{1:N} = (O_1, \ldots, O_N)\) under \(F\), define the restriction \(M_N = \{F_N : F \in M\}\), and let \(R_N : M_N \to \mathbb{R}\) be any such that \(R_N(F_N) = R(F) + o(N^{-1/2})\). A model \(M_N^{\text{para}} \subset M_N\) is a regular parametric submodel if we can write it as \(M_N^{\text{para}} = \{F_{\theta,N} : \theta \in \Theta\}\) where \(\Theta \subset \mathbb{R}^p\) is open, \(F_{0,N} = F_{\theta^*,n}\) for some \(\theta^* \in \Theta\), and \(F_{\theta,N}\) has a differentiable density \(f_{\theta,N}\) such that the matrix inverse in the display equation below exists. Given a regular parametric submodel, define the Cramér-Rao (CR) lower bound as

\[
\text{CR}(M_N^{\text{para}}, R_N) = \nabla_{\theta^T} R_N(F_{N,\theta}) E_{F_{0,N}}[\nabla_{\theta} \log f_{\theta}(O_{1:N}) \nabla_{\theta^T} \log f_{\theta}(O_{1:N})]^{-1} \nabla_{\theta} R_N(F_{N,\theta}) \bigg|_{\theta = \theta^*}.
\]

Notice that we phrased the CR bound in the more general non-iid setting. The CR lower bound is both a lower bound on the variance (times \(n\)) of any unbiased estimator for \(R_N\) (Casella 2002, Theorem 7.3.9) and is the asymptotic variance of the maximum likelihood estimator (MLE) in \(M_N^{\text{para}}\). In the iid setting, we can let \(R_N = R\), the CR bound is independent of \(n\), and the seminal work of Hájek (1970, 1972) shows that the CR bound (times \(n\)) is also a lower bound on the asymptotic MSE of any regular estimator, or of any estimator almost everywhere, or of any estimator in some vanishing neighborhood of \(\theta^*\) (van der Vaart 1998, Theorems 8.8, 8.9, 8.11, respectively).

We define the efficiency bound (EB) for the parameter under the model \(M\) as

\[
\text{EB}(M) = \lim_{N \to \infty} \sup_{\text{regular parametric submodel } M_N^{\text{para}} \subset M_N} N \text{ CR}(M_N^{\text{para}}). \tag{1}
\]

In the rest of the paper we derive the EB for our different models and prove under what conditions our newly proposed estimators have asymptotic MSE that achieves these bounds.

One motivation for the “efficiency” in EB is that, in the iid setting (where the limit in Eq. (1) is unnecessary), a key result of semiparametric inference is that Hájek’s results still apply even when \(M\) is nonparametric: \(\text{EB}(M)\) lower bounds the asymptotic MSE of any regular estimator or of any estimator in a vanishing neighborhood of \(F_0\) (van der Vaart [1998]).

\[\text{For generality, we can also let } M, R \text{ depend on } n \text{ as } M^{(N)}, R^{(N)} \text{ as long as } R^{(N)}(F^{(N)}) = R(F) + o(1/\sqrt{N}).\]
Theorems 25.20 and 25.21, respectively). In particular, if the EB is infinite then every regular estimator (or every estimator, in a vanishing neighborhood) must be inconsistent. This interpretation of Eq. (1) applies when we consider observing a growing number of independent trajectories, as we do in $M_1, M_2$. However, in $M_3$, we can uniquely consider the setting of observing a finite number of growing trajectories (even just one!). In the non-iid case, the meaning of a regular estimator is less clear. There exist different approaches to this (Bickel and Kwon, 2001; Greenwood and Wefelmeyer, 1995). For simplicity and since this question is tangential to our work, similarly to Komunjer and Vuong (2010) and in the spirit of Stein (1956), we simply take Eq. (1) as a definition, compute it for our models, and show that we can find estimators that achieve it. In one simple interpretation, these nonparametric estimators perform as well as MLE would in any well-specified parametric model – a rather high bar.

1.4 Summary of Literature on OPE

OPE is a central problem in both RL and in the closely related dynamic treatment regimes (DTR; Murphy et al., 2001). In RL, one usually assumes that the (time-invariant) MDP model $M_3$ holds. Nonetheless, with some exceptions that we review below, OPE methods in RL have largely not leveraged the additional independence and time-invariance structure of $M_3$ to improve estimation, and in particular, the effect of this structure on efficiency has not previously been studied and no efficient evaluation method has been proposed.

Methods for OPE can be roughly categorized into three types. The first approach is the direct method (DM), wherein we directly estimate the $q$-function and use it to directly estimate the value of the target evaluation policy. One can estimate the $q$-function by a value iteration in a finite-state-and-action-space setting utilizing an approximated MDP based on the empirical distribution (Bertsekas, 2012). More generally, modeling the transition and reward probabilities and using the MDP approximated by the estimates is called the model-based approach (Sutton and Barto, 2018). When the sample space and action space are continuous, we can apply some functional approximation to $q$-function modeling and use the temporal-difference method (Lagoudakis and Parr, 2004). Once we have an estimate $\hat{q}$, the DM estimate is simply

$$\hat{\rho}_{DM} = (1 - \gamma) P_N \left[ E_{\pi^e} [\hat{q}_0 | s_0] \right],$$

where the inner expectation is simply over $a_0 \sim \pi^e(\cdot | s_0)$ and is thus computable as a sum or integral over a known measure and the outer expectation is simply an average over the $N$ observations of $s_0$. For DM, we can leverage the structure of $M_3$ by simply restricting the $q$-function we learn to be the same for all $t$ and solving the fixed point of the Bellman equation. However, DM can fail to be efficient and is also not robust in that, if $q$-functions are inconsistently estimated, the estimate will be inconsistent.

The second approach is importance sampling (IS), which averages the data weighted by the density ratio of the evaluation and behavior policies. Given estimates $\hat{\nu}_t$ of $\nu_t$ (or, $\hat{\nu}_t = \nu_t$ if the behavior policy is known), the IS estimate is simply

$$\hat{\rho}_{IS} = c_T(\gamma) P_N \left[ \sum_{t=0}^T \gamma^t \hat{\nu}_t r_t \right].$$
A common variant the self-normalized IS (SNIS) where we divide the $t^{th}$ summand by $\mathbb{P}_N[\gamma^t \hat{\nu}_t]$. Recall that $T$ here denotes the finite length of the $N$ trajectories in our data. In finite-horizon problems (i.e., when the estimand is $\rho_T^{\pi_e}$), when the behavior policy is known, IS is unbiased and consistent but its variance tends to be large and it is inefficient (Hirano et al., 2003). In infinite-horizon problems, we must need $T$ to grow. But even if $T = \infty$ (our data are full trajectories), IS can have infinite variance because of diminishing overlap, known as the curse of horizon (Liu et al., 2018a). Our results (Table 1) in $\mathcal{M}_1$, $\mathcal{M}_2$ characterize more precisely when this curse applies or not.

The third approach is the doubly robust (DR) method, which combines DM and IS and is given by adding the estimated $q$-function as a control variate (Dudk et al., 2014; Jiang and Li, 2016; Scharfstein et al., 1999). Under $\mathcal{M}_1$, the DR estimate has the form

$$\hat{\rho}_{\text{DR}} = c_T(\gamma) \mathbb{P}_N \left[ \sum_{t=0}^T \gamma^t \left( \hat{\nu}_t(r_t - \hat{q}_t) + \hat{\nu}_{t-1}E_{\pi_e}[\hat{q}_t|s_t] \right) \right].$$

In finite-horizon problems, DR is known to be efficient under $\mathcal{M}_1$ (Kallus and Uehara, 2019b). In infinite horizons, we derive the additional conditions needed for efficiency in $\mathcal{M}_2$ in Section \[3\].

Many variations of DR have been proposed. Thomas and Brunskill (2016) propose both a self-normalized variant of DR and a variant blending DR with DM when density ratios are extreme. Farajtabar et al. (2018) propose to optimize the choice of $\hat{q}(s,a)$ to minimize variance rather than use a plug-in. Kallus and Uehara (2019a) propose a variant that is similarly locally efficient but further ensures asymptotic MSE no worse than DR, IS, and SNIS under misspecification and stability properties similar to self-normalized IS.

However, all of the aforementioned IS and DR estimators do not leverage Markov structure and fail to be efficient under $\mathcal{M}_3$. Recently, in finite horizons, Kallus and Uehara (2019b) derived the efficiency bound of $\rho_T^{\pi_e}$ under $\mathcal{M}_2$ and provided an efficient estimator termed Double Reinforcement Learning (DRL), taking the form

$$\hat{\rho}_{\text{DRL}(\mathcal{M}_2)} = c_T(\gamma) \mathbb{P}_N \left[ \sum_{t=0}^T \gamma^t \left( \hat{\mu}^{(i)}_t(r_t - \hat{q}^{(i)}_t) + \hat{\mu}^{(i)}_{t-1}E_{\pi_e}[\hat{q}^{(i)}_t|s_t] \right) \right],$$

where $\hat{\mu}^{(i)}_t$, $\hat{q}^{(i)}_t$ can either be estimated in-sample ($\hat{q}^{(i)}_t = \hat{q}_t$ and assuming a Donsker condition) or cross-fold (the sample is split and $\hat{q}^{(i)}_t$ is fit on the fold that excludes $i$). DRL’s efficiency depends only on the rates of convergence of these estimates, which can be as slow as $N^{-1/4}$ thus enabling the use of blackbox machine learning methods. In infinite horizons, we derive the additional conditions needed for efficiency in $\mathcal{M}_2$ in Section \[3\].

However, again, all of the aforementioned IS, DR, and DRL estimators do not leverage time-invariance and fail to be efficient under $\mathcal{M}_3$. Our results extend the notion of the curse of dimension and demonstrate that even estimators in $\mathcal{M}_2$, such as the efficient $\hat{\rho}_{\text{DRL}(\mathcal{M}_2)}$, can fail to be consistent as $\mu_t$ can also explode just like $\nu_t$. In contrast, in $\mathcal{M}_3$, regardless of the rate of growth of $\mu_t$, $\nu_t$, consistent evaluation is possible from even just a single trajectory and knowledge of the initial distribution.

Recently, Liu et al. (2018a) proposed a variant of the IS estimator for $\mathcal{M}_3$ that uses the ratio of the stationary distributions in hopes of overcoming the curse of horizon. We describe
this estimator in detail in Section 5.1. Its asymptotic MSE was not previously studied. We provide some results in the parametric setting. The properties in the nonparametric setting are not known. In particular, as we discuss in Section 5.1, its lack of doubly robust structure and its not being an empirical average of martingale differences make analysis particularly challenging. At the same time, these issues also suggest that the estimator is inefficient.

2 Efficiency Bounds in Infinite Horizons

The finite-horizon efficiency bounds for $\rho^p_T$ under $M_1$ and $M_2$ are derived in Kallus and Uehara (2019b) using the unified semiparametric approach (Bickel et al., 1998). We re-derive these efficiency bounds from the more primitive approach of Stein (1956), which allows us to take $T \to \infty$ and apply this to the infinite-horizon problem. Then, we apply this same approach to derive the efficiency bound in $M_3$.

2.1 Efficiency Bounds in Non-Markov and Time-Variant Markov Decision Processes

In this section we address the case of $M_1$ (NMDP) and $M_2$ (TMDP). The unique case of $M_3$ is handled in the next section. Note that, unlike the most of the parts of the paper, only in this section and Section 3 we assume the observed data follows an NMDP or TMDP rather than an MDP.

First, we note that because of the time-variance, if we observe length-$(T + 1)$ trajectories, we can only hope to estimate $\rho^p_T$. This is because as we can infer nothing about the distribution of later time steps. However, as long as $T = \omega(\log^{1/2}(N))$, we have $\rho^p_T = \rho^p + O(N^{-1/2})$, which means the two problems are the same in terms of asymptotic MSE (see Footnote 1). (And, if $T = o(\log^{1/2}(N))$ then consistency is hopeless.)

Specifically, notice that under NMDP,

$$
\rho^p_T = c_T(\gamma) \int \sum_{t=0}^{T} \gamma^t r_t \left\{ \prod_{k=0}^{t} p_k(r_k|H_{a_k}) \pi_k^p(a_k|H_{s_k}) p_k(s_{k+1}|H_{a_k}) \right\} p_0^p(s_0) d\lambda(J_{s_{T+1}}),
$$

where $\lambda$ is a baseline measure (e.g., counting measure for discrete or Lebesgue measure for continuous). Moreover, under TMDP, we can replace $H_{a_k}$ with $(s_k, a_k)$ and $H_{s_k}$ with $s_k$. Given any parametrization of the reward and transition distributions for times $t \leq T$, $p_t(r_t|H_{a_t}; \theta)$, $p_t(s_{t+1}|H_{a_t}; \theta)$, we can use this characterization to compute the CR lower bound for estimating $\rho^p_T$ given $N$ observations of length-$(T + 1)$ trajectories. For any $T = \omega(\log^{1/2}(N))$, the EB for $\rho^p_T$ is the $N \to \infty$ limit of the suprema of these bounds. This EB bounds the possible asymptotic MSE in estimating $\rho^p_T$ from $N$ observations of length-$(T + 1)$ trajectories, where the asymptotic MSE is defined by taking both $N, T \to \infty$. Again, if $T = o(\log^{1/2}(N))$ the asymptotic MSE is infinite.

By carefully picking a particular sequence of parametrizations and showing that they in fact achieve the supremum, we derive the following two results.
Theorem 1 (EB under NMDP). Suppose $T = \omega(\log^{1/2}(N))$. Then

$$EB(\mathcal{M}_1) = (1 - \gamma)^2 \sum_{k=1}^{\infty} E[\gamma^{2(k-1)}\mu_{k-1}^2 \text{var} (r_{k-1} + v_k|\mathcal{H}_{a_{k-1}})].$$  \hspace{1cm} (2)$$

Theorem 2 (EB under TMDP). Suppose $T = \omega(\log^{1/2}(N))$. Then

$$EB(\mathcal{M}_2) = (1 - \gamma)^2 \sum_{k=1}^{\infty} E[\gamma^{2(k-1)}\mu_{k-1}^2 \text{var} (r_{k-1} + v_k|a_{k-1}, s_{k-1})].$$  \hspace{1cm} (3)$$

Remark 1. Equations (2) and (3) are almost the same as the limit as $T \to \infty$ of $c_T(\gamma)$ times the finite-horizon efficiency bounds derived by Kallus and Uehara (2019b). They are the same if we replace the lower summation limit with $k = 0$ instead of $k = 1$ in Eqs. (2) and (3). This is because we here assume $p_{e(0)}$ is known while in Kallus and Uehara (2019b) the assumption is that $p_{b(0)} = p_{e(0)}$ are unknown, the uncertainty due to which increases the efficiency bound. Aside from this, we derive the efficiency bounds here from the primitive approach of taking suprema of CR, in accordance with the notion of efficiency bound described in Section 1.3, rather than the unified path-differentiation approach taken in Kallus and Uehara (2019b).

Corollary 3 (Sufficient conditions for existence of efficiency bounds). If $\|v_k\|_\infty = o(\gamma^{-k})$, then $EB(\mathcal{M}_1) < \infty$. If $\|\mu_k\|_\infty = o(\gamma^{-k})$, then $EB(\mathcal{M}_2) < \infty$. Moreover, if $P_{\mu_b} \in \mathcal{M}_2$ and $EB(\mathcal{M}_1) < \infty$, then $EB(\mathcal{M}_2) < \infty$.

Remark 2 (The curse of horizon in $\mathcal{M}_1$, extended). To demonstrate the curse of horizon, Liu et al. (2018a) gave an example where the IS estimator has a diverging variance as horizon grows. But it is not clear if – and without assuming MDP structure – there might be another estimator that would not suffer from this. Our results show that in fact there is not. If we take any example where $\text{var} (r_{k-1} + v_k|\mathcal{H}_{a_{k-1}})$ are uniformly lower bounded (i.e., state transitions and reward emissions are non-degenerate), then as long as $E[\log(\eta_k)] \geq -\log(\gamma)$ for all $k$, we will necessarily have that $EB(\mathcal{M}_1) = \infty$. (Notice that $E[\log(\eta_k)]$ is Kullback-Leibler divergence.) In this case, as long as we are not restricting the model beyond $\mathcal{M}_1$, we simply cannot break the curse of horizon and it affects all (regular) estimators, not just IS.

Remark 3 (The curse of horizon in $\mathcal{M}_2$, a milder version of the original). Our results further extend the curse of horizon to $\mathcal{M}_2$, providing another refinement of the notion. The curse is milder in $\mathcal{M}_2$ than in $\mathcal{M}_1$, since the EBs are necessarily ordered. It is, in fact, much milder. In particular, rather than involve the growth of the cumulative density ratios, whether $EB(\mathcal{M}_2)$ converges or diverges depends on the growth of the marginal density ratios. These, of course, can also grow and $EB(\mathcal{M}_2)$ can diverge. However, while we can easily make $EB(\mathcal{M}_1) = \infty$ even with a simple MDP example, to make $EB(\mathcal{M}_2)$ diverge we need a more pathological example. It can be verified that if $P_b$ is actually an ergodic MDP and the stationary distributions overlap, then we will necessarily have $\|\mu_k\|_\infty = O(1)$.

This means that, for an MDP, we can overcome the inconsistency of the curse of horizon that affects estimators like $\hat{p}_{DR}$ and $\hat{p}_{IS}$ by using estimators that are efficient under $\mathcal{M}_2$, the first of which was proposed by Kallus and Uehara (2019b), i.e., $\hat{p}_{DRL}(\mathcal{M}_2)$. However, this is still not efficient under $\mathcal{M}_3$. In fact, this is not just a matter of constants: this will not even yield the right scaling of the MSE. We show this in the next section.
2.2 Efficiency Bounds in Time-Invariant Markov Decision Processes

In the previous section, we did not utilize the time-invariant structure of MDPs. In particular, in $\mathcal{M}_3$, it is possible to estimate $\rho^{\pi^*}$ from a single trajectory! In particular, each additional time step provides us useful information for estimating transition and reward probabilities for all time steps. Correspondingly, the MSE should scale inversely with both $N$ and $T$.

In this section, we derive the EB for $\mathcal{M}_3$. In particular, as in the most parts of the paper, unlike the previous section and Section 3, we assume the true distribution is an MDP. Our data consists of $N$ observations of length-$(T + 1)$ trajectories. For the scaling to be correct, we count this as $n = N(T + 1)$ observations. We let $T \to \infty$, while $N \geq 1$ can be growing with $T$ or it can be finite. We therefore index our limits by $T$ only.

To derive the EB, consider any parametric model for the MDP, $\mathcal{M}^\text{para}_3 \subset \mathcal{M}_3$, i.e., a parametrization of the time-invariant $p(r|s, a; \theta)$, $p(s'|s, a; \theta)$. Now, let $\mathcal{M}^\text{para}_{3,T}$ be its restriction to length-$(T + 1)$ trajectories. The following theorem characterizes the limit of the CR lower bound in this parametric model.

**Theorem 4.** Let $g_{r|s,a} = \nabla_\theta \log p(r|s, a; \theta)$ and $g_{s'|s,a} = \nabla_\theta \log p(s'|s, a; \theta)$. Then,

$$\text{CR} \left( \mathcal{M}^\text{para}_{3,T}, \rho^{\pi^*} \right) = N^{-1}(T + 1)^{-1}(A_T I_T^{-1} A_T^\top + C_T J_T^{-1} C_T^\top)$$

where $A_T = c_T(\gamma) E_{\pi^*} \left[ \sum_{t=0}^{T} \gamma^c r_t g_{r_t|s_t,a_t}^\top \right]$, $C_T = c_T(\gamma) E_{\pi^*} \left[ \sum_{t=c+1}^{T} \gamma^{c-1} r_t g_{s_{t+1}|s_{t+1},a_{t+1}}^\top \right]$, $I_T = \frac{1}{T+1} E_{\pi^*} \left[ \sum_{t=0}^{T} g_{r_t|s_t,a_t} g_{r_t|s_t,a_t}^\top \right]$, $J_T = \frac{1}{T+1} E_{\pi^*} \left[ \sum_{t=0}^{T} g_{s_{t+1}|s_t,a_t} g_{s_{t+1}|s_t,a_t}^\top \right]$.

Moreover, if $P_{\pi^*}$ is ergodic, then

$$\lim_{T \to \infty} N(T + 1) \text{CR} \left( \mathcal{M}^\text{para}_{3,T}, \rho^{\pi^*} \right) = A_\infty I_\infty^{-1} A_\infty + C_\infty J_\infty^{-1} C_\infty,$$

where $A_\infty = E_{P_\infty} \left[ r_{s,a} w(s) \eta(a, s) \right]$, $C_\infty = \gamma E_{P_\infty} \left[ v(s') g_{s'|s,a} w(s) \eta(a, s) \right]$, $I_\infty = E_{P_\infty} \left[ g_{r|s,a} g_{r|s,a}^\top \right]$, $J_\infty = E_{P_\infty} \left[ g_{s'|s,a} g_{s'|s,a}^\top \right]$.

Note that while the CR derivation works for any $T$, ergodicity is needed in order to compute the limit of the above time averages. Using this, carefully choosing a sequence of parametric models, and showing that they achieve the supremum, we can derive the following result.

**Theorem 5** (Efficiency bound under MDP). Suppose $P_{\pi^*}$ is ergodic. Then,

$$\text{EB}(\mathcal{M}_3) = E_{P_\infty} \left[ w^2(s) \eta^2(a, s) (r + \gamma v(s') - q(s, a))^2 \right].$$

(4)

**Remark 4** (Comparison to EB$(\mathcal{M}_1)$, EB$(\mathcal{M}_2)$). The comparison between Theorem 5 and Theorems 1 and 2 cannot be made on the basis of the values of the EB in the statements, as the asymptotic MSEs are on different scales: the rate in $\mathcal{M}_3$ is strictly faster. In particular, Theorems 1 and 2 are only relevant when $T = \omega(1)$. And, in this setting, we
have $1/(N(T + 1)) = o(1/N)$. In this sense, efficiency in $\mathcal{M}_3$ corresponds to improvement in the rate, not just the constant, relative to efficiency in $\mathcal{M}_1$ or $\mathcal{M}_2$. This is in contrast to the comparison between $\mathcal{M}_1$ and $\mathcal{M}_2$, which have efficiency bounds that are on the same scale and only differ in the leading coefficient.

3 Efficient Estimators for Infinite Horizons under NMDP and TMDP

Before turning to developing an efficient estimator under the MDP model, we briefly review how we can extend the efficient finite-horizon DRL estimators of Kallus and Uehara (2019b) to be efficient in the infinite-horizon NMDP and TMDP settings.

DRL is a meta-estimator: it takes in as input estimators for $q$-functions and density ratios and combines them in a particular manner that ensures efficiency even when the input estimators may not be well behaved. For example, metric entropy or Donsker assumptions can be avoided by using a cross-fold sample-splitting strategy (Chernozhukov et al., 2018). We proceed by presenting the infinite-horizon extensions of the DRL estimators of Kallus and Uehara (2019b) and their properties. Again, the two DRL estimators present here are not efficient under $\mathcal{M}_3$.

3.1 Non-Markov Decision Process

The infinite-horizon extension of the DRL estimator under $\mathcal{M}_1$ is as follows. Fix some horizon truncation $\omega_N \leq T$ (and recall that $T$ is growing with $N$). Then the estimator is given by

$$\hat{\rho}_{\text{DRL}(\mathcal{M}_1)} = c_{\omega_N}(\gamma) \mathbb{P}_N \left[ \sum_{t=0}^{\omega_N} \gamma^t \left( \hat{\nu}_t(i) r_t - \hat{q}_t(i) \right) + \hat{\nu}_{t-1} \mathbb{E}_{\pi}\left[ \hat{q}_t(i) \mid \mathcal{H}_{s_t} \right] \right],$$

where $\hat{\nu}_t(i), \hat{q}_t(i)$ are some plug-in estimates of $\nu_t, q_t$ to be used for the $i^{th}$ data point in the sample average, $\mathbb{P}_N$. Notice that the inner expectation is only over $a_t \sim \pi_\alpha(\cdot \mid \mathcal{H}_i)$ and computable since we know $\pi_\epsilon$. We can consider two cases. In the adaptive version, $\hat{\nu}_t(i), \hat{q}_t(i)$ are shared among all data points and are estimated on the whole dataset.

The adaptive version of $\hat{\rho}_{\text{DRL}(\mathcal{M}_1)}$ is exactly the DR estimator, $\hat{\rho}_{\text{DR}}$. In the cross-fold version, the sample is evenly split into two folds and $\hat{\nu}_t(i), \hat{q}_t(i)$ are shared within a data points in a fold and are estimated on the opposite fold so that they are independent of data point $i$. Kallus and Uehara (2019b) Section 6) discusses estimation strategies for $\hat{\nu}_t, \hat{q}_t$. In particular, if the behavior policy is known we can simply let $\hat{\nu}_t(i) = \nu_t$.

We can now state a straightforward infinite-horizon extension of the efficiency result of Kallus and Uehara (2019b) Theorems 4 and 6) under $\mathcal{M}_1$ in finite-horizons. Essentially, we just need to be careful about choosing $\omega_N$.

**Theorem 6** (Asymptotic property of $\hat{\rho}_{\text{DRL}(\mathcal{M}_1)}$). Define $\alpha_1, \alpha_2$ such that $\|\hat{q}_t(i) - q_t\|_2 = o_p(N^{-\alpha_1}), \|\hat{\nu}_t(i) - \nu_t\|_2 = o_p(N^{-\alpha_2})$ for $t \geq 0$. Assume (6a) $\nu_t \leq C^t$ and $\gamma C < 1$, (6b) $\hat{q}_t \leq R_{\max}$ and $\hat{\nu}_t \leq C^t$, (6c) $N^{-\min(2\alpha_1, 2\alpha_2)} \omega_N^2 = o_p(1)$, (6d) $\omega_N = \omega((\log N)^{1/2})$, (6e)
Theorem 7. (Asymptotic property of \( \hat{\rho}_{DRL(M_2)} \)). Define \( \alpha_1, \alpha_2 \) such that \( \| \hat{q}_t^{(i)} - q_t \|_2 = o_p(N^{-\alpha_1}), \| \hat{\mu}_t^{(i)} - \mu_t \|_2 = o_p(N^{-\alpha_2}) \) for \( t \geq 0 \). Assume (6a) \( \mu_t \leq C' \) and \( \gamma C' < 1 \), (6b) \( \hat{q}_t \leq R_{\text{max}} \), and \( \hat{\mu}_t \leq C'' \), (6c) \( N^{-\min(2\alpha_1,2\alpha_2)} \omega_N^2 = o_p(1) \), (6d) \( \omega_N = \omega(\log N)^{1/2} \), (6e) \( N^{-\alpha_1 - \alpha_2} \omega_N = o_p(N^{-1/2}) \), and (6f) for the adaptive version only, further assume that \( \hat{\mu}_t, \hat{q}_t \) belong to a Donsker class. Then, \( \sqrt{N} (\hat{\rho}_{DRL(M_2)} - \rho^{\pi_e}) \overset{d}{\to} N(0, \text{EB}(M_2)) \).

Each assumption has the following interpretation. The conditions (6a) is needed to guarantee that the EB is finite. Conditions (6b), (6c) are required to control a term related to a stochastic equicontinuity condition. In particular, even if we observe infinite trajectories \( (T = \infty) \) we cannot set \( \omega_N = \infty \). In the adaptive version, without cross-fitting, we further require a Donsker condition in condition (6f) for the stochastic equicontinuity condition. As before, condition (6d) is needed so that \( \rho_{\omega_N}^{\pi_e} = \rho^{\pi_e} + o(1/\sqrt{N}) \). Essentially, if we choose \( \omega_N \) such that \( \omega_N = \omega((\log N)^{1/2}), \omega_N = o(N^\alpha) \) \( \forall \alpha > 0 \), then the conditions are exactly as in Kallus and Uehara (2019b, Theorems 4 and 6) but enforced to hold for all \( t \geq 0 \). The condition (6e) is needed to show the inflation in variance due to using plug-in estimates is \( o_p(N^{-1/2}) \), that is, the asymptotic variance is not changed because of the plug-in. Because of the mixing bias property (Rotnitzky et al. 2019) of the influence function, the rate is multiplicative in the two estimators’ convergence rate. Finally, note that if we know the behavior policy we can take \( \alpha_2 \to \infty \) and the conditions on \( \alpha_1 \) are quite lax.

3.2 On Time-Variant Markov Decision Process

In finite-horizons, Kallus and Uehara (2019b) proposed the first efficient OPE estimator under TMDP. We now repeat the process in the previous section and show the results can be easily extended to the infinite-horizon case. Fix some horizon truncation \( \omega_N \leq T \), the estimator is given by

\[
\hat{\rho}_{DRL(M_2)} = c_{\omega_N}(\gamma) \mathbb{P}_N \left[ \sum_{t=0}^{\omega_N} \gamma^t \left( \hat{\mu}_t^{(i)} \left( r_t - \hat{q}_t^{(i)} \right) + \hat{\mu}_{t-1} E_{\pi_e}[\hat{q}_t | s_t] \right) \right].
\]

Again, \( \hat{\mu}_t^{(i)}, \hat{q}_t^{(i)} \) can be estimated adaptively or cross-fold. Kallus and Uehara (2019b, Section 6) discusses estimation strategies for \( \hat{\mu}_t, \hat{q}_t \).

We can again state a straightforward infinite-horizon extension of the efficiency result of Kallus and Uehara (2019b, Theorem 9) under \( M_2 \) in finite-horizons.

Theorem 7. (Asymptotic property of \( \hat{\rho}_{DRL(M_2)} \)). Define \( \alpha_1, \alpha_2 \) such that \( \| \hat{q}_t^{(i)} - q_t \|_2 = o_p(N^{-\alpha_1}), \| \hat{\mu}_t^{(i)} - \mu_t \|_2 = o_p(N^{-\alpha_2}) \) for \( t \geq 0 \). Assume (6a) \( \mu_t \leq C' \) and \( \gamma C' < 1 \), (6b) \( \hat{q}_t \leq R_{\text{max}} \), and \( \hat{\mu}_t \leq C'' \), (6c) \( N^{-\min(2\alpha_1,2\alpha_2)} \omega_N^2 = o_p(1) \), (6d) \( \omega_N = \omega((\log N)^{1/2}) \), (6e) \( N^{-\alpha_1 - \alpha_2} \omega_N = o_p(N^{-1/2}) \), and (6f) for the adaptive version only, further assume that \( \hat{\mu}_t, \hat{q}_t \) belong to a Donsker class. Then, \( \sqrt{N} (\hat{\rho}_{DRL(M_2)} - \rho^{\pi_e}) \overset{d}{\to} N(0, \text{EB}(M_2)) \).

3.3 Inefficiency under MDP

Because \( M_3 \) is included in both \( M_1 \) and \( M_2 \), the methods in this section could be applied to an MDP. In fact, many papers using DR-type methods such as \( \hat{\rho}_{DR} \) (equal to the adaptive version of \( \hat{\rho}_{DRL(M_1)} \)) assume that the underlying distribution is MDP when estimating \( q \)-functions: i.e., they fit \( q \)-functions that depend only on \( s_t, a_t \) and that are time-invariant. However, using this additional structure in order to produce better \( q \)-function estimates...
does not improve the asymptotic variance. Indeed, even if we used the oracle \( q \)-functions and oracle density ratios, Theorem \[6\] still apply and inform us that the asymptotic variance is only efficient in \( \mathcal{M}_1 \). The same occurs in \( \mathcal{M}_2 \) by Theorem \[7\].

Per Remark \[4\], this means that even though we might use a total of \( \mathcal{O}(NT) \) observations to get better \( q \)-function estimates, if we use standard DR-type methods, this will get washed out, at least asymptotically, and our variance will only vanish as \( \mathcal{O}(1/N) \). This, of course, much worse than the \( \mathcal{O}(1/(NT)) \) scaling of the efficiency bound under MDP. In this sense, we see that neither cumulative nor marginalized density ratios are the right way to do importance sampling or doubly-robust estimation in MDPs.

### 4 Efficient Estimator for Markov Decision Process

In this section, we propose an estimator that is efficient under the MDP model. To our knowledge it is the first such estimator. The asymptotic regime we consider is \( T \to \infty \), while \( N \geq 1 \) can be growing or fixed, even just equal to 1. We assume throughout this and all following sections that the trajectory is a Harris ergodic chain \[\text{Meyn and Tweedie 2009}\] so that it has a stationary distribution. And, in all that follows, we let the \( L^2 \)-norm \( \| q(s, a, r, s') \|_2 \) be defined with respect to \( p^\infty_b \).

**Assumption 1** (Ergodic MDP). The chains \( \mathcal{C}_b, \mathcal{C}_e \) are Harris ergodic chains and the corresponding stationary density ratio, \( w(s) \), is uniformly upper bounded.

For brevity, we focus on the case where the behavior policy, which is more relevant in RL. So, we have that \( \eta(a, s) \) is known. Our results can be extended to the unknown behavior policy case as well (Remark \[5\] below).

The key to our estimator is the following estimating function, defined for a given \( w \)- and \( q \)-function. We use \( w', q' \) to denote dummy such functions.

\[
\phi(s, a, r, s'; w', q') = (1 - \gamma)E_{p_e^{(0)}}[v'(s_0)] + w'(s)\eta(a, s)(r + \gamma v'(s') - q'(s, a)),
\]

where we use the shorthand that, given \( q' \), we let \( v'(s) = E_{p_e^{(0)}}[q'(s, a) | s] \). Notice that, given a \( q \)-function, the first term is a constant and that it is computable because both \( p_e^{(0)} \) and \( \pi_e \) are known.

Based on this estimating function, our estimator is

\[
\hat{\rho}_{\text{DRL}}(\mathcal{M}_b) = \mathbb{P}_N \mathbb{P}_T[\phi(s, a, r, s'; \hat{w}^{(i)}, \hat{q}^{(i)})]
= (1 - \gamma)\mathbb{P}_N E_{p_e^{(0)}}[\hat{v}^{(i)}(s_0)] + \mathbb{P}_N \mathbb{P}_T[\hat{w}^{(i)}(s)\eta(a, s)(r + \gamma \hat{v}^{(i)}(s') - \hat{q}^{(i)}(s, a))],
\]

where \( \hat{w}^{(i)}, \hat{q}^{(i)} \) are some plug-in estimates of \( w, q \) to be used for the \( i \)th data point in the sample average, \( \mathbb{P}_N \). Recall \( \hat{v}^{(i)} \) is defined in terms of \( \hat{q}^{(i)} \). Again, we consider two cases. In the adaptive version, we have \( \hat{w}^{(i)} = \hat{w}, \hat{q}^{(i)} = \hat{q} \) shared among all data points and estimated on the whole dataset. In the cross-fold version, the sample is split in two folds (over \( N \), not over \( T \)), and \( \hat{w}^{(i)}, \hat{q}^{(i)} \) are shared within a fold and estimated on the opposite fold.

We first discuss the significance of the structure of the estimator before deriving results for the specific two versions of the estimator. First, we note that the structure of our estimator ensures that, if we were to use the oracle values for \( w \) and \( q \), then this estimator will achieve the efficiency bound.
Theorem 8 (Efficiency of $\hat{\rho}_{\text{DRL}(M_3)}$ with oracle $w, q$). Suppose the chain $C_b$ is geometrically ergodic. When $q^{(i)} = q, w^{(i)} = w$, we have $\sqrt{NT}(\hat{\rho}_{\text{DRL}(M_3)} - \rho^{\pi_e}) \overset{d}{\to} N(0, \text{EB}(M_3))$.

The conditions above are used in order to invoke the Markov chain central limit theorem (MC-CLT; see Jones [2004, Corollary 2]). One key structural aspect of our estimator is that, when we use the oracle $q$ function, the variables being time-averaged in the second term in Eq. (6) form a martingale difference sequence. This ensures that covariances across time, which would appear in the MC-CLT, are always zero. This occurs by virtue of the fact that the conditional expectation of the term inside the parentheses is zero by the definition of $q$. This essentially yields the result after some algebra. In terms of showing efficiency of a feasible (rather than oracle) estimator, what remains is to show that our estimator is equal to the above oracle estimator up to error terms that are $o_p((NT)^{-1/2})$.

Critical to this is the doubly robust structure of the estimator. Heuristically, this fact is confirmed as follows (we will prove it formally later). Consider the adaptive version. If the density ratio model is consistent, that is, $\text{plim}_{T \to \infty} \|\hat{q} - q\|_2 = 0$, then we will have

$$\text{plim}_{T \to \infty} \hat{\rho}_{\text{DRL}(M_3)} \approx (1 - \gamma)E_{p_b}^{(0)} [v(s_0)] + E_{p_b}^{(\infty)} \{w^\dagger(s)q(a, s)\{r - q(s, a) + \gamma v(s')\}]$$

$$= (1 - \gamma)E_{p_b}^{(0)} [v(s_0)] = \rho^{\pi_e},$$

where $w^\dagger$ is a convergence point of $\hat{w}$. We use “$\approx$” above because in this heuristic derivation we did not actually account for the interdependence of $\hat{q}, \hat{w}$ and the data. This viewpoint suggests that the estimator $\hat{\rho}_{\text{DRL}(M_3)}$ is given by taking the direct method and adding a control variate term.

On the other hand, if the density ratio model is consistent, that is, $\text{plim}_{T \to \infty} \|\hat{w} - w\| = 0$, then we have that

$$\text{plim}_{T \to \infty} \hat{\rho}_{\text{DRL}(M_3)} \approx E_{p_b}^{(\infty)} \{w(s)q(a, s)r\} + E_{p_b}^{(\infty)} \{w(s)\{-q(a, s)q^\dagger(s, a) + \gamma q(a, s)v^\dagger(s')\}\}$$

$$+ (1 - \gamma)E_{p_b}^{(0)} [v^\dagger(s_0)]$$

$$= E_{p_b}^{(\infty)} \{w(s)q(a, s)r\} + E_{p_b}^{(\infty)} \{w(s)\{-q(a, s)q^\dagger(s, a) + v^\dagger(s)\}\}$$

$$= E_{p_b}^{(\infty)} \{w(s)q(a, s)r\} = \rho^{\pi_e},$$

where $q^\dagger$ is a convergence point of $\hat{q}$. Note that from Eq. (7) to Eq. (8), we have used that for any $f_w(s')$ (see Lemma 13):

$$E_{p_b}^{(\infty)} \{[\gamma w(s)q(a, s) - w(s')]f_w(s')\} + (1 - \gamma)E_{p_b}^{(0)} \{f_w(s)\} = 0$$

We now proceed to prove formally the efficiency and double robustness of our estimator. We note that, relative to the case of NMDP, TMDP, and other standard semiparametric inference settings, there is an additional complexity due to the fact that our data is not iid and we must account for the cross-dependence of variables across a trajectory while still ensuring a $1/T$ scaling. In the following, we assume throughout that the chain $C_b$ generated by $P_b$ is also stationary, i.e., that $p_b^{(0)} = p_b^{(\infty)}$. Since we will eventually reach stationarity, this is a purely technical assumption to ensure that we see enough samples from the stationary
distribution. It is needed in order to invoke uniform laws of large numbers. In particular, the assumption is not necessary for the efficiency of the oracle estimator (Theorem 3), but uniform laws are necessary for controlling the inflation terms due to the estimated plug-ins.

First, we address the case of the cross-fold version, where we can avoid complex metric entropy assumptions by virtue of the unique structure of our estimator.

**Theorem 9** (Efficiency of \( \hat{\rho}_{\text{DRL}(M_3)} \) with cross-fitting). Assume \( \rho_b(0) \), \( \hat{q}(i) \) are uniformly bounded by some constant, \( \rho_b(p) = p_b(\infty) \), \( \sum_{k=1}^{\infty} \rho_k < \infty \), where \( \{ \rho_k \} \) are the \( \rho \)-mixing coefficients of \( C_b \), \( \| \hat{q}(i) - q \|_2 = o_p((NT)^{-\alpha_1}) \), \( \| \hat{w}(i) - w \|_2 = o_p((NT)^{-\alpha_2}) \), \( \alpha_1 > 0, \alpha_2 > 0, \alpha_1 + \alpha_2 \geq 1/2 \). Then, \( \sqrt{NT}(\hat{\rho}_{\text{DRL}(M_3)} - \rho^{\pi_e}) \xrightarrow{d} \mathcal{N}(0, \text{EB}(M_3)) \).

Here, due to cross-fold fitting, we are able to completely avoid any restriction on our estimators, except for requiring a slow rate. In particular, the rate can be subparametric. Crucially, this allows us to potentially use any nonparametric blackbox method, whether we can ensure good metric entropy conditions or not. However, the cross-fold version is only feasible for \( N \geq 2 \) (though \( N \) need not grow). If \( N = 1 \), we must use in-sample estimates.

For the adaptive version of our estimator, we need to control the metric entropy of our plug-in estimators. In particular, we suppose that we are given some class \( F \) of functions, \( \phi(\cdot, \cdot, \cdot; \hat{w}, \hat{q}) \). We let \( J \| (\infty, \phi, L_p(p_0^\infty)) \) be the bracketing integral, i.e., the integral of its square-root-log bracketing number under the \( L_p(p_0^\infty) \) norm (see Kosorok, 2008, p. 17). We will either use the condition that \( J \| (\infty, \phi, L_p(p_0^\infty)) \leq \infty \) for some \( 2 < p < \infty \) or that \( \phi \) is a VC-major class (see Adams and Nobel, 2010 for definition).

**Theorem 10** (Efficiency of \( \hat{\rho}_{\text{DRL}(M_3)} \) with in-sample fitting). Assume \( \rho_b(0) \), \( \hat{w}, \hat{q} \) are uniformly bounded by some constant, \( \rho_b(p) = p_b(\infty) \), \( \sum_{k=1}^{\infty} k^{2/(p-1)} \beta_k < \infty \) for some \( p > 2 \) where \( \{ \beta_k \} \) are the \( \beta \)-mixing coefficients of \( C_b \), \( J \| (\infty, \phi, L_p(p_0^\infty)) \leq \infty \) for some \( 2 < p < \infty \), \( \| \hat{q} - q \|_2 = o_p((NT)^{-\alpha_1}) \), \( \| \hat{w} - w \|_2 = o_p((NT)^{-\alpha_2}) \), \( \alpha_1 > 0, \alpha_2 \geq 0, \alpha_1 + \alpha_2 \geq 1/2 \). Then, \( \sqrt{NT}(\hat{\rho}_{\text{DRL}(M_3)} - \rho^{\pi_e}) \xrightarrow{d} \mathcal{N}(0, \text{EB}(M_3)) \).

To prove this, we invoke a uniform central limit theorem for \( \beta \)-mixing sequences (Kosorok, 2008, Theorem 11.24). The conditions (10a), (10d) are required to control a term corresponding to a stochastic equicontinuity condition. The condition (10c) is required to ensure that the inflation (aka, drift) term due to the use of estimated \( q \)- and \( w \)-functions is \( o_p((NT)^{-1/2}) \).

Next, we formalize the notion of double robustness, which ensures our estimate is consistent even if we inconsistently estimate one of the components.

**Theorem 11** (Double robustness of \( \hat{\rho}_{\text{DRL}(M_3)} \)). Assume \( \phi(\cdot, \cdot, \cdot; \hat{w}, \hat{q}) \) is VC major, \( \rho_b(p) = p_b(\infty) \), \( \| \hat{w} - w \|_2 = o_p(1) \) and \( \| \hat{q} - q \|_2 = o_p(1) \). As long as either \( w \) or \( q \) is consistent, then we have \( \text{plim}_{T \to \infty} \hat{\rho}_{\text{DRL}(M_3)} = \rho^{\pi_e} \).

The condition (11a) and (11b) are needed to invoke a uniform law of large numbers for an ergodic sequence (Adams and Nobel, 2010). Condition (11c) is a common condition to state the double robustness (Scharfstein et al., 1999).

Theorem 11 does not provide a rate or an asymptotic distribution. We next strengthen the result (and, correspondingly, the conditions) to ensure a \( 1/(NT) \) scaling and asymptotic
normality. This kind of double robustness is sometimes called model double robustness [Smucler et al., 2019] because the rates needed essentially correspond to parametric estimation and therefore the conditions refer to whether these parametric models are well-specified.

**Theorem 12** (Model double robustness of $\hat{\rho}_\text{DRL}(M_3)$). Assume (10a)-(10d) and suppose either $\|q - q^\dagger\|_2 = o_p(1)$, $\|\hat{w} - w\|_2 = o_p((NT)^{-1/2})$ or $\|q - q\|_2 = o_p((NT)^{-1/2})$, $\|\hat{w} - w\|_2 = o_p(1)$ holds. Then, $\sqrt{NT}(\hat{\rho}_\text{DRL}(M_3) - \rho^{\pi^*}) \overset{d}{\to} \mathcal{N}(0, V)$ for some $V$.

**Remark 5** (When the density of behavior policy is unknown). All of results are easily extended to the case where the behavior policy is unknown by replacing $\hat{w}(s)\hat{\eta}(s,a)$ with $\hat{w}(s)\tilde{\eta}(s,a)$, where $\tilde{\eta}(s,a)$ is some estimator for $\eta(s,a)$, e.g., $\pi^e(a|s)/\tilde{\pi}^b(a|s)$, where $\tilde{\pi}^b(a|s)$ is some estimator for the behavior policy. All of the results stay the same where conditions on $\|\hat{w} - w\|_2$ are simply replaced with the same conditions on $\|\hat{w}\tilde{\eta} - w\eta\|_2$ instead.

The remaining question is how to consistently estimate $q$-functions and stationary density ratios from a single (finite) trajectory. We next discuss how to estimate $q$ in Section 5 and how to estimate $w$ in Section 5.

### 5 Modeling the Ratio of Average Visitation Distributions

Our DRL estimator in $M_3$ relied on having an estimator for the the ratio of average visitation distributions, $w(s)$. In this section, we discuss its estimation from semiparametric inference perspective. These estimates can then be plugged into $\hat{\rho}_\text{DRL}(M_3)$.

#### 5.1 Importance Sampling Using Stationary Density Ratios

Before discussing how to estimate $w(s)$, we consider an IS-type estimator for MDPs using $w(s)$. We can transform our DRL estimator to an IS-type estimator by simply choosing $\hat{q}^{(i)} = 0$. This leads to the ergodic importance sampling (EIS) estimator

$$
\hat{\rho}_\text{EIS} = P_N P_T [\eta(a,s)\hat{w}(s)r], \quad \hat{w}(s) \approx w(s) = \frac{p_b^{(\infty)}(s)}{p_b^{(\infty)}(s)}. \quad (9)
$$

Where “$\approx$” above means “estimating.” Note that this is different than the IS estimator proposed by [Liu et al., 2018a], which is defined as an empirical approximation of

$$
\mathbb{E}_{p_b^{(\infty)}}[\eta(a,s)\hat{w}(s)r], \quad \hat{w}(s) \approx w(s) = \frac{p_{b,\gamma}^{(\infty)}(s)}{p_{b,\gamma}^{(\infty)}(s)}. \quad (10)
$$

The difference between two methods is that we use $p_b^{(\infty)}$ instead of $p_{b,\gamma}^{(\infty)}$ in the denominator of the density ratio. There are a few benefits to this. Intuitively, since we have samples from $p_b^{(\infty)}$, the former (using $p_b^{(\infty)}$) can be more efficient because, to get a sample from the distribution $p_{b,\gamma}^{(\infty)}$, we would essentially have to throw away samples with a geometric probability $(1 - \gamma)$. In fact, the performance of IS estimator based on Eq. (10) behaves badly when $\gamma < 1$ [Liu et al., 2018a, Figure 3(d)]. Moreover, using $p_b^{(\infty)}$ means we can express the estimator as a time average.
Nonetheless, unlike $\hat{\rho}_{\text{DRL}(M_3)}$, the estimator $\hat{\rho}_{\text{EIS}}$ does not have a martingale difference structure. This means that the covariance terms across the time in the MC-CLT do not drop out, potentially inflating the variance of the $\mathbb{P}_T$ average. Moreover, because it lacks a doubly robust structure, there is an inflation term due to the plug-in of an estimate, $\hat{w}$, of $w$, unlike $\hat{\rho}_{\text{DRL}(M_3)}$. This occurs even if the estimate has a parametric rate, $\|\hat{w} - w\|_2 = O_p(T^{-1/2})$, because there is no second convergence rate to cancel it. These two factors make it difficult to analyze the asymptotic MSE of $\hat{\rho}_{\text{EIS}}$. They also suggest the estimator might not be efficient.

5.2 Efficient Semiparametric Estimation

The remaining question is how to estimate $w(s) = p(\infty, \gamma)(s)/p(\infty)(s)$. Here, we take a semiparametric approach. First, we consider a characterization of $w(s)$ by modifying Theorem 4 in Liu et al. (2018a). We obtain the following lemma.

Lemma 13 (Characterization of $w(s)$). Define

$$L(w', f_w) = E_{p_b}(\infty)[(\gamma w'(s)\eta(a, s) - w'(s')) f_w(s')] + (1 - \gamma)E_{p_e}(0)[f_w(s)].$$

(11)

Then, $w(s) = p_b(\infty)(s)/p_b(\infty)(s)$ if and only if $L(w', f_w) = 0$ for all test functions $f_w(s)$.

Lemma 13 has the following intuitive interpretation. Heuristically, when $\gamma = 1$ (rigorously, a normalization condition is needed as in Liu et al., 2018a, Theorem 1), Eq. (11) is reduced to

$$E_{p_b}(\infty)[w(s)\eta(a, s) - w(s')|s'] = 0.$$  

(12)

This is closely related to a similar key relation of $\mu_k(s_k)$ used in Section 3.2, namely, $E[\nu_{k-1}|s_k] = \mu_k(s_k)$, which implies

$$E[\mu_{k-1}(s_{k-1})\eta(a_{k-1}, s_{k-1}) - \mu_k(s_k)|s_k] = 0.$$  

(13)

By taking a limit of Eq. (13) as $k \to \infty$ and replacing $\lim_{k \to \infty} \mu_k(s)$ with $w(s)$, we get Eq. (12). Notice that in Eq. (13), we obtain $\mu_k$ from $\mu_{k-1}$, whereas in Eq. (12) we obtain $w$ from itself, i.e., it solves a fixed-point equation. This change is analogous to the change in $q$-equations between the time-variant finite-horizon problem and the time-invariant infinite-horizon problem.

Suppose first that we assume a parametric model $w(s) = w(s; \beta^*)$. Then, $\beta^*$ can be estimated as a solution to an empirical approximation of Eq. (11), that is,

$$\mathbb{P}_N\mathbb{P}_T[(\gamma w(s; \beta)\eta(a, s) - w(s'; \beta)) f_w(s')] + (1 - \gamma)E_{p_e}(0)[f_w(s)] = 0,$$

(14)

for some vector-valued function $f_w$. We denote the estimator as $\hat{\beta}_{f_w}$. Note $E_{p_e}(0)[\phi(s)]$ can be exactly calculated because $p_e(0)$ is known.
Example 1 (Linear regression approach). Consider a case when our model is linear in some features of \( s \), i.e., \( w(s; \beta) = \beta^\top \phi(s) \). Then, as in linear regression, a natural choice for \( f_w(s) \) is \( \phi(s) \). The estimator of \( \hat{\beta}_\phi \) is constructed as the solution to

\[
\frac{1}{N(T + 1)} \sum_{i=1}^{N} \sum_{k=0}^{T} \phi(s_k^{(i)}) \left( \gamma \eta(a_k^{(i)}; s_k^{(i)}) \phi^\top(s_{k+1}^{(i)}) - \phi^\top(s_k^{(i)}) \right) \beta + (1 - \gamma) E_{\hat{p}_e(0)}[\phi(s)] = 0.
\]

In the finite-state-space setting, we can use \( \phi(s) = (I(s^{s1} = s), \ldots, I(s^{sd} = s)^\top \), where \( S = \{s^{s1}, \ldots, s^{sd}\} \).

More generally, for a linear or non-linear model, under the correct specification assumption, that is, there exists \( \beta^* \) such that \( w(s) = w(s; \beta^*) \), we have the following result.

Theorem 14 (Efficient estimation of \( w(s; \beta^*) \)). Define

\[
\Delta(s,a,s';\beta) = \{\gamma w(s; \beta) \eta(a, s) - w(s'; \beta)\}.
\]

Suppose the model \( w(s; \beta) \) is well-specified and that a vector-valued \( f_w \) is given such that \( L(w(s; \beta), f_w) = 0 \iff \beta = \beta^* \). Further assume standard regularity conditions, i.e., that the chain \( C_b \) is geometrically ergodic, that the parameter space of \( \beta \) is compact, that \( \beta^* \) is in the interior of the parameter space, that \( w(s; \beta) \) is a \( C^2 \)-function with respect to \( \beta \) and the first and second derivatives are uniformly bounded, and that for any \( \alpha \) with \( ||\alpha|| = 1 \) we have \( \epsilon > 0 \) with \( E[|\Delta(s,a,s'; \beta)\alpha^\top f_w(s')|^{2+\epsilon}]_{\beta=\beta^*} < \infty \). The lower bound for the asymptotic MSE for estimating \( \beta^* \) scaled by \( NT \) is

\[
E_{\hat{p}_b(\infty)}[\nabla_\beta m_w(s'; \beta) v_w^{-1}(s'; \beta) \nabla_\beta^\top m_w(s'; \beta)]^{-1}_{\beta=\beta^*},
\]

where \( m_w(s'; \beta) = E_{\hat{p}_b(\infty)}[\Delta(s,a,s'; \beta)|s'], v_w(s'; \beta) = \text{var}_{\hat{p}_b(\infty)}[\Delta(s,a,s'; \beta)|s'] \).

This bound is achieved when the estimator \( \hat{\beta}_{f_w} \) with

\[
f_w(s) = \nabla_\beta m_w(s; \beta) v_w^{-1}(s; \beta)|_{\beta=\beta^*}.
\]

(15)

Importantly, regardless of the choice of \( f_w \), the rate of \( ||\hat{w}(s; \beta_{f_w}) - w(s)||_2 \) will be \( O_p((NT)^{-1/2}) \). Still, efficient estimation is preferred so that the constant term can be smaller. Practically, we do not know the efficient \( f_w(s) \) in Eq. (15). One way is to parametrically estimate it. This type of estimator would be locally efficient estimator in the sense that it is efficient when the model for \( f_w(s) \) is well-specified (Tsiatis, 2006). Another approach is to use a sieve GMM estimator, using a basis expansion for \( f_w(s) \) (Carrasco and Florens, 2014; Hahn, 1997).

To extend the above approach to a nonparametric estimation of \( w \), we can also take a basis expansion \( w \). This is most easily done using the linear regression approach as in Example 1. We can let \( w(s; \beta_N) = \sum_{j=1}^{d_N} \beta_j \phi_j(s) \) where \( \phi_1, \phi_2, \ldots \) is a basis expansion of \( L^2 \) and \( d_N \to \infty \) as we collect more data. Under appropriate regularity conditions and smoothness conditions on \( w \), we can obtain rates on \( ||w(\cdot; \beta_N) - w||_2 \) without assuming correct parametric specification (Chen and Shen, 1998). This provides a means to estimate \( w \) for \( \hat{p}_{\text{DRL}(M_3)} \), either parametrically or nonparametrically.

Because of the doubly robust structure of \( \hat{p}_{\text{DRL}(M_3)} \), it did not matter how we estimated \( w \) as long as we had a (subparametric) rate. This is not true for \( \hat{p}_{\text{EIS}} \). We can, however, derive its asymptotics for the particular parametric approach above.
Theorem 15 (Asymptotic property of $\hat{\rho}_{\text{EIS}}$). Suppose the conditions of Theorem 14 hold and that $\mathbb{G}_{N,T}[r\eta(a,s)w(s;\beta_{f_w})] - \mathbb{G}_{N,T}[r\eta(a,s)w(s;\beta^*)] = o_p(1)$, where $\mathbb{G}_{N,T} = \sqrt{N}\mathbb{E}[(\mathbb{P}_N - \mathbb{P}) - \mathbb{E})]$ is the empirical process. Then, $\hat{\rho}_{\text{EIS}}$ is $\sqrt{N}$-consistent. More specifically,

$$\hat{\rho}_{\text{EIS}} = o_p((NT)^{-1/2}) + \mathbb{P}_N\mathbb{P}_T \left[ w(s)\eta(a,s)r(s,a) \right] + E[\nabla_\beta w(s;\beta)\eta(a,s)r(s,a)]E[f_w(s')\nabla_\beta \Delta(s,a,s';\beta)]^{-1}\Delta(s,a,s';\beta)f_w(s') | \beta = \beta^*]. \quad (16)$$

Note the technical condition $\mathbb{G}_{N,T}[r\eta(a,s)w(s;\beta_{f_w})] - \mathbb{G}_{N,T}[r\eta(a,s)w(s;\beta^*)] = o_p(1)$ can potentially be verified as in the proof of Theorems 9 and 10. Also note that the efficient $f_w$ in Eq. (15) for estimating $w$ does not necessarily minimize the asymptotic MSE of $\hat{\rho}_{\text{EIS}}$ because the covariance term of two terms in right hand side of Eq. (16) is not zero.

6 Modeling the $q$-function

In this section, we discuss from a semiparametric inference perspective how to estimate the $q$-function in an off-policy manner, potentially from only one trajectory. Our approach can be seen as a generalization of LSTDQ (Lagoudakis and Parr 2004). The estimated $q$-function we obtain can be used in our estimator, $\hat{\rho}_{\text{DRL}(\mathcal{M}_I)}$.

By definition, the $q$-function is characterized as a solution to

$$q(s_k,a_k) = E[r_k|s_k,a_k] + \gamma E[\pi' [q(s_{k+1},a_{k+1})|s_{k+1}] | s_k,a_k].$$

Assume a parametric model for the $q$-function, $q(s,a) = q(s,a;\beta)$. Then, the parameter $\beta$ can be estimated using the following recursive estimating equation:

$$E[\epsilon_q(s_k,a_k, r_k, s_{k+1};\beta)|s_k,a_k] = 0,$$

where $\epsilon_q(s,a,r,s'\beta) = r + \gamma E_{\pi'}(q(s',a';\beta)|s') - q(s,a)\beta$.

This implies that for any test function $f_q(s,a)$,

$$E_{\pi'}(f_q(s,a)|\epsilon_q(s,a,r,s';\beta)] = 0. \quad (17)$$

More specifically, given a vector-valued $f_q(s,a)$, we can define an estimator $\hat{\beta}_{\hat{f}_q}$ as the solution to

$$\mathbb{P}_N\mathbb{P}_T[f_q(s,a)|\epsilon_q(s,a,r,s';\beta)] = 0. \quad (18)$$

Example 2 (LSTDQ). When $q(s,a;\beta) = \beta^\top \phi(s,a)$ and $f_q(s,a) = \phi(s,a)$, this leads to the LSTDQ method (Lagoudakis and Parr 2004):

$$\left( \sum_{i=0}^{N} \sum_{k=0}^{T} \phi(s_k^{(i)}, a_k^{(i)})[\phi^\top(s_k^{(i)}, a_k^{(i)})] - \gamma E_{\pi'}[\phi^\top(s_{k+1}^{(i)}, a_{k+1}^{(i)})|s_{k+1}^{(i)}] \right)^{-1} \left\{ \sum_{i=0}^{N} \sum_{k=0}^{T} r_k^{(i)} \phi(s_k^{(i)}, a_k^{(i)}) \right\}.$$

More generally, for a linear or non-linear model, under the correct specification assumption, that is, that there exists some $\beta^*$ such that $q(s,a) = q(s,a;\beta^*)$, we have the following result.
Theorem 16 (Efficient estimation of $q(s,a;\beta)$. Suppose the model $q(s,a;\beta)$ is well-specified and that a vector-valued $f_q$ is given such that (Eq. [17] hold) $\iff \beta = \beta^*$. Further assume standard regularity conditions, i.e., that the chain $\mathcal{C}_b$ is geometrically ergodic, that the parameter space is compact, that $\beta^*$ is in the interior of the parameter space, that $q(s,a;\beta)$ is $C^2$-function with respect to $\beta$ and that the first and second derivatives are uniformly bounded, and that for any $\alpha$ with $\|\alpha\| = 1$ we have $\epsilon > 0$ with $E_{p_b}(\|e_q(s,a,r,s';\beta)\alpha^T f_q(s,a)\|^{2+\epsilon}) |_{\beta=\beta^*} > 0$. The lower bound for the asymptotic MSE for estimating $\beta^*$ scaled by $NT$ is

$$V_\beta = E_{p_b}(\|\nabla_\beta m_q(s,a;\beta) v_q^{-1}(s,a;\beta) \nabla_\beta m_q(s,a;\beta)\|^{-1}) |_{\beta=\beta^*}$$

where $m_q(s,a;\beta) = E_{p_b}(e_q(s,a,r,s';\beta)|s,a]$, $v_q(s,a) = \text{var}_{p_b}(e_q(s,a,r,s';\beta)|s,a]$. This bound is achieved when

$$f_q(s,a) = \nabla_\beta m_q(s,a;\beta) v_q^{-1}(s,a;\beta) |_{\beta=\beta^*}. \quad (19)$$

Importantly, regardless of the choice of $f_q$, the rate $\|q(\cdot,\cdot;\beta_f) - q\|_2$ is $O_p((NT)^{-1/2})$. Nonetheless, efficient estimation is preferred. Practically, we do not know the efficient $f_q$ in Eq. [19]. One way is parametrically estimating it and the other way is a sieve generalized method of moments (GMM) estimator, using a basis expansion for $f_q$.

We can also extend the approach to achieve nonparametric estimation of $q$. This most easily done by extending the LSTDQ approach in Example 2. We simply let $q(s,a;\beta_N) = \sum_{j=1}^{d_N} \beta_j \phi_j(s,a)$ where $\phi_1,\phi_2,\ldots$ is a basis expansion of $L^2$ and $d_N \to \infty$ as we collect more data. Given regularity conditions and smoothness conditions on $q$, we can obtain rates on $\|q(\cdot,\cdot;\beta) - q\|_2$ without assuming correct parametric specification (Chen and Shen 1998). This provides a means to estimate $q$ for $\hat{\rho}_{\text{DRL(M3)}}$, either parametrically or nonparametrically.

If we use $q$ as estimated parametrically above, we can also establish the asymptotic behavior of $\hat{\rho}_{\text{DM}}$. Again, as in the case of $\hat{\rho}_{\text{EIS}}$, because $\hat{\rho}_{\text{DM}}$ lacks the doubly robust structure, we must have parametric rates on $q$-estimation in order to achieve $1/(NT)$ MSE scaling in the below, unlike the case of $\hat{\rho}_{\text{DRL(M3)}}$ where $q$-estimation can have slow nonparametric rates.

Theorem 17 (Asymptotic property of $\hat{\rho}_{\text{DM}}$). Let $\hat{\rho}_{\text{DM}} = (1-\gamma)E_{p_c}(E_{\pi}\{q(s,a;\hat{\beta}_{f_q})|s\}).$ Suppose the assumptions of Theorem 16 hold. Then $\sqrt{NT}(\hat{\rho}_{\text{DM}} - \rho^*) \overset{d}{\to} N(0,V_{\text{DM}})$ where

$$V_{\text{DM}} = (1-\gamma)^2E_{p_c}(E_{\pi}\{\nabla_\beta q(s,a;\beta)|s\})\nabla_\beta E_{p_c}(E_{\pi}\{\nabla_\beta q(s,a;\beta)|s\}) |_{\beta=\beta^*}.$$ 

Remark 6. Luckett et al. (2018); Ueno et al. (2011) considered related semiparametric estimation techniques for the $v$-function. For our estimator, we need $q$-function estimates.

7 Experimental Results

In this section, we conduct experiments to compare our method with existing off-policy evaluation methods. We focus on methods that take plug-in estimates of nuisances such as
the standard IS, DR, and DM. The comparison is therefore on how we use these plug-ins. We conduct our experiment in the Taxi environment. For detail on this environment, see Liu et al. (2018a).

We set our target evaluation policy to be the final policy \( \pi^e = \pi^* \) after running \( q \)-learning for 1000 iterations. We set another policy \( \pi^+ \) as the result after 150 iterations. The behavior policy is then defined as \( \pi^b = \alpha \pi^* + (1 - \alpha) \pi^+ \), where we range \( \alpha \) to vary the overlap. We show results for \( \alpha = 0.2, 0.6 \) here and provide additional results for \( \alpha = 0.4, 0.8 \) in Appendix C. We consider the case with the behavior policy known and set \( \gamma = 0.98 \). Note that this \( \pi^* \), \( \pi^+ \) are fixed in each setting.

We estimate all \( w \)-functions following Example 1. For \( q \)-functions, we use a value iteration for the approximated MDP based on the empirical distribution. Then, we compare \( \hat{\rho}_{IS} \), \( \hat{\rho}_{DR}(M_1) \), \( \hat{\rho}_{EIS} \), \( \hat{\rho}_{DM} \), and \( \hat{\rho}_{DR}(M_3) \). We consider observing a single trajectory \( (N = 1) \) of increasing length \( T \), \( T \in [50000, 100000, 200000, 400000] \). For each, we consider 200 replications. Note that we use adaptive (in-sample) fitting and not cross-fitting because \( N = 1 \). In addition, we do not compare to a marginalized importance sampling estimator or to \( \hat{\rho}_{DR}(M_2) \) because \( \mu_t \) cannot be estimated with \( N = 1 \) (e.g., the empirical estimated marginal importance \( \hat{\mu}_t \) is just \( \nu_t \)).

To study the effect of double robust property, we consider three settings.

1. Both \( w \)-model and \( q \)-model are correct.
2. Only \( w \)-model is correct: we add noise \( N(1.0, 1.0) \) to \( \hat{q}(s,a) \).
3. Only \( q \)-model is correct: we add noise \( N(1.0, 1.0) \) to \( \hat{w}(s) \).

### 7.1 Results and Discussion

We report the resulting MSE over the replications for each estimator in each setting in Figs. 1 to 6.

First, we note that the estimator \( \hat{\rho}_{DR}(M_3) \) handily outperforms the standard IS and DR estimators, \( \hat{\rho}_{IS} \), \( \hat{\rho}_{DR}(M_1) \), \( \hat{\rho}_{DR}(M_3) \), in every setting. This is owed to the fact that these do not leverage the MDP structure. The competitive comparison is of course to DM and EIS.

We find that, in the large-sample regime, \( \hat{\rho}_{DR}(M_3) \) dominates all other estimators across all settings. First, for \( T = 400000 \), it has the lowest MSE among all estimators for each setting. Second, while in some settings it has MSE similar to another method, it beats it handily in another setting. Compared to DM, the MSE is similar when the \( q \)-function is well-specified but \( \hat{\rho}_{DR}(M_3) \) does much better when \( q \) is ill-specified. Compared to EIS, the MSE is similar when both the \( w \)-function is well-specified and there is good overlap but \( \hat{\rho}_{DR}(M_3) \) performs much better when either specification or overlap fails. This is of course owed to the doubly robust structure and the efficiency of \( \hat{\rho}_{DR}(M_3) \).

In the small-to-medium sample regime, \( \hat{\rho}_{DR}(M_3) \) performs the best among all estimators except when overlap is good (\( \alpha = 0.6 \)) and \( w \) is well specified (settings (2) and (3)). In these cases, for the small-to-medium sample regime, EIS performs better. However, as in the large-sample regime, it performs much worse in small-to-medium samples too when overlap is bad or when \( w \) is misspecified. In particular, in setting (2) with \( \alpha = 0.2 \), \( \hat{\rho}_{DR}(M_3) \) has performance much better than all other estimators across the sample-size regimes.
Because having either parametric misspecification or nonparametric rates for \( \hat{w} \) and \( \hat{q} \) is unavoidable in practice (for continuous state-action spaces), the estimator \( \hat{\rho}_{\text{DRL}(M_a)} \) is superior. This is doubly true when overlap can be weak.
8 Conclusions

We established the efficiency bound for OPE in a time-invariant Markov decision process in the regime where $N$ is (potentially) finite and $T \to \infty$. This novel lower bound quantifies how fast one could hope to estimate policy value in a model usually assumed in RL. According to our results, many IS and DR OPE estimators used in RL are in fact not leveraging this structure to the fullest and are inefficient. This leads to MSE that is suboptimal in rate, not just in leading coefficient. We instead proposed the first efficient estimator achieving the efficiency bound, while also enjoying a double robustness property at the same time. We hope our work inspires others to further develop estimators that build on ours by leveraging MDP structure as we have here and perhaps combining this with ideas like balancing [Kallus 2018], stability [Kallus and Uehara 2019a], or blending [Thomas and Brunskill 2016] that can improve the finite-sample performance in addition to our asymptotic efficiency.

References

T. Adams and A. Nobel. Uniform convergence of vapnik-chervonenkis classes under ergodic sampling. *Annals of Probability*, 38, 2010.

D. P. Bertsekas. *Dynamic programming and optimal control*. Athena Scientific optimization and computation series. Athena Scientific, Belmont, Mass, 4th ed. edition, 2012.

P. J. Bickel and J. Kwon. Inference for semiparametric models: Some questions and an answer. *Statistica Sinica*, 11:863–886, 2001.

P. J. Bickel, C. A. J. Klaassen, Y. Ritov, and J. A. Wellner. *Efficient and Adaptive Estimation for Semiparametric Models*. Springer, 1998.

M. Carrasco and J.-P. Florens. On the asymptotic efficiency of gmm. *Econometric Theory*, 30:372–406, 2014.

G. Casella. *Statistical inference*. Duxbury advanced series. Duxbury/Thomson Learning, Australia ; Pacific Grove, Calif., 2nd ed. edition, 2002.

X. Chen and X. Shen. Sieve extremum estimates for weakly dependent data. *Econometrica*, 66:289–314, 1998.

V. Chernozhukov, D. Chetverikov, M. Demirer, E. Duflo, C. Hansen, W. Newey, and J. Robins. Double/debiased machine learning for treatment and structural parameters. *Econometrics Journal*, 21:C1–C68, 2018.

M. Dudk, D. Erhan, J. Langford, and L. Li. Doubly robust policy evaluation and optimization. *Statistical Science*, 29:485–511, 2014.

M. Farajtabar, Y. Chow, and M. Ghavamzadeh. More robust doubly robust off-policy evaluation. *In Proceedings of the 35th International Conference on Machine Learning*, pages 1447–1456, 2018.
O. Gottesman, F. Johansson, M. Komorowski, A. Faisal, D. Sontag, F. Doshi-Velez, and L. A. Celi. Guidelines for reinforcement learning in healthcare. *Nat Med*, 25:16–18, 2019.

P. E. Greenwood and W. Wefelmeyer. Efficiency of empirical estimators for markov chains. *The Annals of Statistics*, 23:132–143, 1995.

J. Hahn. Efficient estimation of panel data models with sequential moment restrictions. *Journal of Econometrics*, 79:1–21, 1997.

J. Hájek. A characterization of limiting distributions of regular estimates. *Zeitschrift für Wahrscheinlichkeitstheorie und verwandte Gebiete*, 14:323–330, 1970.

J. Hájek. Local asymptotic minimax and admissibility in estimation. In *Proceedings of the sixth Berkeley symposium on mathematical statistics and probability*, volume 1, pages 175–194, 1972.

K. Hirano, G. Imbens, and G. Ridder. Efficient estimation of average treatment effects using the estimated propensity score. *Econometrica*, 71:1161–1189, 2003.

N. Jiang and L. Li. Doubly robust off-policy value evaluation for reinforcement learning. In *Proceedings of the 33rd International Conference on International Conference on Machine Learning-Volume*, pages 652–661, 2016.

G. L. Jones. On the markov chain central limit theorem. *Probab. Surveys*, 1(299-320): 299–320, 2004.

N. Kallus. Balanced policy evaluation and learning. In *Advances in Neural Information Processing Systems*, pages 8895–8906, 2018.

N. Kallus and M. Uehara. Intrinsically efficient, stable, and bounded off-policy evaluation for reinforcement learning. *arXiv preprint arXiv:1906.03735*, 2019a.

N. Kallus and M. Uehara. Double reinforcement learning for efficient off-policy evaluation in markov decision processes. *arXiv preprint arXiv:1908.08526*, 2019b.

I. Komunjer and Q. Vuong. Semiparametric efficiency bound in time-series models for conditional quantiles. *Econometric Theory*, 26:383–405, 2010.

M. R. Kosorok. *Introduction to Empirical Processes and Semiparametric Inference*. Springer Series in Statistics. Springer New York, New York, NY, 2008.

M. Lagoudakis and R. Parr. Least-squares policy iteration. *Journal of Machine Learning Research*, 4:1107–1149, 2004.

L. Li, R. Munos, and C. Szepesvari. Toward minimax off-policy value estimation. In *Proceedings of the 18th International Conference on Artificial Intelligence and Statistics*, pages 608–616, 2015.

Q. Liu, L. Li, Z. Tang, and D. Zhou. Breaking the curse of horizon: Infinite-horizon off-policy estimation. In *Advances in Neural Information Processing Systems 31*, pages 5356–5366. 2018a.
Y. Liu, O. Gottesman, A. Raghu, M. Komorowski, A. A. Faisal, F. Doshi-Velez, and E. Brunskill. Representation balancing mdps for off-policy policy evaluation. In Advances in Neural Information Processing Systems 31, pages 2644–2653. 2018b.

D. J. Luckett, E. B. Laber, A. R. Kahkoska, D. M. Maahs, E. Mayer-Davis, and M. R. Kosorok. Estimating dynamic treatment regimes in mobile health using v-learning. Journal of the American Statistical Association, pages 1–34, 2018.

A. R. Mahmood, H. P. van Hasselt, and R. S. Sutton. Weighted importance sampling for off-policy learning with linear function approximation. In Advances in Neural Information Processing Systems 27, pages 3014–3022. 2014.

T. Mandel, Y. Liu, S. Levine, E. Brunskill, and Z. Popovic. Off-policy evaluation across representations with applications to educational games. In Proceedings of the 13th International Conference on Autonomous Agents and Multi-agent Systems, pages 1077–1084, 2014.

S. Meyn and R. L. Tweedie. Markov Chains and Stochastic Stability. Cambridge University Press, New York, 2nd ed. edition, 2009.

R. Munos, T. Stepleton, A. Harutyunyan, and M. Bellemare. Safe and efficient off-policy reinforcement learning. In Advances in Neural Information Processing Systems 29, pages 1054–1062. 2016.

S. A. Murphy. Optimal dynamic treatment regimes. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 65:331–355, 2003.

S. A. Murphy, M. J. Van Der Laan, and J. M. Robins. Marginal mean models for dynamic regimes. Journal of the American Statistical Association, 96:1410–1423, 2001.

D. Precup, R. Sutton, and S. Singh. Eligibility traces for off-policy policy evaluation. In Proceedings of the 17th International Conference on Machine Learning, pages 759–766, 2000.

A. Rotnitzky, E. Smucler, and J. Robins. Characterization of parameters with a mixed bias property. arXiv preprint arXiv:1509.02556, 2019.

D. Scharfstein, A. Rotnizky, and J. M. Robins. Adjusting for nonignorable dropout using semi-parametric models. Journal of the American Statistical Association, 94:1096–1146, 1999.

E. Smucler, A. Rotnitzky, and J. M. Robins. A unifying approach for doubly-robust $\ell_1$ regularized estimation of causal contrasts. arXiv preprint arXiv:1904.03737, 2019.

C. Stein. Efficient nonparametric testing and estimation. Proc. Third Berkeley Symp. on Math. Statist. and, Prob.(Vol.1):187–195, 1956.

R. S. Sutton and A. G. Barto. Reinforcement learning: An introduction. MIT press, Cambridge, 2018.
P. Thomas and E. Brunskill. Data-efficient off-policy policy evaluation for reinforcement learning. *In Proceedings of the 33rd International Conference on Machine Learning*, pages 2139–2148, 2016.

G. Tripathi. A matrix extension of the Cauchy-Schwarz inequality. *Economics Letters*, 63:1–3, 1999.

A. A. Tsiatis. *Semiparametric Theory and Missing Data*. Springer Series in Statistics. Springer New York, New York, NY, 2006.

T. Ueno, M. Kawanabe, T. Morii, S.-I. Maeda, and S. Ishii. Generalized td learning. *Journal of Machine Learning Research*, 12:1977–2020, 2011.

A. W. van der Vaart. *Asymptotic statistics*. Cambridge University Press, Cambridge, UK, 1998.

T. Xie, Y. Ma, and Y.-X. Wang. Optimal off-policy evaluation for reinforcement learning with marginalized importance sampling. *arXiv preprint arXiv:1906.03393*, 2019.
A Notation

We first summarize the notation we use in Table 2 and the abbreviations we use in Appendix A. Notice in particular that, following empirical process theory literature, in the proofs we also use $\mathbb{P}$ to denote expectations (interchangeably and even simultaneously with E).

Table 2: Notation

| Notation | Description |
|----------|-------------|
| $(S, A, R, p, \gamma)$ | MDP |
| $p^{(0)}_b(s), p^{(0)}_e(s)$ | Initial distributions |
| $J$ | $\{s_t, a_t, r_t\}_{t=0}^\infty$ |
| $J_{s_t}, J_{a_t}$ | History up to $s_t, a_t$, respectively |
| $\mathcal{H}_{s_t}, \mathcal{H}_{a_t}$ | History up to $s_t, a_t$, respectively, excluding reward variables |
| $r_t, s_t, a_t$ | Reward, state, and action at $t$ |
| $\rho^\pi$ | Policy value, $\lim_{T \to \infty} c_T(\gamma) \mathbb{E}_{\pi} \left[ \sum_{t=0}^T \gamma^t r_t \right]$ |
| $\rho^\pi_T$ | $c_T(\gamma) \mathbb{E}_{\pi} \left[ \sum_{t=0}^T \gamma^t r_t \right]$ |
| $p_{\pi, \gamma}^{(\infty)}(s)$ | Average visitation distribution of the policy $\pi$ with discount rate $\gamma$ |
| $p_{\pi}^{(\infty)}(s)$ | Stationary distribution |
| $p_{\pi}^{(\infty)}(s, a, r, s')$ | $p_{\pi}^{(\infty)}(s)\pi(a|s)p(s'|s, a)p(r|s, a)$ |
| $w(s)$ | $p_{\pi, \gamma}^{(\infty)}(s)/p_{\pi}^{(\infty)}(s)$ |
| $\nabla_\beta$ | Differentiation with respect to $\beta$ |
| $\pi^e(a|s), \pi^b(a|s)$ | Target and behavior policies respectively |
| $v(s)$ | Value function |
| $q(s, a)$ | $q$-function |
| $\nu_t(\mathcal{H}_{a_t})$ | Cumulative density ratio $\prod_{k=0}^t \pi_k^e/\pi_k^b$ |
| $\mu_t(s_t, a_t)$ | Marginal density ratio $\mathbb{E}[\nu_t | s_t, a_t]$ |
| $\eta(s, a)$ | Instantaneous density ratio $\pi^e(a|s)/\pi^b(a|s)$ |
| $C, R_{\text{max}}$ | Upper bound of density ratio and reward, respectively |
| $\| \cdot \|_p$ | $L^p$-norm $\mathbb{E}[|f|^p]^{1/p}$ |
| $\preceq$ | Inequality up to constant |
| $\mathbb{E}_{\pi}[\cdot], \mathbb{P}_{\pi}$ | Expectation with respect to a sample from a policy $\pi$ |
| $\mathbb{E}[\cdot], \mathbb{P}$ | Same as above for $\pi = \pi^b$ |
| $\mathbb{E}_N[\cdot], \mathbb{P}_N, \mathbb{P}_T$ | Empirical or time average (based on sample from a behavior policy) |
| $\mathcal{D}_1, \mathcal{D}_2$ | The split samples when using cross-fold fitting, $\mathcal{D}_1 \cup \mathcal{D}_2 = \{1, \ldots, N\}$ |
| $N_j$ | The size of $\mathcal{D}_j$ |
| $\mathbb{E}_{N_j}, \mathbb{P}_{N_j}$ | Empirical expectation on $\mathcal{D}_j$ |
| $\mathbb{G}_N$ | Empirical process $\sqrt{N}(\mathbb{P}_N - \mathbb{P})$ |
| $A_N = o_p(a_N)$ | The term $A_N/a_N$ converges to zero in probability |
| $A_N = O_p(a_N)$ | The term $A_N/a_N$ is bounded in probability |
B Proofs

Proof of Theorems 1 and 2. We prove Theorem 2. The proof of Theorem 1 is similar. Consider some parametric models given by parameterizing the reward and transition probabilities up to $T$: $p_t(r_t|s_t, a_t; \theta_t)$, $p_t(s_{t+1}|s_t, a_t; \theta_t)$, and $\theta = (\theta_{1T}, \theta_{2T}, \ldots, \theta_{ST})^\top$. Here, because of the independence of the trajectories, we have

$$\text{NCR} \left[ \{p_t(r_t^{(i)}|s_t^{(i)}, a_t^{(i)}; \theta_t)\}_{t=0}^T, \{p_t(s_{t+1}^{(i)}|s_t^{(i)}, a_t^{(i)}; \theta_t)\}_{t=0}^T, \rho_T^{\pi^{(i)}} \right]$$

$$= \text{CR} \left[ \{p_t(r_t|s_t, a_t; \theta_t)\}_{t=0}^T, \{p_t(s_{t+1}|s_t, a_t; \theta_t)\}_{t=0}^T, \rho_T^{\pi} \right]$$

By some algebra, Cramér-Rao lower bound

$$\text{CR} \left[ \{p_t(r_t|s_t, a_t; \theta_t)\}_{t=0}^T, \{p_t(s_{t+1}|s_t, a_t; \theta_t)\}_{t=0}^T, \rho_T^{\pi} \right]$$

is

$$\sum_{c=0}^T I^n_c J_c^{-1} I^n_c + \sum_{c=0}^T J^n_c J_c^{-1} J^n_c,$$

(20)

where

$$g_{r_c|s_c,a_c} = \nabla_{\theta} \log p_c(r_c|s_c, a_c; \theta_c), g_{s_{c+1}|s_c,a_c} = \nabla_{\theta} \log p_c(s_{c+1}|s_c, a_c; \theta_c),$$

$$I_c = E[g_{r_c|s_c,a_c}g_{r_c|s_c,a_c}^\top], J_c = E[g_{s_{c+1}|s_c,a_c}g_{s_{c+1}|s_c,a_c}^\top],$$

$$I^n_c = \sum_{c=0}^T E_{\pi^b} \left[ \gamma^c \mu_c(s_c, a_c) \{ r_c - E(r_c|s_c, a_c) \} g_{r_c|s_c,a_c}^\top \right],$$

$$J^n_c = E_{\pi^b} \left[ \gamma^c \mu_c(s_c, a_c) \left( \sum_{t=c+1}^T r_t|s_{t+1} \right) - E_{\pi^c} \left( \sum_{t=c+1}^T r_t|s_c, a_c \right) \right] g_{s_{c+1}|s_c,a_c}^\top.$$

By Cauchy-Schwarz inequality (Tripathi 1999), we have

$$E_{p(x)}[a(x)b(x)] \leq E_{p(x)}[a^2(x)] E_{p(x)}[b^2(x)].$$

Then, Eq. (20) is upper bounded by

$$\sum_{c=0}^{T-1} E_{\pi^b} \left[ \gamma^{2c} \mu_c(s_c, a_c)^2 \{ (r_c - E(r_c|s_c, a_c))^2 + (v_{c+1}(s_{c+1}) - q_c(s_c, a_c) + E[r_c|s_c, a_c])^2 \} \right]$$

$$+ E_{\pi^b}[\gamma^T \mu_T(s_T, a_T)^2(r_T - E[r_T|s_T, a_T])]$$

$$= \sum_{c=0}^{T-1} E_{\pi^b}[\gamma^{2c} \mu_c(s_c, a_c)^2(r_c - E(r_c|s_c, a_c))^2 + v_{c+1}(s_{c+1}) - q_c(s_c, a_c) + E[r_c|s_c, a_c])^2]$$

$$+ E_{\pi^b}[\gamma^T \mu_T(s_T, a_T)^2(r_T - E[r_T|s_T, a_T])^2]$$

$$= \sum_{c=0}^T E_{\pi^b}[\gamma^{2c} \mu_c(s_c, a_c)^2(r_c + v_{c+1}(s_{c+1}) - q_c(s_c, a_c))^2]$$

$$+ E_{\pi^b}[\gamma^T \mu_T(s_T, a_T)^2(r_T - E[r_T|s_T, a_T])^2]$$

$$= \sum_{c=1}^{T+1} E_{\pi^b}[\gamma^{2c-1} \mu_{c-1}(s_{c-1}, a_{c-1})^2 \text{var}[r_{c-1} + v_{c}(s_c)|s_{c-1}, a_{c-1}]],$$

(24)
where $v_{T+1} = 0$.

From Eq. (21) to Eq. (22), we use the fact that the crossing term is zero:

$$E_{\pi_b} [\mu_c(s_c, a_c) \{v_{c+1}(s_{c+1}) − q_c(s_c, a_c) + E(r_c|s_c, a_c)\}] = E_{\pi_b} [\mu_c(s_c, a_c) \{E(r_c|s_c, a_c) − E(r_c|s_c, a_c)\}] = 0.$$

From Eq. (23) to Eq. (24), we use a variance decomposition:

$$E[\mu_c(s_c, a_c)^2] = \text{var}[\mu_c(s_c, a_c)] + E[\text{var}[\mu_c(s_c, a_c)|s_c, a_c]]$$

where $c$ and $p$ are such as Fourier series functions.

Lemma 18. Define regular parametric models given by and $\pi_c(s_t+1|s_t, a_t)$ \(\pi_c(s_t+1|s_t, a_t) = \exp(\theta_{s_t}^\top b(s_t, a_t))\)
and $p_t(s_t+1|s_t, a_t)$ \(p_t(s_t+1|s_t, a_t) = \exp(\theta_{s_t}^\top b(s_t, a_t))\), where $\theta_{s_t}$, $\theta_{s_t}$ are components of $\theta$ and $b(s_t, a_t)$ is a vector of some truncated basis functions expanding mean zero $L^2$-space such as Fourier series functions.

Finally, we will show that the upper bound is actually the supremum over parametric models. Define regular parametric models given by and $\pi_t(r_t|s_t, a_t; \theta_{r_t}) \propto p_t(r_t|s_t, a_t)$ \(p_t(r_t|s_t, a_t) = \exp(\theta_{r_t}^\top b(s_t, a_t))\)
and $p_t(s_t+1|s_t, a_t)$ \(p_t(s_t+1|s_t, a_t) = \exp(\theta_{s_t}^\top b(s_t, a_t))\), where $\theta_{r_t}$, $\theta_{s_t}$ are components of $\theta$ and $b(s_t, a_t)$ is a vector of some truncated basis functions expanding mean zero $L^2$-space such as Fourier series functions.

To proceed, we first prove the following general result.

**Lemma 18.**

$$\lim_{N \to \infty} NCR \left[ \left\{ p_t(r_t|s_t, a_t; \theta_{r_t}) \right\}_{t=0, i=1}, \left\{ p_t(s_t+1|s_t, a_t; \theta_{s_t}) \right\}_{t=0, i=1} \right], c_T(\gamma) \rho_T^\pi.$$
Then, the statement is concluded by noting that the score functions of \( p_t(\tau_t|s_t, a_t; \theta_t) \) \( \propto p(\tau_t|s_t, a_t) \exp(\theta^T b(s_t, a_t)) \) and \( p_t(s_{t+1}|s_t, a_t; \theta_{s_{t+1}}) \propto p(s_{t+1}|s_t, a_t) \exp(\theta^{s_{t+1}} b(s_t, a_t)) \) at \( \theta_{s_t} = \theta_{\tau_t} = 0 \) are \( b(s_t, a_t) \).

**Proof of Corollary 3.** We prove the statement for NMDP. For TMDP, the statement is confirmed similarly. We have

\[
\lim_{T \to \infty} (1 - \gamma)^2 \sum_{k=0}^{T} E[\gamma^{2(k-1)} \nu_k^2 \var{r_k + v(s_k)|s_{k-1}, a_{k-1}}] \\
\preceq \lim_{T \to \infty} (1 - \gamma)^2 \sum_{k=0}^{T} \gamma^{2(k-1)} ||\nu_k||^2 < \infty.
\]

The final statement is clear because TMDP is inincluded in NMDP.

**Proof of Theorems 4 and 5.** For simplicity, we assume \( N = 1 \). The extension to general \( N \) is straightforward. By some algebra, the scaled Cramér-Rao lower bound

\[
\lim_{T \to \infty} (T + 1) CR \left( \{p(r_i|s_i, a_i; \theta_{r_i})\}_{i=0}^{T}, \{p(s_{i+1}|s_i, a_i; \theta_{s_i})\}_{i=0}^{T} \right), c_T(\gamma) \rho_T^c
\]

is

\[
A_\infty I_\infty^{-1} A_\infty + C_\infty J_\infty^{-1} C_\infty
\]

where \( A_\infty = \lim_{T \to \infty} A_T, C_\infty = \lim_{T \to \infty} C_T, \\
A_T = c_T(\gamma) E_{\pi^c} \left[ \sum_{c=0}^{T} \gamma^c r_c g^T_{r_{c+1}|s_{c+1}, a_{c+1}} \right], C_T = c_T(\gamma) \gamma \sum_{c=0}^{T} \gamma^c \sum_{t=c+1}^{T} E_{\pi^c} \left[ \gamma^{t-(c+1)} r_t g^T_{s_{t+1}|s_{t}, a_{t}} \right], \\
g^{r}_{|s,a} = \nabla_{\theta_r} \log p(r|s, a; \theta_r), g^{s'}_{|s,a} = \nabla_{\theta_s} \log p(s'|s, a; \theta_s).
\]

Under ergodicity assumption, this is calculated as

\[
A_\infty = \lim_{T \to \infty} c_T(\gamma) E_{\pi^c} \left[ \sum_{c=0}^{T} \gamma^c r_c g^T_{r_{c+1}|s_{c+1}, a_{c+1}} \right] = E_{\rho_{p,c,\gamma}}[r g^T_{r|s,a}],
\]

\[
C_\infty = \lim_{T \to \infty} c_T(\gamma) \gamma \sum_{c=0}^{T} \gamma^c \sum_{t=c+1}^{T} E_{\pi^c} \left[ \gamma^{t-(c+1)} r_t g^T_{s_{t+1}|s_{t}, a_{t}} \right]
\]

\[
= \lim_{T \to \infty} c_T(\gamma) \gamma \sum_{c=0}^{T} \gamma^c E_{\pi^c} \left[ v(s_{c+1}) g^T_{s_{c+1}|s_{c}, a_{c}} \right] = \gamma E_{\rho_{p,c,\gamma}}[v(s') g^T_{s'|s,a}],
\]

Therefore, \( (A_\infty I_\infty^{-1} A_\infty + C_\infty J_\infty^{-1} C_\infty) \) is

\[
\left[ \begin{array}{c}
\rho_{p,c,\gamma}(s) \eta(a, s) g^T_{r|s,a} \\
\rho_{p,c,\gamma}(s) \eta(a, s) g^T_{r|s,a}
\end{array} \right] E_{\rho_{p,c,\gamma}}[g_{r|s,a} g^T_{r|s,a}]^{-1} \left[ \begin{array}{c}
\rho_{p,c,\gamma}(s) \eta(a, s) g^T_{r|s,a} \\
\rho_{p,c,\gamma}(s) \eta(a, s) g^T_{r|s,a}
\end{array} \right] + \\
\gamma^2 E_{\rho_{p,c,\gamma}} \left[ \begin{array}{c}
\rho_{p,c,\gamma}(s) \eta(a, s) g^T_{r|s,a} \\
\rho_{p,c,\gamma}(s) \eta(a, s) g^T_{r|s,a}
\end{array} \right] E_{\rho_{p,c,\gamma}}[g_{s'|s,a} g^T_{s'|s,a}]^{-1} E_{\rho_{p,c,\gamma}} \left[ \begin{array}{c}
\rho_{p,c,\gamma}(s) \eta(a, s) g^T_{r|s,a} \\
\rho_{p,c,\gamma}(s) \eta(a, s) g^T_{r|s,a}
\end{array} \right].
\]

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Noting

\[
E_{p_b}(\infty) \left[ \frac{p_{\epsilon,\gamma}(\infty)(s)}{p_b(\infty)(s)} r \eta(a, s) g_r^\top s, a \right] = E_{p_b}(\infty) \left[ \frac{p_{\epsilon,\gamma}(\infty)(s)}{p_b(\infty)(s)} \{ r - E[r|s, a]\} \eta(a, s) g_r^\top s, a \right],
\]

\[
E_{p_b}(\infty) \left[ \frac{p_{\epsilon,\gamma}(\infty)(s)}{p_b(\infty)(s)} v(s') \eta(a, s) g_{s'}^\top s, a \right] = E_{p_b}(\infty) \left[ \frac{p_{\epsilon,\gamma}(\infty)(s)}{p_b(\infty)(s)} \{ v(s') - E[v(s')|s, a]\} \eta(a, s) g_{s'}^\top s, a \right],
\]

from Cauchy-Schwarz inequality, \(A_{\infty}J_{\infty}^{-1}A_{\infty} + C_{\infty}J_{\infty}^{-1}C_{\infty}\) is upper bounded by

\[
E_{p_b}(\infty) \left[ \left( \frac{p_{\epsilon,\gamma}(\infty)(s)}{p_b(\infty)(s)} \right)^2 \eta(a, s)^2 \{ (r - E[r|s, a])^2 + \gamma^2 (v(s') - E[v(s')|s, a])^2 \} \right]
\]

\[
= E_{p_b}(\infty) \left[ \left( \frac{p_{\epsilon,\gamma}(\infty)(s)}{p_b(\infty)(s)} \right)^2 \eta(a, s)^2 (r - E[r|s, a] + \gamma v(s') - \gamma E[v(s')|s, a])^2 \right]
\]

\[
= E_{p_b}(\infty) \left[ \left( \frac{p_{\epsilon,\gamma}(\infty)(s)}{p_b(\infty)(s)} \right)^2 \eta(a, s)^2 (r + \gamma v(s') - q(s, a))^2 \right].
\]

From Eq. (25) to Eq. (26), we use

\[
E[(r - E[r|s, a])(v(s') - E[v(s')|s, a])]
= E[(E[r|s, a, s'] - E[r|s, a, s'])(v(s') - E[v(s')|s, a])] = 0.
\]

From Eq. (26) to Eq. (27), we use \(q(s, a) = E[r + \gamma v(s')|s, a]\).

The statement that the upper bound is actually a supremum is concluded as in the proof of Theorem 2 utilizing Lemma 18.

\[\Box\]

**Proof of Theorem 4** Define \(\phi(\{\hat{v}_k\}, \{\hat{q}_k\})\) as:

\[
\sum_{k=0}^{\infty} \hat{v}_k r_k - \{ \hat{v}_{k-1} \hat{q}_k - \hat{v}_k E_{\pi^e}[\hat{q}_k(s_k, a_k)|s_k]\}.
\]

The estimator \(\hat{\rho}_{\text{DRL}(M_1)}\) is given by

\[
\frac{N_0}{N} \mathbb{P}_{N_0} \phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) + \frac{N_1}{N} \mathbb{P}_{N_1} \phi(\{\hat{v}_k^{(0)}\}, \{\hat{q}_k^{(0)}\}),
\]

where \(\mathbb{P}_{N_0}\) is an empirical approximation based on a set of samples such that \(J = 0\), \(\mathbb{P}_{N_1}\) is an empirical approximation based on a set of samples such that \(J = 1\). Then, we have

\[
\sqrt{N}(\mathbb{P}_{N_0} \phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \rho^{\pi^e}) = \sqrt{N/N_0} \mathbb{G}_{N_0} \phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \phi(\{v_k\}, \{q_k\})
\]

\[
+ \sqrt{N/N_0} \mathbb{G}_{N_0} \phi(\{v_k^{(1)}\}, \{q_k^{(1)}\})
\]

\[
+ \sqrt{N}(E[\phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\})|\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}] - \rho^{\pi^e}).
\]

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We analyze each term. To do that, we use the following relation:

\[ \phi(\{\hat{v}_k\}, \{\hat{q}_k\}) - \phi(\nu_k), \{q_k\}) = D_1 + D_2 + D_3, \quad \text{where} \]

\[ D_1 = \sum_{k=0}^{W_N} (\hat{v}_k - \nu_k)(-\hat{q}_k + q_k) + (\hat{v}_{k-1} - \nu_{k-1})(-\hat{v}_k + v_k), \]

\[ D_2 = \sum_{k=0}^{W_N} \nu_k(\hat{q}_k - q_k) + \nu_{k-1}(\hat{v}_k - v_k), \]

\[ D_3 = \sum_{k=0}^{W_N} (\hat{v}_k - \nu_k)(r_k - q_k + v_{k+1}). \]

First, we show the term Eq. (28) is \( o_p(1) \).

**Lemma 19.** The term Eq. (28) is \( o_p(1) \).

**Proof.** If we can show that for any \( \epsilon > 0 \),

\[ \lim_{n \to \infty} N_0 P[ \mathbb{P}_{N_0} \phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \phi(\nu_k), \{q_k\})] \]

\[ - E[\phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \phi(\nu_k), \{q_k\})] + \epsilon |D_1| = 0, \]

Then, by bounded convergence theorem, we would have

\[ \lim_{n \to \infty} N_0 P[ \mathbb{P}_{N_0} \phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \phi(\nu_k), \{q_k\})] \]

\[ - E[\phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \phi(\nu_k), \{q_k\})] + \epsilon = 0, \]

yielding the statement.

To show Eq. (31), we show that the conditional mean is 0 and conditional variance is \( o_p(1) \). The conditional mean is

\[ E[\mathbb{P}_{N_0} [\phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \phi(\nu_k), \{q_k\})] | |D_1] = 0. \]

Here, we leveraged the sample splitting construction, that is, \( \hat{v}_k^{(1)} \) and \( \hat{q}_k^{(1)} \) only depend on \( D_1 \). The conditional variance is

\[ \text{var}[\sqrt{N_0} \phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \phi(\nu_k), \{q_k\})] | |D_1] \]

\[ = E[D_1^2 + D_2^2 + D_3^2 + 2D_1D_2 + 2D_2D_3 + 2D_2D_3 | |D_1] \]

\[ = \omega^2 N \max\{o_p(N^{-1/3}), o_p(N^{-2/3}), o_p(N^{-1/2}) \} = o_p(1). \]

Here, we used the convergence rate assumption and the relation \( ||\hat{v}_k^{(1)} - v_k||_2 < ||\hat{q}_k^{(1)} - q_k||_2 \) arising from the fact that the former is the marginalization of the latter over \( \pi_k^e \). Then, from Chebyshev’s inequality:

\[ \sqrt{N_0} P[ \mathbb{P}_{N_0} [\phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \phi(\nu_k), \{q_k\})] - E[\phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\})] \]

\[ - \phi(\nu_k), \{q_k\}) | |D_1] > \epsilon | |D_1] \]

\[ \leq \frac{1}{\epsilon^2} \text{var}[\sqrt{N_0} \mathbb{P}_{N_0} [\phi(\{\hat{v}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \phi(\nu_k), \{q_k\})] | |D_1] = o_p(1). \]
Lemma 20. The term Eq. (30) is $o_p(1)$.

Proof.

$$\sqrt{N}\mathbb{E}[\phi(\{\hat{\nu}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \mathbb{E}[\phi(\{\nu_k\}, \{q_k\})|\{\hat{\nu}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}]
= \sqrt{N}\mathbb{E}\sum_{k=0}^{\omega_N}(\hat{\nu}_k^{(1)} - \nu_k)(-\hat{q}_k^{(1)} + q_k) + (\hat{\nu}_{k-1}^{(1)} - \nu_{k-1})(-\hat{q}_{k-1} + q_k)|\{\hat{\nu}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}
+ \sqrt{N}\sum_{k=0}^{\omega_N}\nu_k(\hat{q}_k^{(1)} - q_k) + \nu_{k-1}(\hat{q}_{k-1} - q_k)|\{\hat{\nu}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}
+ \sqrt{N}\sum_{k=0}^{\omega_N}(\hat{\nu}_k^{(1)} - \nu_k)(r_k - q_k + v_k)|\{\hat{\nu}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}
= \sqrt{N}\sum_{k=0}^{\omega_N}\mathcal{O}(\|\hat{\nu}_k^{(1)} - \nu_k\|_2\|\hat{q}_k^{(1)} - q_k\|_2) = \sqrt{N}\sum_{k=0}^{\omega_N}c_p(N^{-\alpha_1})c_p(N^{-\alpha_2}) = o_p(1).$$

Finally, we get

$$\sqrt{N}(\mathbb{P}_{N_0}\phi(\{\hat{\nu}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \rho^{\pi^c}) = \sqrt{N}/N_0\mathcal{G}_{N_0}[\phi(\{\nu_k\}, \{q_k\})] + o_p(1).$$

Therefore,

$$\sqrt{N}(\hat{\rho}_{\text{DRL}(M_1)} - \rho^{\pi^c})
= N_0/N\sqrt{N}\phi(\{\hat{\nu}_k^{(1)}\}, \{\hat{q}_k^{(1)}\}) - \rho^{\pi^c} + N_1/N\sqrt{N}(\mathbb{P}_{N_1}\phi(\{\nu_k\}, \{q_k\}) - \rho^{\pi^c})
= \sqrt{N_0}/N\mathcal{G}_{N_0}[\phi(\{\nu_k\}, \{q_k\})] + \sqrt{N_1}/N\mathcal{G}_{N_1}[\phi(\{\nu_k\}, \{q_k\})] + o_p(1)
= \mathcal{G}_{N}[\phi(\{\nu_k\}, \{q_k\})] + o_p(1),$$

concluding the proof.

Proof of Theorem 4 The proof is similar to that of Theorem 3.

Proof of Theorem 5 For the ease of the notation, we assume $N = 1$. The extension to general $N$ is straightforward.

We use the MC-CLT result in [Jones 2004 Corollary 2]. The required moment condition is satisfied because we assume that $w(s)$ is bounded by some constant.

Then, $\sqrt{T}(\hat{\rho}_{\text{DRL}(M_1)} - \rho^{\pi^c})$ converges to the normal distribution with mean and variance

$$\var_{\rho_b}(e(s_0, a_0, r_0, s_0)) + 2 \sum_{i=1}^{\infty} \cov_{\rho_b}(e(s_0, a_0, r_0, s_0), e(s_i, a_i, r_i, s_i)),$$

where $e(s, a, r, s') = w(s)\eta(a, s)\{r + \gamma v(s') - q(s, a)\}$. The first term in Eq. (32) is

$$\var_{\rho_b}(e(s_0, a_0, r_0, s_0)e(s_0, a_0, r_0, s_0)).$$
The second term in Eq. (32) is zero because
\[ E_{p_b}^{(\infty)} [e(s_0, a_0, r_0, s_0) e(s_i, a_i, r_i, s_{i+1})] = E_{p_b}^{(\infty)} [e(s_0, a_0, r_0, s_0) E_{p_b}^{(\infty)} [e(s_i, a_i, r_i, s_{i+1}) | s_{i-1}, a_{i-1}, r_{i-1}, s_i]] = 0. \]

**Proof of Theorem 9.** Define \( \phi(\hat{w}, \hat{q}) \) as
\[ \phi(s, a, r, s'; w, q) = (1 - \gamma) E_{p_e}^{(0)} [v(s)] + w(s) \eta(a, s) \{ r + \gamma v(s') - q(s, a) \}. \]

Then, the estimator \( \hat{\rho}_{DRL(M3)} \) is given by
\[ N_0 \frac{P_{N_0}}{N_0} P_T \phi(\hat{w}^{(1)}, \hat{q}^{(1)}) + \frac{N_1}{N} P_{N_1, T} \phi(\hat{u}^{(0)}, \hat{q}^{(0)}), \]
where \( P_{N_0} \) is an empirical approximation based on a set of samples such that \( J = 0 \), \( P_{N_1} \) is an empirical approximation based on a set of samples such that \( J = 1 \). Then, we have
\[ \sqrt{NT} \left( P_{N_0} P_T \phi(\hat{w}^{(1)}, \hat{q}^{(1)}) - \rho^{\pi_0} \right) = \sqrt{N/N_0} G_{N_0, T} [\phi(\hat{w}^{(1)}, \hat{q}^{(1)}) - \phi(w, q)] \]
\[ + \sqrt{N/N_0} G_{N_0, T} [\phi(w, q)] + \sqrt{NT} (E[\phi(\hat{w}^{(1)}, \hat{q}^{(1)})] - \rho^{\pi_0}), \] (34)

where \( G_{N_0, T} \) is an empirical process defined over the all sample in the first fold. We analyze each term. First, we show the term Eq. (33) is \( o_p(1) \).

**Lemma 21.** The term Eq. (33) is \( o_p(1) \).

**Proof.** Consider the case \( N_0 = 1 \). If we can show that for any \( \epsilon > 0 \),
\[ \lim_{T \to \infty} \sqrt{T} P[\phi(\hat{w}^{(1)}, \hat{q}^{(1)}) - \phi(w, q)] \]
\[ - E[\phi(\hat{w}^{(1)}, \hat{q}^{(1)}) - \phi(w, q) | \hat{w}^{(1)}, \hat{q}^{(1)}] > \epsilon | D_1] = 0, \] (35)

Then, by bounded convergence theorem, we would have
\[ \lim_{T \to \infty} \sqrt{T} P[\phi(\hat{w}^{(1)}, \hat{q}^{(1)}) - \phi(w, q)] \]
\[ - E[\phi(\hat{w}^{(1)}, \hat{q}^{(1)}) - \phi(w, q) | \hat{w}^{(1)}, \hat{q}^{(1)}] > \epsilon = 0, \]
yielding the statement.

To show Eq. (35), we show that the conditional mean is 0 and conditional variance is \( o_p(1) \). The conditional mean is
\[ E[\phi(\hat{w}^{(1)}, \hat{q}^{(1)}) - \phi(w, q) | \hat{w}^{(1)}, \hat{q}^{(1)}] \]
\[ - P[\phi(\hat{w}^{(1)}, \hat{q}^{(1)}) - \phi(w, q) | D_1] = 0. \]
Then, we obtain two lemmas.

Then, from Chebyshev’s inequality:

\[
\var\left[\sqrt{T}\mathbb{P}_T[\phi(\hat{w}(1), \hat{q}(1)) - \phi(w, q)]\right|D_1
\]

\[
= \frac{1}{T} \left[ \sum_{i=0}^{T} \max\{o_p(N^{-2\alpha_1}), o_p(N^{-2\alpha_2})\} + 2 \sum_{i,j} \rho_{\|i-j\|} \max\{o_p(N^{-2\alpha_1}), o_p(N^{-2\alpha_2})\} \right]
\]

\[
= o_p(1).
\]

Then, from Chebyshev’s inequality:

\[
\sqrt{T}\mathbb{P}_T[\phi(\hat{w}(1), \hat{q}(1)) - \phi(w, q)] - E[\phi(\hat{w}(1), \hat{q}(1)) - \phi(w, q)|\hat{w}(1), \hat{q}(1)] > \epsilon|D_1
\]

\[
\leq \frac{1}{\epsilon^2} \var\left[\sqrt{T}\mathbb{P}_T[\phi(\hat{w}(1), {\{\hat{q}(1)\}}) - \phi(w, q)]\right|D_1 = o_p(1). \quad \Box
\]

**Lemma 22.** \(\sqrt{NT} \mathbb{E}_{p(\infty)}[\phi(\hat{w}, \hat{q})|\hat{w}, \hat{q}] - \rho^{\mathcal{M}_3} = o_p(1).\)

**Proof.** Same as the proof of Lemma 24 \(\Box\)

Combining all lemmas and from Eq. (36),

\[
\sqrt{NT}(\hat{\rho}_{\text{DRL}(\mathcal{M}_3)} - \rho^{\pi^*}) = \mathcal{G}_{NT}(\phi(w, q) + o_p(1).
\]

Then, from MC-CLT, the statement is concluded as Theorem 8 \(\Box\)

**Proof of Theorem 10** For the ease of the notation, we assume \(N = 1\). The extension to general \(N\) is straightforward.

We have the following decomposition;

\[
\sqrt{T}(\hat{\rho}_{\text{DRL}(\mathcal{M}_3)} - \rho^{\pi^*}) = \mathcal{G}_T(\phi(\hat{w}, \hat{q}) - \mathcal{G}_T\phi(\hat{w}, q) + \mathcal{G}_T\phi(\hat{w}, q) + \sqrt{T}\mathbb{E}_{p(\infty)}[\phi(\hat{w}, \hat{q})|\hat{w}, \hat{q}] - \rho^{\pi^*})
\]

(36)

where

\[
\phi(s, a, r, s'; w, q) = (1 - \gamma)\mathbb{E}_{p(o)}[v(s)] + w(s)\eta(a, s){r + \gamma v(s') - q(s, a)}.
\]

Here, we have

\[
\mathbb{P}_T\phi(s, a, r, s'; \hat{w}, \hat{q}) - \mathbb{P}_T\phi(s, a, r, s'; w, q)
\]

\[
= \mathbb{P}_T\{[\hat{w}(s) - w(s)]\eta(a, s){r - q(s, a) + \gamma v(s')}] + \mathbb{P}_T[w(s)\eta(a, s){q(s, a) - \hat{q}(s, a) + \gamma \hat{v}(s') - \gamma v(s')} + (1 - \gamma)\mathbb{E}_{p(o)}[v'(s) - v(s)] + \mathbb{P}_T\{[\hat{w}(s) - w(s)]\eta(a, s){q(s, a) - \hat{q}(s, a) + \gamma \hat{v}(s') - \gamma v(s')} \}
\]

Then, we obtain two lemmas.

**Lemma 23.** \(\mathcal{G}_T\phi(\hat{w}, \hat{q}) - \mathcal{G}_T\phi(\hat{w}, q) = o_p(1).\)

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Proof. From Theorem 11.24 (Kosorok 2008) based on the assumptions (10a)-(10d), \( G_T \rightarrow^d H \) in \( L_\infty(p_b^{(\infty)}) \), where \( H \) is a tight mean zero Gaussian process with some covariance. If \( \|\phi(\hat{w}, \hat{q}) - \phi(w, q)\|_2 = o_p(1) \), from Lemma 18.5 (van der Vaart 1998), the statement is concluded. The equation \( \|\phi(\hat{w}, \hat{q}) - \phi(w, q)\|_2 = o_p(1) \) is proved from (10e).

Lemma 24. \( \sqrt{T}(E_{p_b^{(\infty)}}[\phi(\hat{w}, \hat{q})]\hat{w}, \hat{q}) - \rho^{M_3}) = o_p(1) \).

Proof. Noting \( E_{p_b^{(\infty)}}[(\hat{q} - q)^2] \geq E_{p_b^{(\infty)}}[(\hat{v} - v)^2] \),

\[
\sqrt{T}E_{p_b^{(\infty)}}[\phi(s, a, r, s'; \hat{w}, \hat{q}) - \phi(s, a, r, s'; w, q)]\hat{w}, \hat{q}) = \sqrt{T}E_{p_b^{(\infty)}}[(\hat{w}(s) - w(s))\eta(a, s)(r - q(s, a) + \gamma v(s'))\hat{w}, \hat{q}) + \\
\sqrt{T}E_{p_b^{(\infty)}}[w(s)\eta(a, s)\{q(s, a) - \hat{q}(s, a) + \gamma \hat{v}(s') - \gamma v(s')\}] + (1 - \gamma)E_{p_b^{(\infty)}}[\hat{v}(s) - v(s)]\|\hat{w}, \hat{q}) + \\
\sqrt{T}E_{p_b^{(\infty)}}[(\hat{w}(s) - w(s))\eta(a, s)\{q(s, a) - \hat{q}(s, a) + \gamma \hat{v}(s') - \gamma v(s')\}]\|\hat{w}, \hat{q})
\]

\[
= \sqrt{T}[\|\hat{w}(s) - w(s)\|_2\|q(s, a) - \hat{q}(s, a) + \gamma \hat{v}(s') - \gamma v(s')\|] = o_p(1).
\]

Here, we have used an assumption (10e).

Combining all lemmas and from Eq. (36),

\[
\sqrt{T}(\hat{\rho}_{DRL(M_3)} - \rho^{M_3}) = G_T\phi(w, q) + o_p(1).
\]

Then, from MC-CLT, the statement is concluded as Theorem 8.

Proof of Theorem 14. Define

\[
\phi(s, a, r, s'; w, q) = (1 - \gamma)E_{p_b^{(\infty)}}[v(s)] + w(s)\eta(a, s)\{r + \gamma v(s') - q(s, a)\}.
\]

Then, we have

\[
P_T\phi(\hat{w}, \hat{q}) = \sup_{f \in F}[P_Tf - E_{p_b^{(\infty)}}[f]] + E_{p_b^{(\infty)}}[\phi(\hat{w}, \hat{q})]\hat{w}, \hat{q}) = o_p(1) + E_{p_b^{(\infty)}}[\phi(\hat{w}, \hat{q})]\hat{w}, \hat{q}].
\]
Here, we have used an uniform law of large numbers of stationary sequence [Adams and Nobel, 2010] based on the condition (11a) and (11b). Then, we have

\[
E_{\hat{p}_b(\infty)}[\phi(\hat{w}, \hat{q})|\hat{w}, \hat{q}]
= E_{\hat{p}_b(\infty)}\{(\hat{w}(s) - w^\dagger(s))\eta(a, s)\{r - \hat{q}(s, a) + \gamma v^\dagger(s')\}\} + E_{\hat{p}_b(\infty)}[w^\dagger(s)\eta(a, s)\{q^\dagger(s, a) - \hat{q}(s, a) + \gamma \hat{v}(s') - \gamma v^\dagger(s')\}] + (1 - \gamma)E_{\hat{p}_b(\infty)}[v^\dagger(s) - v^\dagger(s)]
+ E_{\hat{p}_b(\infty)}\{(\hat{v}(s) - v^\dagger(s))\eta(a, s)\{q^\dagger(s, a) - \hat{q}(s, a) + \gamma \hat{v}(s') - \gamma v^\dagger(s')\}] + E_{\hat{p}_b(\infty)}\{(\hat{v}(s) - v^\dagger(s)) - \hat{q}(s, a) + q^\dagger(s, a)\}|\hat{w}, \hat{q}]
+ E_{\hat{p}_b(\infty)}[\phi(w^\dagger, q^\dagger)|\hat{w}, \hat{q}]
= O(||\hat{w}(s) - w^\dagger(s)||_2, ||\hat{q}(s, a) - q^\dagger(s, a)||_2, ||\hat{v}(s) - v^\dagger(s)||_2) + E_{\hat{p}_b(\infty)}[\phi(w^\dagger, q^\dagger)]
= \alpha_p(1) + E_{\hat{p}_b(\infty)}[\phi(w^\dagger, q^\dagger)].
\]

\textbf{q-model is well-specified.} Consider the case where \(q^\dagger(s, a) = q(s, a)\);

\[
E_{\hat{p}_b(\infty)}[\phi(w^\dagger, q^\dagger)] = E_{\hat{p}_b(\infty)}[(1 - \gamma)E_{\hat{p}_b(\infty)}[v^\dagger(s)] + w^\dagger(s)\eta(a, s)\{r + \gamma v(s') - q(s, a)\}]
= (1 - \gamma)E_{\hat{p}_b(\infty)}[v^\dagger(s)] = \rho^{n_e}.
\]

This implies unless q-model is consistent, the estimator \(\hat{\rho}_{DRL(M_3)}\) is also consistent.

\textbf{w-model is well-specified.} Consider the case where \(w^\dagger(s) = w(s)\);

\[
E_{\hat{p}_b(\infty)}[\phi(w^\dagger, q^\dagger)] = E[(1 - \gamma)E_{\hat{p}_b(\infty)}[v^\dagger(s)] + w(s)\eta(a, s)\{r + \gamma v(s') - q^\dagger(s, a)\}]
= (1 - \gamma)E_{\hat{p}_b(\infty)}[v^\dagger(s)] + E_{\hat{p}_b(\infty)}[w(s)\eta(a, s)r] + E_{\hat{p}_b(\infty)}[w(s)\eta(a, s)\gamma v^\dagger(s')]
- E_{\hat{p}_b(\infty)}[w(s)\eta(a, s)q^\dagger(s, a)]
= E_{\hat{p}_b(\infty)}[w(s)\eta(a, s)r] + E_{\hat{p}_b(\infty)}[w(s)v^\dagger(s)] - E_{\hat{p}_b(\infty)}[w(s)\eta(a, s)q^\dagger(s, a)]
= E_{\hat{p}_b(\infty)}[w(s)\eta(a, s)r] = \rho^{n_e}.
\]

From Eq. (37) to Eq. (38), we use a result

\[
(1 - \gamma)E_{\hat{p}_b(\infty)}[v^\dagger(s)] + E_{\hat{p}_b(\infty)}[w(s)\eta(a, s)\gamma v^\dagger(s')] = E_{\hat{p}_b(\infty)}[w(s)v^\dagger(s)]
\]

from Lemma \textit{13}. From Eq. (38) to Eq. (39), we use a result

\[
E_{\hat{p}_b(\infty)}[w(s)\eta(a, s)q^\dagger(s, a)] = E_{\hat{p}_b(\infty)}[w(s)E[\eta(a, s)q^\dagger(s, a)|s]] = E_{\hat{p}_b(\infty)}[w(s)v^\dagger(s)].
\]

This implies unless the ratio model is consistent, the estimator \(\hat{\rho}_{DRL(M_3)}\) is also consistent. \(\square\)
Proof of Theorem 12. For the ease of the notation, we assume \( N = 1 \). The extension to general \( N \) is straightforward. We have the following decomposition:

\[
\sqrt{T} (\hat{\rho}_{\text{DRL}(M_2)} - \rho^{\pi^c}) = \mathbb{G}_T \phi(\hat{w}, \hat{q}) - \mathbb{G}_T \phi(w^\top, q^\top) + \sqrt{T} (\mathbb{E}_{p^\phi_b(\infty)} [\phi(\hat{w}, \hat{q}) | \hat{w}, \hat{q}] - \mathbb{E}_{p^\phi_b(\infty)} [\phi(w^\top, q^\top)]) + \sqrt{T} (\mathbb{E}_{p^\phi_b(\infty)} [\phi(w^\top, q^\top)] - \rho^{\pi^c}) + \mathbb{G}_T \phi(w^\top, q^\top).
\]

The term Eq. (40) is \( o_p(1) \) from Lemma 23. The term Eq. (41) is also \( o_p(1) \) from Lemma 24. The term Eq. (42) is 0 following the argument in the proof of Theorem 11. Then, we get \( \sqrt{T} (\hat{\rho}_{\text{DRL}(M_2)} - \rho^{\pi^c}) = \mathbb{G}_T \phi(w^\top, q^\top) + o_p(1) \). From MC-CLT, the statement is concluded as Theorem 8. \( \square \)

Proof of Lemma 13. Define

\[
\delta(g, s') = \gamma \int p(s' | s) g(s) d\lambda(s) - g(s') + (1 - \gamma) p_e^{(0)}(s'),
\]

where \( g(s) \) is any function and \( p(s' | s) \) is a marginal distribution of \( p(s' | s, a) \pi^c(a | s) \). We have \( g(s) = p_{e, \gamma}^{(\infty)}(s) \) if and only if \( \delta(g, s') = 0 \) and any \( s' \). Then,

\[
\begin{align*}
L(w, f_w) &= \mathbb{E}_{p^\phi_b(\infty)} [\gamma w(s) \eta(a, s) - w(s')] f_w(s') \right) + (1 - \gamma) \mathbb{E}_{p^\phi_e(\infty)} [f_w(s)] \\
&= \mathbb{E}_{p^\phi_b(\infty)} [\gamma w(s) \eta(a, s) f_w(s')] - \mathbb{E}_{p^\phi_b(\infty)} [w(s) f_w(s)] + (1 - \gamma) \mathbb{E}_{p^\phi_e(\infty)} [f_w(s)] \\
&= \mathbb{E}_{p^\phi_e(\infty)} [(p^\phi_e(\infty) / p^\phi_b(\infty))(s)]^{-1} \gamma w(s) \eta(a, s) f_w(s') - \mathbb{E}_{p^\phi_e(\infty)} [(p^\phi_e(\infty) / p^\phi_b(\infty)(s))]^{-1} w(s) f_w(s)] + (1 - \gamma) \mathbb{E}_{p^\phi_e(\infty)} [f_w(s)] \\
&= \int \delta(g, s') f_w(s') d\lambda(s'),
\end{align*}
\]

where we have \( g(s) = p_{e, \gamma}^{(\infty)}(s) \{p_{e, \gamma}^{(\infty)}(s) / p^\phi_b(\infty)(s)\}^{-1} w(s) \). Therefore, \( L(w, f_w) = 0 \) for any \( f_w \) is equivalent to \( \delta(g, s') = 0 \) for any \( s' \). This is equivalent to \( g(s) = p_{e, \gamma}^{(\infty)}(s) \), that is, \( w(s) = \pi^c(a | s) / \pi^b(a | s) \). \( \square \)

Proof of Theorem 14. For the ease of the notation, we assume \( N = 1 \). In the first step, we calculate the asymptotic variance for general \( f_w(s) \). Then, we prove the upper bound.

Step 1 Prove that the asymptotic MSE is given by

\[
\mathbb{E}_{p^\phi_b(\infty)} [f_w(s') \nabla_{\beta^\top} \Delta(s, a, s')] \mathbb{E}_{p^\phi_b(\infty)} [\nabla_{\beta} \Delta(s, a, s') f_w(s')^\top] \mathbb{E}_{p^\phi_b(\infty)} [\nabla_{\beta} \Delta(s, a, s') f_w(s')]^{-1} |_{\beta^*}.
\]

For simplicity, we assume \( \beta \) is one-dimensional. Using a mean value theorem, we have

\[
\sqrt{T} (\hat{\beta}_f - \beta^*) = -\mathbb{E} [f_w(s') \nabla_{\beta^\top} \Delta(s, a, s')] |_{\beta^*} \sqrt{T} \mathbb{E} [f_w(s') \Delta(s, a, s')] |_{\beta^*},
\]

39
where $\beta^t$ is a value between $\hat{\beta}$ and $\beta^*$. The first term in right hand size of Eq. (44) converges to

$$\mathbb{P}_{T}[f_w(s')\nabla_{\beta^T} \Delta(s, a, s')]|_{\beta^t} \overset{P}{\rightarrow} \mathbb{E}_{p_\infty}^\beta[f_w(s')\nabla_{\beta^T} \Delta(s, a, s')]|_{\beta^*}. \tag{45}$$

This is proved by an uniform convergence condition coming from Lipschitz condition and $\beta^t \overset{P}{\rightarrow} \beta^*$. (Consistency is easily proved (van der Vaart, 1998, Theorem 5.7))

Next, we calculate the second term in right hand size of Eq. (44). By MC-CLT, we have

$$\sqrt{T}(\mathbb{P}_{T}[f_w(s')\Delta(s, a, s')]|_{\beta^*} - \mathbb{E}_{p_\infty}^\beta[f_w(s')\Delta(s, a, s')]|_{\beta^*}) \overset{d}{\rightarrow} \mathcal{N}(0, \sigma^2), \tag{46}$$

where

$$\sigma^2 = \lim_{t \rightarrow \infty} \text{var}[\Delta(z_t)f_w(s_{t+1})]|_{\beta^*} + 2\lim_{t \rightarrow \infty} \sum_{t'=1}^{\infty} \text{cov}(\Delta(z_t)f_w(s_{t+1}), \Delta(z_{t+t'})f_w(s_{t+1+t'}))|_{\beta^*}, \tag{47}$$

where $z_t$ is $(s_t, a_t, r_t, s_{t+1})$. The first term in Eq. (47) is

$$\lim_{t \rightarrow \infty} \text{var}[\Delta(z_t)f_w(s_{t+1})]|_{\beta^*} = \text{var}_{p_\infty}^\beta[\Delta(s, a, s')f_w(s')]|_{\beta^*}.$$

where $z_t = (s_t, a_t, s_{t+1})$. On the other hand, the second term in Eq. (47) is zero. This is because for $0 \leq t < t'$,

$$\mathbb{E}_{p_\infty}^\beta[\Delta(z_t)f_w(s_{t+1})\Delta(z_{t+t'})f_w(s_{t+1+t'})]|_{\beta^*} = \mathbb{E}_{p_\infty}^\beta[\Delta(z_t)f_w(s_{t+1})f_w(s_{t+1+t'})|_{\beta^*}.\tag{48}$$

To sum up,

$$\sigma^2 = \text{var}_{p_\infty}^\beta[\Delta(s, a, s')f_w(s')]|_{\beta^*}.\tag{49}$$

Combining Eq. (45) and Eq. (46), by Slutsky’s theorem, the statement Eq. (43) is obtained.

**Step 2** Use a Cauchy Schwarz inequality for

$$\mathbb{E}_{p_\infty}^\beta[f_w(s')\nabla_{\beta^T} \Delta(s, a, s')]^{-1} \mathbb{E}_{p_\infty}^\beta[\Delta(s, a, s')f_w(s')]\mathbb{E}_{p_\infty}^\beta[\nabla_{\beta^T} \Delta(s, a, s')f_w(s')^{-1}]|_{\beta^*}^{-1} = A_w^{-1}B_wA_{w^*}^{-1},$$

where

$$A_w = \mathbb{E}_{p_\infty}^\beta[f_w(s')\nabla_{\beta^T} \Delta(s, a, s')]|_{\beta^*},$$

$$B_w = \mathbb{E}_{p_\infty}^\beta[\text{var}_{p_\infty}^\beta[\Delta(s, a, s')f_w(s')f_w(s')^{-1}]|_{\beta^*}.$$
The lower bound of this value is
\[ \mathbb{E}_{\hat{p}_b^{(\infty)}}[\nabla_\beta m_w(s')v_w^{-1}(s')\nabla_\beta^\top m_w(s')]^{-1}|_{\beta^*}, \]
where
\[ m_w(s') = \mathbb{E}_{\hat{p}_b^{(\infty)}}[\nabla_\beta \Delta(s,a,s')|s'], \quad v_w(s') = \text{var}_{\hat{p}_b^{(\infty)}}[\Delta(s,a,s')|s']. \]

**Proof of Theorem 15.** For the ease of the notation, we assume \( N = 1 \).

\[
\sqrt{T}(\hat{\rho}_{\text{EIS}} - \rho_{\infty}^*) = G_T[w(s; \hat{\beta}_{f_w})\eta(a,s)r] - G_T[w(s)\eta(a,s)r] + G_T[w(s)\eta(a,s)r] + \sqrt{T}(E[w(s; \hat{\beta}_{f_w})\eta(a,s)r|\hat{\beta}_{f_w}] - \rho_{\infty}^*) .
\]

Here, from the standard argument,
\[
\sqrt{T}(E[w(s; \hat{\beta}_{f_w})\eta(a,s)r] - \rho_{\infty}^*) = E[\nabla_\beta^\top w(s; \beta)\eta(a,s)r]E[f_w(s')\nabla_\beta^\top \Delta(s,a,s'; \beta)]^{-1}[\mathbb{P}_T\Delta(s,a,s'; \beta)f_w(s')|_{\beta^*} + o_p(1)].
\]

This concludes the proof. \( \square \)

**Proof of Theorems 16 and 17.** Same as the proof of Theorem 14. \( \square \)

**C Additional results of Experiment**

Here, we provide additional results from the experiment in Section 7 with \( \alpha = 0.4, 0.8 \). The results are given in the below figures.
