Minimax Weight and Q-Function Learning for Off-Policy Evaluation

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Abstract

We provide theoretical investigations into off-policy evaluation in reinforcement learning using function approximators for (marginalized) importance weights and value functions. Our contributions include:
(1) A new estimator, MWL, that directly estimates importance ratios over the state-action distributions, removing the reliance on knowledge of the behavior policy as in prior work (Liu et al., 2018).
(2) Another new estimator, MQL, obtained by swapping the roles of importance weights and value-functions in MWL. MQL has an intuitive interpretation of minimizing average Bellman errors and can be combined with MWL in a doubly robust manner.
(3) Several additional results that offer further insights into these methods, including the sample complexity analyses of MWL and MQL, their asymptotic optimality in the tabular setting, how the learned importance weights depend the choice of the discriminator class, and how our methods provide a unified view of some old and new algorithms in RL.

1. Introduction

In reinforcement learning (RL), off-policy evaluation (OPE) refers to the problem of estimating the performance of a new policy using historical data collected from a different policy, which is of crucial importance to the real-world applications of RL. The problem is genuinely hard as any unbiased estimator has to suffer a variance exponential in horizon in the worst case (Li et al., 2015; Jiang and Li, 2016), known as the curse of horizon.

Recently, a new family of estimators based on marginalized importance sampling (MIS) receive significant attention from the community (Liu et al., 2018; Xie et al., 2019), as they overcome the curse of horizon with relatively mild representation assumptions. The basic idea is to learn the marginalized importance weight that converts the state distribution in the data to that induced by the target policy, which sometimes have much smaller variance than the cumulative importance weight on action sequences used by standard sequential IS. Among these works, Liu et al. (2018) constructs an objective function based on the Bellman equation for state distributions with the help of a discriminator value-function class, and learn the importance weights by solving a minimax optimization problem.

In this work, we investigate more deeply the space of algorithms that utilize a value-function class and an importance weight class. Our main contributions are:

• (Section 4) A new estimator, MWL, that directly estimates importance ratios over the state-action distributions, removing the reliance on knowledge of the behavior policy as in prior work.
• (Section 5) By swapping the roles of importance weights and Q-functions in MWL, we obtain a new estimator that learns a Q-function using importance weights as discriminators, with an intuitive interpretation of minimizing average Bellman errors (Jiang et al., 2017). The estimation procedure and the guarantees of MQL show an interesting symmetry w.r.t. those of MWL. We also combine MWL and MQL in a doubly robust manner and provide their sample complexity guarantees (Section 6).

• (Section 7) We investigate the statistical efficiency of MWL and MQL, and show that by modeling state-action (value and importance weight) functions, MWL and MQL are able to achieve the semiparametric lower bound of OPE in the tabular setting while their state-function variants fail to do so.

• Our framework provides a unified view that connects many old and new algorithms in RL. For example, we show that when both importance weights and value functions are modeled using the same linear class, we recover LSTDQ (Lagoudakis and Parr, 2004) and off-policy LSTD (Bertsekas and Yu, 2009; Dann et al., 2014) as special cases of MWL/MQL and their state-function variants. This gives LSTD algorithms a novel interpretation that is very different from the standard TD intuition.

• We also show that (tabular) model-based OPE and step-wise importance sampling—two algorithms that are so different that we seldom connect them to each other—are both special cases of MWL, and discuss how the learned importance weights depend on the choice of the discriminators.

2. Preliminaries

An infinite-horizon discounted MDP is often specified by a tuple $\langle S, A, P, R, \gamma \rangle$ where $S$ is the state space, $A$ is the action space, $P : S \times A \rightarrow \Delta(S)$ is the transition function, $R : S \times A \rightarrow \Delta([0, R_{\text{max}}])$ is the reward function, and $\gamma \in [0, 1)$ is the discount factor. We also use $\mathcal{X} := S \times A$ to denote the space of state-action pairs. Given an MDP, a (stochastic) policy $\pi : S \rightarrow \Delta(A)$ and a starting state distribution $d_0 \in \Delta(S)$ together determine a distribution over trajectories of the form $s_0, a_0, r_0, s_1, a_1, r_1, \ldots$, where $s_0 \sim d_0$, $a_t \sim \pi(s_t)$, $r_t \sim R(s_t, a_t)$, and $s_{t+1} \sim P(s_t, a_t)$ for $t \geq 0$. The ultimate measure of the performance of a policy is the (normalized) expected discounted return, defined as

$$R_\pi := (1 - \gamma)E_{d_0, \pi}\left[\sum_{t=0}^{\infty} \gamma^t r_t\right],$$

where the expectation is taken over the randomness of the trajectory determined by the initial distribution and the policy on the subscript, and $(1 - \gamma)$ is the normalization factor.

A concept central to this paper is the notion of (normalized) discounted occupancy:

$$d_{\pi, \gamma} := (1 - \gamma)\sum_{t=0}^{\infty} \gamma^t d_{\pi,t},$$

where $d_{\pi,t} \in \Delta(\mathcal{X})$ is the distribution of $(s_t, a_t)$ under policy $\pi$. (The dependence on $d_0$ is made implicit in this notation.) We will sometimes also write $s \sim d_{\pi, \gamma}$ for sampling from its
marginal distribution over states. An important property of discounted occupancy, which we will make heavy use of, is

$$R_\pi = E_{(s,a) \sim d_{\pi,\gamma}, r \sim R(s,a)}[r].$$

(2)

It will also be useful to define the policy-specific Q-value function:

$$Q^\pi(s,a) := E[\sum_{t=0}^{\infty} \gamma^t r_t | s_0 = s, a_0 = a; a_t \sim \pi(s_t) \forall t > 0].$$

The corresponding state-value function is $$V^\pi(s) := Q^\pi(s,\pi(s))$$, where for any function $$f$$, $$f(s,\pi)$$ is the shorthand for $$E_{a \sim \pi(s)}[f(s,a)]$$.

**Off-Policy Evaluation (OPE)** We are concerned with estimating the expected discounted return of an evaluation policy $$\pi_e$$ under a given initial distribution $$d_0$$, using data collected from a possibly different behavior policy $$\pi_b$$. For our methods, we will consider the following data generation protocol, where we have a dataset consisting of $$n$$ i.i.d. tuples $$(s,a,r,s')$$ generated according to the distribution:

$$s \sim d_{\pi_b}, a \sim \pi_b(s), r \sim R(s,a), s' \sim P(s,a).$$

Here $$d_{\pi_b}$$ is some exploratory state distribution that well covers the state space, and the technical assumptions required on this distribution will be discussed in later sections. With a slight abuse of notation we will also refer to the joint distribution over $$(s,a,r,s')$$ or its marginal on $$(s,a)$$ as $$d_{\pi_b}$$, e.g., whenever we write $$(s,a,r,s') \sim d_{\pi_b}$$ or $$(s,a) \sim d_{\pi_b}$$, the variables are always distributed according to the above generative process. We will use $$E[\cdot]$$ to denote the exact expectation, and use $$E_n[\cdot]$$ as its empirical approximation using the $$n$$ data points.

Note that although we assume i.i.d. data for concreteness and the ease of exposition, the actual requirement on the data is very mild: Even if the $$n$$ data points are dependent of each other, our method works as long as the empirical expectation (over $$n$$ data points) concentrates around the exact expectation w.r.t. $$(s,a,r,s') \sim d_{\pi_b}$$. This holds, for example, when the Markov chain induced by $$\pi_b$$ is ergodic, and our data is a single long trajectory generated by $$\pi_b$$ without resetting. As long as the induced chain has nice mixing properties, it is well known that the empirical expectation over the single trajectory will concentrate around the true expectation, and in this case $$d_{\pi_b}(s)$$ corresponds to the stationary distribution of the Markov chain. In fact, we consider precisely this setting in Section 6 and show that we can prove sample complexity bounds for the estimator under additional standard assumptions (such as the trajectory being $$\beta$$-mixing).

3. Overview of OPE Methods

In this section we briefly survey the popular approaches to OPE.

**Direct Methods** A straightforward approach to OPE is to estimate an MDP model from data, and then compute the quantity of interest from the estimated model. An alternative but closely related approach is to fit $$Q^{\pi_e}$$ directly from data using standard approximate
Table 1: Summary of some of the OPE Methods. For methods that require knowledge of $\pi_b$, the policy can be estimated from data to form a “plug-in” estimator. In the function approximation column, we use blue color to mark the conditions for the discriminator classes for minimax-style methods. For Liu et al. (2018), we use $W_S$ and $F_S$ for the function classes to emphasize that their functions are over the state space (ours are over the state-action space). Although they assumed $V_{\pi_e} \in F_S$ (*), this assumption on the discriminator class can also be relaxed to $V_{\pi_e} \in \text{conv}(F)$ as in our analyses. Also note that the assumption for the main function classes ($W_S$, $W$, and $Q$) can be relaxed as discussed in Examples 1 and 3, and we put realizability conditions here only for simplicity.

Importance Sampling (IS) IS forms an unbiased estimate of the expected return by collecting full-trajectory behavioral data and reweighting each trajectory according to its likelihood under $\pi_e$ over $\pi_b$ (Precup et al., 2000). Such a ratio can be computed as the cumulative product of the importance weight over action ($\frac{\pi_e(a|s)}{\pi_b(a|s)}$) for each time step, which is the cause of high variance in IS: even if $\pi_e$ and $\pi_b$ only has constant divergence per step, the divergence will be amplified over the horizon, causing the cumulative importance weight to have exponential variance, thus the “curse of horizon”. Although techniques that combine IS and direct methods can partially reduce the variance, the exponential variance of IS simply cannot be improved when the MDP has significant stochasticity (Jiang and Li, 2016). Furthermore, IS explicitly uses the knowledge of $\pi_b$, and when it is not available the policy has to be estimated from data (Hanna et al., 2019).

Marginalized Importance Sampling (MIS) MIS improves over IS by observing that, if $\pi_b$ and $\pi_e$ induces marginal distributions over states that have substantial overlap—which is often the case in many practical scenarios—then reweighting the reward $r$ in each data

| Method          | $\pi_b$ known? | Target object | Func. approx. | Tabular optimality |
|-----------------|----------------|---------------|---------------|-------------------|
| MSWL (Liu et al.) | Yes            | $w_{\pi_e/\pi_b}$ (Eq.(3)) | $w_{\pi_e/\pi_b} \in W^S$, $V_{\pi_e} \in F^S$ (*) | No                |
| MWL (Sec 4)     | No             | $w_{\pi_e/\pi_b}$ (Eq.(4))  | $w_{\pi_e/\pi_b} \in W$, $Q_{\pi_e} \in \text{conv}(F)$ | Yes               |
| MQL (Sec 5)     | No             | $Q_{\pi_e}$   | $Q_{\pi_e} \in Q$, $w_{\pi_e/\pi_b} \in \text{conv}(G)$ | No                |
| Fitted-Q        | No             | $Q_{\pi_e}$   | $Q$ closed under $B_{\pi_e}$ | Yes               |
point \((s, a, r, s')\) with the following ratio
\[
    w^S_{\pi^e/\pi_b}(s) \cdot \frac{\pi_e(a|s)}{\pi_b(a|s)}, \quad \text{where} \quad w^S_{\pi_e/\pi_b}(s) := \frac{d_{\pi_e,\gamma}(s)}{d_{\pi_b}(s)} \tag{3}
\]
can potentially have much lower variance than reweighting the entire trajectory (Liu et al., 2018). The difference between IS and MIS is essentially performing importance sampling using Eq.(1) vs. Eq.(2). However, the weight \(w^S_{\pi_e/\pi_b}\) is not directly available and has to be estimated from data. Liu et al. (2018) proposes to estimate such a weighting function by leveraging the Bellman equation for distributions. The method requires two function approximators, one for modeling the weighting function \(w^S_{\pi_e/\pi_b}(s)\), and the other for modeling \(V^\pi_b\) which is used as a discriminator class for distribution learning. Compared to the direct methods, MIS only requires standard realizability conditions for the two function classes, though it also needs the knowledge of \(\pi_b\). A related method for finite horizon problems has been developed by Xie et al. (2019).

4. MWL: Learning Importance Weights with Q-Function Discriminators

In this section we propose a simple extension to Liu et al. (2018) that is agnostic to the knowledge of \(\pi_b\). The key observation is that the estimator in the prior work uses a discriminator class that contains \(V^\pi_e\) to learn the marginalized importance weight on state distributions (see Eq.(3)). If the discriminator class is slightly more powerful—for example, it is a Q-function class that realizes \(Q^\pi_e\)—then we may be able to learn the importance weight over state-action pairs directly:
\[
    w_{\pi_e/\pi_b}(s, a) := \frac{d_{\pi_e,\gamma}(s, a)}{d_{\pi_b}(s, a)}. \tag{4}
\]
We can use it to directly re-weight the rewards without having to know \(\pi_b\), as \(R_{\pi_e} = R_w[w_{\pi_e/\pi_b}(s, a)] := E_{\pi_b}[w_{\pi_e/\pi_b}(s, a) \cdot r]\). It will be also useful to define the empirical approximation of \(R_w[\cdot]\) as \(R_{\pi,e,n}[\cdot], \) where \(R_{\pi,e,n}[w] := E_n[w(s, a) \cdot r]\). Here \(E_n[\cdot]\) applies the function inside \([\cdot]\) on each data point \((s, a, r, s')\) and then takes the average.

In the rest of this section, we provide theoretical results that this simple idea works. We start with two assumptions that we will use throughout the paper, most notably that the state-action distribution in data well covers the discounted occupancy induced by \(\pi_b\).

Assumption 1. Assume \(\mathcal{X} = \mathcal{S} \times \mathcal{A}\) is a compact space. Let \(\nu\) be its Lebesgue measure over \(\mathcal{X}\). \(^1\)

Assumption 2. There exists \(C_w < +\infty\) such that \(w_{\pi_e/\pi_b}(s, a) \leq C_w \forall (s, a) \in \mathcal{X}\).

Loss Function Next, we define the loss function central to our estimation procedure:
\[
    L_w(w, f) := E_{(s,a,r,s') \sim d_{\pi_e}}[\gamma w(s, a) \cdot f(s', \pi_e) - w(s, a) f(s, a)] + (1 - \gamma) E_{d_0 \times \pi_e}[f(s, a)].
\]
Here \((s, a) \sim d_0 \times \pi_e \iff s \sim d_0, a \sim \pi_e(a|s),\) and recall that \(f(s', \pi_e) := E_{a' \sim \pi_e(a')}[f(s', a')].\) The loss function satisfies the following property, that it is always zero when \(w = w_{\pi_e/\pi_b}\).

\(^1\) When \(\nu\) is a counting measure (tabular setting), every method can be still applied, and all of the statements hold with minor modification.
Such a solution is also unique if we require $L_w(w, f) = 0$ for a rich set of functions and $d_{\pi_b}$ is supported on the entire $\mathcal{X}$, formalized as the following lemma:

**Lemma 1.** $L_w(w_{\pi_c/\pi_b}, f) = 0 \forall f \in L^2(\mathcal{X}, \nu):= \{f : \int f(s, a)^2 d\nu < \infty\}$. Moreover, under additional technical assumptions, $w_{\pi_c/\pi_b}$ is the only function that satisfies such a property.

This motivates the following estimator, which uses two function classes: a class $\mathcal{W} : \mathcal{X} \rightarrow \mathbb{R}$ to model the $w_{\pi_c/\pi_b}$ function, and another class $\mathcal{F} : \mathcal{X} \rightarrow \mathbb{R}$ to serve as the discriminators.

$$\hat{w}(s, a) = \arg \min_{w \in \mathcal{W}} \max_{f \in \mathcal{F}} L_w(w, f)^2.$$  

(5)

Note that this is the ideal estimator that assumes exact expectations (or equivalently, infinite amount of data). In reality, we will only have access to a finite sample, and the real estimator replaces $L_w(w, f)$ with its sample-based estimation, defined as

$$L_{w,n}(w, f) := \mathbb{E}_n[\{\gamma w(s, a) f(s, \pi) - w(s, a) f(s, \pi)\}] + (1 - \gamma)\mathbb{E}_{d_0 \times \pi_c}[f(s, a)].$$  

(6)

So the sample-based estimator is

$$\hat{w}_n(s, a) := \arg \min_{w \in \mathcal{W}} \max_{f \in \mathcal{F}} L_{w,n}(w, f)^2.$$  

(7)

We call this estimation procedure MWL (minimax weight learning).

As Lemma 1 has indicated, $w_{\pi_c/\pi_b}$ can be uniquely identified if we use a very rich $\mathcal{F}$ class. However, this may cause serious sample complexity issues, as we need to pay the statistical complexity of $\mathcal{W}$ and $\mathcal{F}$ (see Section 6), and hence cannot afford to use rich classes such as $L^2(\mathcal{X}, \nu)$. Fortunately, for the purpose of off-policy evaluation, the real representation requirement on $\mathcal{F}$ is much weaker: as long as $Q^{\pi_c}$ is captured by the convex hull of $\mathcal{F}$, $\max_{f \in \mathcal{F}} L_w(w, f)$ will be an upper bound on the approximation error of the OPE estimator obtained by re-weighting rewards by $w$. This is formalized in the following result.

**Theorem 2.** For any given $w : \mathcal{X} \rightarrow \mathbb{R}$, define $R_w[w] = \mathbb{E}_{d_{\pi_b}}[w(s, a) \cdot r]$. If $Q^{\pi_c} \in \text{conv}(\mathcal{F})$, where $\text{conv}()$ denotes the convex hull of a function class,

$$|R_{\pi_c} - R_w[w]| \leq \max_{f \in \mathcal{F}} |L_w(w, f)|, \quad |R_{\pi_c} - R_w[\hat{w}]| \leq \min_{w \in \mathcal{W}} \max_{f \in \mathcal{F}} |L_w(w, f)|.$$  

A few comments are in order:

1. To guarantee that the estimation is accurate, all we need is $Q^{\pi_c} \in \text{conv}(\mathcal{F})$, and $\min_w \max_f |L_w(w, f)|$ is small. While the latter can be guaranteed by realizability of $\mathcal{W}$, i.e., $w_{\pi_c/\pi_b} \in \mathcal{W}$, we show in an example below that realizability is sufficient but not always necessary: in the extreme case where $\mathcal{F}$ only contains $Q^{\pi_c}$, even a constant $w$ function can satisfy $\max_f |L_w(w, f)| = 0$ and hence provide accurate OPE estimation.

2. All proofs of this section can be found in Appendix B

3. As we will see, the uniqueness/identifiability of $w_{\pi_c/\pi_b}$ is not crucial to the OPE goal, so we defer the technical assumptions to a formal version of the lemma in Appendix B. Despite this, the identifiability may still be of interest if we use the same formulation for learning $w_{\pi_c/\pi_b}$. In the appendix, we also show that the same statement holds when $\mathcal{F}$ is an ISPD kernel; see Theorem 16 for details.
Example 1 (Realizability of \( \mathcal{W} \) can be relaxed). When \( \mathcal{F} = \{Q^{\pi_e}\} \), as long as \( w_0 \in \mathcal{W} \) where \( w_0 \) is a constant function that always evaluates to \( R_{\pi_e}/R_{\pi_b} \), we have \( R_{\pi_e}[w] = R_{\pi_e} \).

Proof. Suppose \( w_0(s,a) = C \forall (s,a) \). Then, for \( f = Q^{\pi_e} \) we have

\[
L_w(w_0, f) = CE_{d_{\pi_b}}[(\gamma V^{\pi_e}(s') - Q^{\pi_e}(s,a)) + (1-\gamma)E_{d_0 \times \pi_e}[Q^{\pi_e}(s,a)]
= CR_{\pi_b} - R_{\pi_e}.
\]

Hence \( C = R_{\pi_e}/R_{\pi_b} \) satisfies that \( L_w(w_0, f) = 0, \forall f \in \mathcal{F} \). From Theorem 2, \( |R_{\pi_e} - R_{\pi_e}[w]| \leq \min_w \max_f |L_w(w, f)| \leq \max_f |L_w(w_0, f)| = 0 \).

2. For the condition that \( Q^{\pi_e} \in \text{conv}(\mathcal{F}) \), we can further relax the convex hull to the linear span, though we will need to pay the \( \ell_1 \) norm of the combination coefficients (which is 1 for convex combinations) in the later sample complexity analysis and we do not consider this relaxation for simplicity. Also note that relaxing \( \mathcal{F} \) to \( \text{conv}(\mathcal{F}) \) is not useful when \( \mathcal{F} \) itself is linear, but can provide improper learning benefits when \( \mathcal{F} \) is a non-linear class. We will see an intuitive example in an analogous situation for the MQL estimator in the next section.

3. Although Eq.\((5)\) uses \( L_w(w, f)^2 \) in the objective function, the square is mostly for optimization convenience and is not vital in determining the statistical properties of the estimator. In later sample complexity analysis, it will be much more convenient to work with the equivalent objective function that uses \( |L_w(w, f)| \) instead.

4. When the behavior policy \( \pi_b \) is known, we can incorporate this knowledge by setting \( \mathcal{W} = \{ s \mapsto w(s)_{\pi_e(a|s)} : w \in \mathcal{W}^S \} \), where \( \mathcal{W}^S \) is some function class over the state space.

The derived estimator is still different from Liu et al. (2018) since our discriminator class is still over the state-action space.

4.1 Efficient Implementation with RKHS

The estimator in Eq.\((6)\) requires solving a minimax optimization problem, which can be computationally challenging. Following Liu et al. (2018) we show that the inner maximization has a closed form solution when we choose \( \mathcal{F} \) to correspond to a reproducing kernel Hilbert space (RKHS) \( \mathcal{H}_K \) be a RKHS associated with kernel \( K(\cdot,\cdot) \). Let \( \langle \cdot, \cdot \rangle_{\mathcal{H}_K} \) be the inner product of \( \mathcal{H}_K \), which satisfies the reproducing property \( f(x) = \langle f, K(\cdot, x) \rangle_{\mathcal{H}_K} \).

Lemma 3. When \( \mathcal{F} = \{ f \in (\mathcal{X} \to \mathbb{R}) : \langle f, f \rangle_{\mathcal{H}_K} \leq 1 \} \), the term \( \max_{f \in \mathcal{F}} L_w(w, f)^2 \) has a closed form expression:

\[
\max_{f \in \mathcal{F}} L_w(w, f)^2 = E_{d_{\pi_b}}[\gamma^2 w(s, a)w(\tilde{s}, \tilde{a})E_{d' \sim \pi_e(s'), \tilde{a}' \sim \pi_e(\tilde{s}')}[K((s', a'), (\tilde{s}', \tilde{a}'))] + \\
+ E_{d_{\pi_b}}[w(s, a)w(\tilde{s}, \tilde{a})K((s, a), (\tilde{s}, \tilde{a}))] + (1-\gamma)^2 E_{d_0 \times \pi_e}[K((s, a), (\tilde{s}, \tilde{a}))] + \\
- 2E_{d_{\pi_b}}[\gamma w(s, a)w(\tilde{s}, \tilde{a})E_{d' \sim \pi_e(s')}[K((s', a'), (\tilde{s}, \tilde{a}))]] + \\
+ 2\gamma(1-\gamma)E_{(s, a) \sim d_{\pi_b}, (\tilde{s}, \tilde{a}) \sim d_0 \times \pi_e}[\gamma w(s, a)E_{d' \sim \pi_e(s')}[K((s', a'), (\tilde{s}, \tilde{a}))]] + \\
- 2(1-\gamma)E_{(s, a) \sim d_{\pi_b}, (\tilde{s}, \tilde{a}) \sim d_0 \times \pi_e}[w(s, a)w(\tilde{s}, \tilde{a})K((s, a), (\tilde{s}, \tilde{a}))].
\]
In the above expression, all $a'$ and $\tilde{a}'$ terms are marginalized out in the inner expectations, and when they appear together they are always independent. Similarly, in the first 3 lines when $(s, a, s')$ and $(s, a, \tilde{s}')$ appear together in the outer expectation, they are i.i.d. following the distribution specified in the subscript.

Below is a further special case when both $W$ and $F$ are linear classes under the same state-action features $\phi: \mathcal{X} \rightarrow \mathbb{R}^d$. The resulting algorithm has a close connection to LSTDQ (Lagoudakis and Parr, 2004), and we will discuss this connection in more detail later.

**Example 2.** Let $w(s, a; \alpha) = \phi(s, a)\trans\alpha$ where $\phi(s, a) \in \mathbb{R}^d$ is some basis function and $\alpha$ is the parameters. If we use the same linear function space as $F$, i.e., $F = \{(s, a) \mapsto \phi(s, a)\trans\beta : \|\beta\|_2 \leq 1\}$, then the parameter $\alpha$ can be estimated as

$$\hat{\alpha} = \mathbb{E}[\mathbb{E}[-\gamma \phi(s', \pi_e)\phi(s, a)\trans\hat{\alpha} + \phi(s, a)\phi(s, a)\trans\hat{\alpha} - (1 - \gamma)\mathbb{E}[\phi(s, a)]]].$$

The sample-based estimator for the OPE problem is

$$R_{w, n}[\hat{w}_n] = \mathbb{E}[\mathbb{E}[-\gamma \phi(s', \pi_e)\phi(s, a)\trans\hat{\alpha} + \phi(s, a)\phi(s, a)\trans\hat{\alpha} - (1 - \gamma)\mathbb{E}[\phi(s, a)]]].$$

Just as our method corresponds to LSTDQ in the linear setting, it is worth pointing out that the method of Liu et al. (2018)—which we will call MSWL (minimax state weight learning) for distinction and easy reference—corresponds to off-policy LSTD (Bertsekas and Yu, 2009; Dann et al., 2014); see Appendix B.2 for details.

### 4.2 Connections to related work

Nachum et al. (2019) has recently proposed a version of MIS with a similar goal of being agnostic to the knowledge of $\pi_b$. In fact, their estimator and ours have an interesting connection, as our Lemma 1 can be obtained by taking the functional derivative of their loss function; we refer interested readers to Appendix B.1 for details. That said, there are also important differences between our methods. First, our loss function can be reduced to single-stage optimization when using an RKHS discriminator, just as in Liu et al. (2018). In comparison, the estimator of Nachum et al. (2019) cannot avoid two-stage optimization. Second, they do not directly estimate $w_{\pi_e/\pi_b}(s, a)$, and instead estimate $\nu^*(s, a)$ such that $\nu^*(s, a) - \gamma \mathbb{E}[\mathbb{E}[-\gamma \phi(s', \pi_e)\phi(s, a)\trans\nu^*(s', a') - (1 - \gamma)\mathbb{E}[\phi(s, a)]]] = w_{\pi_e/\pi_b}(s, a)$, which is more indirect.

In the special case of $\gamma = 0$, i.e., when the problem is a contextual bandit, our method essentially becomes kernel mean matching when using an RKHS discriminator (Gretton et al., 2012), so this estimator can be viewed as a natural extension of kernel mean matching in the sequential decision-making setting.

### 5. MQL: Learning $Q$-Functions using Importance Weight Discriminators

In Section 4, we show how to use value-function class as discriminators to learn the importance weight function. In this section, by swapping the roles of $w$ and $f$, we derive a new estimator that learns $Q^{\pi_e}$ from data using importance weights as discriminators. The resulting objective function has an intuitive interpretation of average Bellman errors, which has many nice properties and interesting connections to prior works in other areas of RL.
**Setup** We assume that we have a class of state-action importance weighting functions \( \mathcal{G} \subseteq (\mathcal{X} \to \mathbb{R}) \) and a class of state-action value functions \( \mathcal{Q} \subseteq (\mathcal{X} \to \mathbb{R}) \). To avoid confusion we do not reuse the symbols \( W \) and \( F \) in Section 4, but when we apply both estimators on the same dataset (and possibly combine them via doubly robust), it can be reasonable to choose \( \mathcal{Q} = \mathcal{F} \) and \( \mathcal{G} = \mathcal{W} \). For now it will be instructive to assume that \( \mathcal{Q}^\pi_e \) is captured by \( \mathcal{Q} \) (we will relax this assumption later), and the goal is to find \( q \in \mathcal{Q} \) such that

\[
R_q[q] := (1 - \gamma)E_{d_0 \times \pi_e}[q]
\]  
(i.e., the estimation of \( R_{\pi_e} \) as if \( q \) were \( \mathcal{Q}^\pi_e \)) is an accurate estimate of \( R_{\pi_e} \).

**Loss Function** The loss function we will use in this section is

\[
L_q(q, g) = E_{d_{\pi_b}}[g(s, a)(r + \gamma v(s') - q(s, a))], \text{ where } v(s') := q(s', \pi_e).
\]

**Interpretation** As we alluded to earlier, if \( g \) is the importance weight that converts the data distribution (over \( (s, a) \)) \( d_{\pi_b} \) to any other distribution \( \mu \), then the loss function becomes \( E_{\mu}[r + \gamma v(s') - q(s, a)] \), which is essentially the average Bellman error defined by Jiang et al. (2017). An important property of this quantity is that, if \( \mu = d_{\pi_e, \gamma} \), then by (a variant of) Lemma 1 of Jiang et al. (2017), we immediately have

\[
R_{\pi_e} - R_q[q] = E_{d_{\pi_e, \gamma}}[r + \gamma v(s') - q(s, a)] \overset{\text{def}}{=} L_q(q, w_{\pi_e/\pi_b}).
\]

Based on this observation, we introduce the following estimator of \( R_{\pi_e} \):

\[
\hat{q} = \arg \min_{q \in \mathcal{Q}} \max_{g \in \mathcal{G}} L_q(q, g)^2.
\]

We call this method MQL (minimax Q-function learning). Similar to Section 4, we use \( \hat{q}_n \) to denote the estimator based on a finite sample of size \( n \) (which replaces \( L_q(q, g) \) with its empirical approximation \( L_{q,n}(q, g) \)), and develop the formal results that parallel those in Section 4 for MWL. All proofs and additional results can be found in Appendix C.

**Lemma 4.** \( L_q(Q^{\pi_e}, g) = 0 \) for \( \forall g \in L^2(\mathcal{X}, \nu) \). Moreover, if we further assume that \( d_{\pi_b}(s, a) > 0 \ \forall (s, a) \), then \( Q^{\pi_e} \) is the only function that satisfies such a property.

Similar to the case of MWL, we show that under certain representation conditions, the estimator will provide accurate estimation to \( R_{\pi_e} \).

**Theorem 5.** The following holds if \( w_{\pi_e/\pi_b} \in \text{conv}(\mathcal{G}) \):

\[
|R_{\pi_e} - R_q[q]| \leq \max_{g \in \mathcal{G}} |L_q(q, g)|, \quad |R_{\pi_e} - \hat{q}[\hat{q}]| \leq \min_{q \in \mathcal{Q}} \max_{g \in \mathcal{G}} |L_q(q, g)|.
\]

4. Note that \( R_q[\cdot] \) only requires knowledge of \( d_0 \) and can be computed directly. This is different from the situation in MWL, where \( R_{w,\cdot} \) still requires knowledge of \( d_{\pi_b} \) even if the importance weights are known, and the actual estimator needs to use the empirical approximation \( R_{w,n}[\cdot] \).
5.1 Case Studies

We proceed to give several special cases of this estimator corresponding to different choices of \(G\) to illustrate its properties. In the first example, we show the analogy of Example 1 for MWL, which demonstrates that requiring \(\min_g \max_q L_q(q, g) = 0\) is weaker than realizability \(Q^{\pi_e} \in \mathcal{Q}\).

**Example 3** (Realizability of \(Q\) can be relaxed). When \(\mathcal{G} = \{w_{\pi_e/\pi_b}\}\), as long as \(q_0 \in \mathcal{Q}\), where \(q_0\) is a constant function that always evaluates to \(R_{\pi_e}/(1 - \gamma)\), we have \(R_q[\hat{q}] = R_{\pi_e}\).

**Proof.** Suppose \(q_0(s, a) = C\). Then, for \(g = w_{\pi_e/\pi_b}\), we have

\[
L_q(q, g) = E_{d_{\pi_b}}[w_{\pi_e/\pi_b}(s, a)(r + \gamma C - C)]
= E_{d_{\pi_b}}[w_{\pi_e/\pi_b}(s, a)r] - (1 - \gamma)C = R_{\pi_e} - (1 - \gamma)C.
\]

Therefore \(C = R_{\pi_e}/(1 - \gamma)\) satisfies \(L_q(q, g) = 0\) \(\forall g \in \mathcal{G}\). From Theorem 5 we further have \(R_q[\hat{q}] = R_{\pi_e}\).

Next, we show a simple and intuitive example where \(w_{\pi_e/\pi_b} \notin \mathcal{G}\) but \(w_{\pi_e/\pi_b} \in \text{conv}(\mathcal{G})\), i.e., there are cases where relaxing \(\mathcal{G}\) to its convex hull yields stronger representation power and the corresponding theoretical results provide a better description of the algorithm’s behavior.

**Example 4.** Suppose \(X\) is finite. Let \(\mathcal{Q}\) be the tabular function class, and \(\mathcal{G}\) is the set of state-action indicator functions. Then \(w_{\pi_e/\pi_b} \notin \mathcal{G}\) but \(w_{\pi_e/\pi_b} \in \text{conv}(\mathcal{G})\), and \(R_q[\hat{q}] = 0\). Furthermore, the sample-based estimator \(\hat{q}_n\) coincides with the model-based solution, as \(L_{q, n}(q, g) = 0\) for each \(g\) is essentially the Bellman equation on the corresponding state-action pair in the estimated MDP model. (In fact, the solution remains the same if we replace \(\mathcal{G}\) with the tabular function class.)

In the next example, we choose \(\mathcal{G}\) to be a rich \(L^2\)-class with bounded norm, and recover the usual (squared) Bellman error as a special case. A similar example has been given by Feng et al. (2019).

**Example 5** (\(L^2\)-class). When \(\mathcal{G} = \{g(s, a); E_{d_{\pi_b}}[g^2] \leq 1\}\),

\[
\max_{g \in \mathcal{G}} L_q(q, g)^2 = E_{d_{\pi_b}}[((B^\pi q)(s, a) - q(s, a))^2],
\]

where \(B^\pi\) is the Bellman update operator \((B^\pi q)(s, a) := E_{r \sim \mathcal{R}(s, a), s' \sim P(s, a)}[r + \gamma q(s', \pi)]\).

Note that the standard Bellman error cannot be directly estimated from data when the state space is large, even if the \(\mathcal{Q}\) class is realizable (Szepesvari and Munos, 2005; Sutton and Barto, 2018; Chen and Jiang, 2019). From our perspective, this difficulty can be explained by the fact that squared Bellman error corresponds to an overly rich discriminator class that demands an unaffordable sample complexity.

The next example is RKHS class which yields a closed-form solution to the inner maximization as usual.

---

5. Strictly speaking we need to multiply these indicator functions by \(C_w\) to guarantee \(w_{\pi_e/\pi_b} \in \text{conv}(\mathcal{G})\); see the comment on linear span after Theorem 2
Example 6 (RKHS class). When $\mathcal{G} = \{g(s, a); \langle g, g \rangle_{\mathcal{H}_K} \leq 1\}$, we have the following result.

**Lemma 6.** Assume $\mathcal{G} = \{g(s, a); \langle g, g \rangle_{\mathcal{H}_K} \leq 1\}$. Then, we have

$$\max_{g \in \mathcal{G}} L_q(q, g)^2 = E_{d_{x_2}}[\Delta^q(q; s, a, r, s')\Delta^q(q; \tilde{s}, \tilde{a}, \tilde{r}, \tilde{s}')K((s, a), (\tilde{s}, \tilde{a}))],$$

where $\Delta^q(g; s, a, r, s') = g(s, a)(r + \gamma v(s') - q(s, a))$.

Finally, the linear case.

**Example 7.** Let $q(s, a; \alpha) = \phi(s, a)^\top \alpha$ where $\phi(s, a) \in \mathbb{R}^d$ is some basis function and $\alpha$ is the parameters. If we use the same linear function space as $\mathcal{G}$, i.e., $\mathcal{G} = \{(s, a) \mapsto \phi(s, a)^\top \beta : \|\beta\|_2 \leq 1\}$, then the parameter $\alpha$ can be estimated as

$$\hat{\alpha} = E_n[-\gamma \phi(s, a)\phi(s', \pi_e)^\top + \phi(s, a)\phi(s, a)^\top]^{-1}E_n[r\phi(s, a)].$$

The resulting $q(s, a; \hat{\alpha})$ as an estimation of $Q^{\pi_e}$ is precisely LSTDQ (Lagoudakis and Parr, 2004). In addition, the final OPE estimator $R_q[\hat{g}_n]$ is

$$R_q[\hat{g}_n] = (1 - \gamma)E_{d_0 \times \pi_c}[\phi(s, a)^\top]E_n[-\gamma \phi(s, a)\phi(s', \pi_e)^\top + \phi(s, a)\phi(s, a)^\top]^{-1}E_n[r\phi(s, a)].$$

which is the same as $R_{w, n}[\hat{w}_n]$ when $\mathcal{W}$ and $\mathcal{F}$ are the same linear class.

5.2 Connection to Kernel Loss (Feng et al., 2019)

Feng et al. (2019) has recently proposed a loss function that can learn from on-policy data. By some transformations, we may rewrite their loss function over state-value function $v$ as

$$\max_{g \in \mathcal{G}^S} E_{\pi_e}[\{r + \gamma v(s') - v(s)\}g(s)]^2,$$

where $\mathcal{G}^S$ is an RKHS over the state space. While their method is very similar to MQL when written as the above expression, they focus on learning a state-value function and need to be on-policy for policy evaluation. In contrast, our goal is OPE (i.e., estimating the expected return instead of the value function), and we learn a Q-function as an intermediate object and hence are able to learn from off-policy data. More importantly, the importance weight interpretation of $g$ has eluded their paper and they interpret this loss purely from a kernel perspective. In contrast, by leveraging the importance weight interpretation, we are able to establish approximation error bounds based on representation assumptions that are fully expressed in quantities directly defined in the MDP. We also note that their loss for policy optimization (i.e., learning $v^*$) can be similarly interpreted as minimizing average Bellman errors under a set of distributions.

Furthermore, it is easy to extend their estimator to the OPE task using knowledge of $\pi_b$. The loss functions for state-value function $v$ can be defined in two ways:

$$\max_{g \in \mathcal{G}^S} E_{\pi_b} \left[ \pi_e(a|s) \pi_e(s') \{r + \gamma v(s') - v(s)\}g(s) \right]^2,$$

$$\max_{g \in \mathcal{G}^S} E_{\pi_b} \left[ \pi_e(a|s) \pi_b(s') \{r + \gamma v(s') - v(s)\}g(s) \right]^2.$$

For distinction and easy reference, we will call this method MVL (minimax value learning) in later sections. Again, just as we discussed in Appendix B.2 on MSWL, when we use linear classes for both value functions and importance weights, the above estimators become two variants of off-policy LSTDQ (Dann et al., 2014; Bertsekas and Yu, 2009) and coincide with MSWL and its variant.
6. Doubly Robust Extension and Sample Complexity of MWL/MQL

In the previous sections we have seen two different ways of using a value-function class and an importance-weight class for OPE. Which one should we choose?

In this section we show that there is no need to make a choice. In fact, we can combine the two estimates naturally through the doubly robust trick (Kallus and Uehara, 2019a), whose ideal version (with exact expectations) is:

\[ R[w, q] = (1 - \gamma)E_{d_0}[v(s)] + E_{d_\pi_b}[w(s, a)\{r + \gamma v(s') - q(s, a)\}] \]  \hspace{1cm} (9)

As before, we write \( R_n[w, q] \) as the empirical analogue of \( R[w, q] \). While it is often instructive to think of them as the estimators obtained by MWL and MQL, sometimes we will treat \( w \) and \( q \) as arbitrary functions from the \( W \) and \( Q \) classes to keep our results general. By combining the two estimators, we obtain the usual doubly robust property, that when either \( w = w_{\pi_e/\pi_b} \) or \( q = Q_{\pi_e} \), we have \( R[w, q] = R_{\pi_e} \), that is, as long as either one of the models works well, the final estimator behaves well.

Besides being useful as an estimator, Eq.(9) also provides a unified framework to analyze the previous estimators, which are all its special cases: Note that \( R[0, q] = R_{\pi_b} \) and \( R[w, 0] = R_{\pi_e} \), where 0 means a constant function that always evaluates to 0. Below we first prove a set of results that unify and generalize the results in Sections 4 and 5, and then state the sample complexity guarantees for the proposed estimators.

**Lemma 7.**

\[ R[w, q] - R_{\pi_e} = E_{d_\pi_b}[\{w(s, a) - w_{\pi_e/\pi_b}(s, a)\}\{\gamma V_{\pi_e}(s') - \gamma v(s') + q(s, a) - Q_{\pi_e}(s, a)\}] \]

**Theorem 8.** Fixing any \( q' \in Q \), if \( [Q_{\pi_e} - q'] \in \text{conv}(F), \)

\[ |R[w, q'] - R_{\pi_e}| \leq \max_{f \in F} |L_w(w, f)|, \text{ and } |R[w, q'] - R_{\pi_e}| \leq \min_{w \in W} \max_{f \in F} |L_w(w, f)|. \]

Similarly, fixing any \( w' \in W \), if \( [w_{\pi_e/\pi_b} - w'] \in \text{conv}(G), \)

\[ |R[w', q] - R_{\pi_e}| \leq \max_{g \in G} |L_q(q, g)|, \text{ and } |R[w', q] - R_{\pi_e}| \leq \min_{q \in Q} \max_{g \in G} |L_q(q, g)|. \]

**Remark 1.** When \( q' = 0 \), the first statement is reduced to Theorem 2. When \( w' = 0 \), the second statement is reduced to Theorem 5.

**Theorem 9** (Double robust inequality for discriminators (i.i.d case)). Recall that

\[ \hat{w}_n = \arg \min_{w \in W} \max_{f \in F} L_{w,n}(w, f)^2, \text{ and } \hat{q}_n = \arg \min_{q \in Q} \max_{g \in G} L_{q,n}(q, g)^2, \]

where \( L_{w,n} \) and \( L_{q,n} \) are the empirical losses based on a set of \( n \) i.i.d samples. We have the following two statements.

1. Assume \( [Q_{\pi_e} - q'] \in \text{conv}(F) \) for some \( q' \), and \( \forall f \in F, \|f\|_\infty < C_f \). Then, with probability at least \( 1 - \delta \),

\[ |R[\hat{w}_n, q'] - R_{\pi_e}| \leq \min_{w \in W} \max_{f \in F} |L_w(w, f)| + R_n(F, W) + C_f C_w \sqrt{\frac{\log(1/\delta)}{n}}. \]
where $\mathcal{R}_n(W, F)$ is the Rademacher complexity \(^7\) of the function class
\[
\{(s, a, s') \mapsto (w(s, a)(\gamma f(s', \pi_e) - f(s, a))) : w \in W, f \in F\}.
\]

(2) Assume $[w_{\pi_e}, w_{\pi_b} - w'] \in \text{conv}(G)$ for some $w'$, and $\forall g \in G$, $\|g\|_\infty < C_g$. Then, with probability at least $1 - \delta$, 
\[
|R[w', q_a] - R_{\pi_e}| \leq \min_{q \in Q} \max_{g \in G} |L_q(q, g)| + \mathcal{R}_n(Q, G) + C_g R_{\text{max}} \frac{\log(1/\delta)}{n},
\]
where $\mathcal{R}_n(Q, G)$ is the Rademacher complexity of the function class
\[
\{(s, a, r, s') \mapsto (g(s, a)(r + \gamma q(s', \pi_e) - q(s, a))) : q \in Q, g \in G\}.
\]

Here $A \lesssim B$ means there exists the constant $C$ not depending on $n, C_f, C_g, R_{\text{max}}, \gamma$ such that $A < CB$. Note that we can immediately extract the sample complexity guarantees for the MWL and the MQL estimators as the corollaries of this general guarantee by letting $q' = \mathbf{0}$ and $w' = \mathbf{0}$. \(^8\)

**Relaxing the i.i.d. assumption** Although the previous sample complexity results are for i.i.d. data, we show that under standard assumptions we can also handle dependent data and obtain almost the same results. For simplicity, we only include the result for $\hat{w}_n$.

In particular, we consider the setting mentioned in Section 2, that our data is a single long trajectory generated by policy $\pi_b$:
\[
s_1, a_1, r_1, s_2, a_2, r_2, \ldots, s_T, a_T, r_T, s_{T+1}.
\]

We assume that the Markov chain induced by $\pi_b$ is ergodic, and $s_1$ is sampled from its stationary distribution so that the chain is stationary. In this case, $d_{\pi_b}$ corresponds to such a stationary distribution, which is also the marginal distribution of any $s_t$. We convert this trajectory into a set of transition tuples $\{(s_i, a_i, r_i, s'_i)\}_{i=1}^n$ with $n = T$ and $s'_i = s_{i+1}$, and then apply our estimator on this data. Under the standard $\beta$-mixing condition \(^9\) (see e.g., Antos et al., 2008), we can prove a similar sample complexity result:

**Corollary 10.** Assume $\{s_i, a_i, r_i, s'_i\}_{i=1}^n$ follows a stationary $\beta$-mixing distribution with $\beta$-mixing coefficient $\beta(k)$ for $k = 0, 1, \cdots$. For any $a_1, a_2 > 0$ with $2a_1a_2 = n$ and $\delta > 4(a_1 - 1)\beta(a_2)$, with probability at least $1 - \delta$, we have (all other assumptions are the same as in Theorem 9(1))
\[
|R[\hat{w}_n, q] - R_{\pi_e}| \leq \min_{w \in W} \max_{f \in F} |L_w(w, f)| + \hat{\mathcal{R}}_{a_1}(F, W) + C_f C_w \sqrt{\frac{\log(1/\delta')}{a_1}}
\]
where $\hat{\mathcal{R}}_{a_1}(F, W)$ is the empirical Rademacher complexity of the function class $\{(s, a, s') \mapsto \{w(s, a)(\gamma f(s', \pi_e) - f(s, a)) : w \in W, f \in F\}$ based on a selected subsample of size $a_1$ from the original data (see Mohri and Rostamizadeh (2009, Section 3.1) for details), and $\delta' = \delta - 4(a_1 - 1)\beta(a_2)$.

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7. Refer to Bartlett and Mendelson (2003) regarding the definition.
8. Strictly speaking, when $q' = \mathbf{0}$, $R[\hat{w}_n, q'] = R_w[\hat{w}_n]$ is very close to but slightly different from the sample-based MWL estimator $R_w[\hat{w}_n]$, but their difference can be bounded by a uniform deviation bound over the $W$ class in a straightforward manner. The MQL analysis does not have this issue as $R_a[\cdot]$ does not require empirical approximation.
9. Refer to Meyn and Tweedie (2009) regarding the definition.
7. Statistical Efficiency of MWL and MQL in the Tabular Setting

As we have discussed earlier, both MWL and MQL are equivalent to LSTDQ when we use the same linear class for all function approximators. Here we show that in the tabular setting, which is a special case of the linear setting, MWL and MQL can achieve the semiparametric lower bound of OPE (Kallus and Uehara, 2019b), because they coincide with the model-based solution. This is a desired property that many OPE estimators fail to obtain, including MSWL and MVL.

**Theorem 11.** Assume the whole data set \( \{(s, a, r, s')\} \) is geometrically ergodic \(^{10}\). Then, in the tabular setting, \( \sqrt{n}(R_{w,n}[^{\hat{w}}]_n - R_{\pi_e}) \) and \( \sqrt{n}(R_{q[^{\hat{q}}]}_n - R_{\pi_e}) \) weakly converge to the normal distribution with mean 0 and variance

\[
E_{d_{\pi_e}}[w_{\pi_e}^2(s, a)(r + \gamma V_{\pi_e}(s') - Q_{\pi_e}(s, a))^2].
\]

This variance matches the semiparametric lower bound for OPE given by Kallus and Uehara (2019b, Theorem 5).

The details of this theorem and further discussions can be found in Appendix E, where we also show that MSWL and MVL have an asymptotic variance greater than this lower bound. To back up this theoretical finding, we also conduct empirical experiments in the Taxi environment (Dietterich, 2000) following Liu et al. (2018, Section 5), and compare three methods, all using the tabular representation: MSWL with exact \( \pi_e \), MSWL with estimated \( \pi_e \) (“plug-in”), and MWL (same as MQL). As we have mentioned, this comparison is essentially among off-policy LSTD, plug-in off-policy LSTD, and LSTDQ. From Figure 1, we can see that MWL/MQL performs significantly better than MSWL with exact \( \pi_e \) and slightly better than plug-in MSWL. While it can be counterintuitive that plug-in MSWL is better than MSWL, it is well understood that plug-in based on MLE with a well specified model for the policy can be viewed as a form of control variates (Henm and Eguchi, 2004; Hanna et al., 2019). Whether the plug-in MSWL can achieve the semiparametric lower bound remains as future work.

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\(^{10}\) Regarding the definition, refer to Meyn and Tweedie (2009)
8. Further Discussions

We conclude the paper with further discussions and open questions.

On the dependence of $\hat{w}$ on $\mathcal{F}$

In Example 1, we have shown that with some special choice of the discriminator class in MWL, the algorithm is able to pick up very simple weighting functions—such as constant functions—that are very different from the “true” $w_{\pi_e/\pi_b}$ and nevertheless produce accurate OPE estimates with very low variance.\(^{11}\) Therefore, the function $w$ that satisfies $L_w(w, f) = 0 \forall f \in \mathcal{F}$ may not be unique, and the set of feasible $w$ functions highly depend on the choice of $\mathcal{F}$. This leads to several additional questions we would like to investigate in the future, such as how to choose $\mathcal{F}$ to allow for these simple solutions, and how to use regularization techniques to choose a simple function for best bias-variance trade-off.\(^{12}\)

In case it is not clear enough that the set of feasible $w$ functions generally depends on $\mathcal{F}$, we provide two additional examples which are also of independent interest themselves. The first example actually shows that standard sequential step-wise IS can be viewed as a special case of MWL, when we choose a very rich discriminator class of history-dependent functions.

**Example 8 (Step-wise IS as a Special Case of MWL).** We show that step-wise IS (Precup et al., 2000) in discounted episodic problems can be viewed as a special case of MWL, and sketch the proof as follows. In addition to the setup in Section 2, we also assume that the MDP always goes to the absorbing state in $H$ steps from any starting state drawn from $d_0$. The data are trajectories generated by $\pi_b$. We first convert the MDP into an equivalent history-based MDP, i.e., a new MDP where the state is the history of the original MDP (absorbing states are still treated specially). We use $h_t$ to denote a history of length $t$, i.e., $h_t = (s_0, a_0, r_0, s_1, \ldots, s_t)$. Since the history-based MDP still fits our framework, we can apply MWL as-is to the history-based MDP. In this case, each data trajectory will be converted into $H$ tuples in the form of $(h_t, a_t, r_t, h_{t+1})$.

We choose the following $\mathcal{F}$ class for MWL, which is the space of all functions over histories (of various lengths up to $H$). Assuming all histories have non-zero density under $\pi_e$ (this assumption can be removed), from Lemma 1 we know that the only $w$ that satisfies $\forall f \in \mathcal{F}, L_w(w, f) = 0$ is

$$
\frac{d_{\pi_e, \gamma}(h_t, a_t)}{d_{\pi_b}(h_t, a_t)} = \frac{(1 - \gamma)\gamma^t}{1/H} \prod_{t'=0}^{t} \frac{\pi_e(a_{t'}|s_{t'})}{\pi_b(a_{t'}|s_{t'})}.
$$

Note that $R_w[w]$ with such an $w$ is precisely the step-wise IS estimator in discounted episodic problems. Furthermore, the true marginalized importance weight in the original MDP

\(^{11}\) Using notations from Example 1, the variance of (sample-based version of) $R_w[w_0]$ is in general much smaller than that of $R_w[w_{\pi_e/\pi_b}]$.

\(^{12}\) Such a trade-off is relatively well understood in the contextual bandit setting (Kallus, 2017; Hirshberg and Wager, 2017), though extension to sequential decision-making is not obvious.

\(^{13}\) Here the term $(1-\gamma)^t/t^H$ appears because a state at time step $t$ is discounted in the evaluation objective but its empirical frequency in the data is not. Other than that, the proof of this equation is precisely how one derives sequential IS, i.e., density ratio between histories is equal to the cumulative product of importance weights on actions.
\( \frac{d\pi_e, \gamma(s,a)}{d\pi_b(s,a)} \) is not feasible under this “overly rich” history-dependent discriminator class (see also related discussions in Jiang (2019)).

**Example 9** (Bisimulation). Assume \( \phi \) is a bisimulation state abstraction (see Li et al. (2006) for the definition), \( \pi_e \) and \( \pi_b \) only depend on \( s \) through \( \phi(s) \), and \( \mathcal{F} \) only contains functions that are piece-wise constant under \( \phi \), then \( w(s,a) = \frac{d\pi_e, \gamma(\phi(s),a)}{d\pi_b(\phi(s),a)} \) also satisfies \( L_w(w,f) = 0, \forall f \in \mathcal{F} \).

**“Duality” between MWL and MQL**

From Sections 4 and 5, one can observe an obvious symmetry between MWL and MQL from the estimation procedures to the guarantees. Such a symmetry reminds us a lot about the duality between state-value functions and state-action distributions in linear programming for MDPs. Is there any formal sense where MWL and MQL are dual to each other? This is an open question we would like to address in the future.

Moreover, MWL and MQL are perhaps just two special cases of a larger family of algorithms that leverage the interesting interplay between value functions and importance weights for policy evaluation and optimization. The other message of our work is that from a theoretical viewpoint, value functions and importance weights seem to be every bit as important as each other in batch learning, whereas traditionally batch model-free RL algorithms have largely focused on value function learning and ignored importance weights. A possible future direction is to investigate algorithms that put more emphases on importance weight learning, discover the connections to their value-function learning counterparts, and understand this rich family of algorithms under a unified framework.

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Appendix A. Table of Notations

Table 2: Notation

| Notation | Description |
|----------|-------------|
| \(\pi_e, \pi_b\) | Evaluation policy, Behavior policy |
| \(\{(s_i, a_i, r_i, s'_i)\}_{i=1}^n\) | Finite sample of data |
| \((\mathcal{S}, \mathcal{A}, P, \mathcal{R}, \gamma, d_0), \mathcal{X}\) | MDP, \(\mathcal{X} = \mathcal{S} \times \mathcal{A}\) |
| \(d_{\pi_b}\) | Data distribution over \((s, a, r, s')\) or its marginals |
| \(d_{\pi_e, \gamma}\) | Discounted occupancy induced by \(\pi_e\) |
| \(\beta_{\pi_e/\pi_b}(a, s)\) | Importance weight on action: \(\pi_e(a|s)/\pi_b(a|s)\) |
| \(w_{\pi_e/\pi_b}(s, a)\) | \(d_{\pi_e, \gamma}(s, a)/d_{\pi_b}(s, a)\) |
| \(C_w\) | Bound on \(\|w_{\pi_e/\pi_b}\|_{\infty}\) |
| \(V_{\pi_e}\) | Value function |
| \(Q_{\pi_e}\) | Q-value function |
| \(R_{\pi_e}\) | Expected discounted return of \(\pi_e\) |
| \(R_{w}[:]\) | OPE estimator using \((\cdot)\) as the weighting function (population version) |
| \(R_{w,n}[:]\) | OPE estimator using \((\cdot)\) as the weighting function (sample-based version) |
| \(R_{q}[:]\) | OPE estimator using \((\cdot)\) as the approximate Q-function |
| \(\mathbb{E}_n\) | Empirical approximation |
| \(\mathcal{W}, \mathcal{F}\) | Function classes for MWL |
| \(\mathcal{Q}, \mathcal{G}\) | Function classes for MQL |
| \(\langle \cdot, \cdot \rangle_{H_K}\) | Inner product of RKHS with a kernel \(K\) |
| \(\text{conv}(\cdot)\) | convex hull |
| \(\nu\) | Uniform measure over the compact space \(\mathcal{X}\) |
| \(L^2(\mathcal{X}, \nu)\) | \(L^2\)-space on \(X\) with respect to measure \(\nu\) |
| \(\mathcal{N}_n(\cdot)\) | Rademacher complexity |
| \(\lesssim\) | Inequality without constant |

Appendix B. Proofs and Additional Results of Section 4

We first give the formal version of Lemma 1, which is Lemmas 12 and 13 below, and then provide the proof.

**Lemma 12.** For any function \(g(s, a)\), define the map; \(g \rightarrow \delta(g, s', a')\);

\[
\delta(g, s', a') = \gamma \int P(s'|s, a)\pi_e(a'|s')g(s, a)d\nu(s, a) - g(s', a') + (1 - \gamma)d_0(s')\pi_e(a'|s').
\]

Then, \(\delta(d_{\pi_e, \gamma}, s', a') = 0 \forall (s', a')\).
Proof of Lemma 12. We have

\[ d_{\pi_e,\gamma}(s', a') = (1 - \gamma) \sum_{t=0}^{\infty} \gamma^t d_{\pi_e,t}(s', a') \]

\[ = (1 - \gamma) \left\{ d_0(s') \pi_e(a'|s') + \sum_{t=1}^{\infty} \gamma^t d_{\pi_e,t}(s', a') \right\} \]

\[ = (1 - \gamma) \left\{ d_0(s') \pi_e(a'|s') + \sum_{t=0}^{\infty} \gamma^{t+1} d_{\pi_e,t+1}(s', a') \right\} \]

\[ = (1 - \gamma) \left\{ d_0(s') \pi_e(a'|s') + \gamma \sum_{t=0}^{\infty} \int P(s'|s, a) \pi_e(a'|s') \gamma^t d_{\pi_e,t}(s, a) d\nu(s, a) \right\} \]

\[ = (1 - \gamma) d_0(s') \pi_e(a'|s') + \gamma \int P(s'|s, a) \pi_e(a'|s') \gamma d_{\pi_e,\gamma}(s, a) d\nu(s, a). \]

This concludes \( \delta(d_{\pi_e,\gamma}, s', a') = 0 \forall (s', a'). \)

Lemma 13. \( L_w(w_{\pi_e/\pi_b}, f) = 0 \forall f \in L^2(\mathcal{X}, \nu) := \{ f : \int f(s, a)^2 d\nu < \infty \}. \) Moreover, if we further assume that \( (a) d_{\pi_b}(s, a) > 0 \forall (s, a), (b) g(s, a) = d_{\pi_e,\gamma}(s, a) \) if and only if \( \delta(g, s', a') = 0 \forall (s', a') \), then \( w_{\pi_e/\pi_b} \) is the only function that satisfies such a property.

Proof of Lemma 13. Here, we denote \( \beta_{\pi_e/\pi_b}(s, a) = \pi_e(a|s)/\pi_b(a|s) \). Then, we have

\[ L_w(w, f) = E_{d_{\pi_b}}[\gamma w(s, a) f(s', a) - w(s, a) f(s, a)] + (1 - \gamma) E_{d_0 \times \pi_e}[f(s, a)] \]

\[ = E_{d_{\pi_b}}[\gamma w(s, a) \beta_{\pi_e/\pi_b}(a', s') f(s', a')] - E_{d_{\pi_b}}[w(s, a) f(s, a)] + (1 - \gamma) E_{d_0 \times \pi_e}[f(s, a)] \]

\[ = \gamma \int f(s', a') P(s'|s, a) \pi_e(a'|s') d_{\pi_b}(s, a) w(s, a) d\nu(s, a, s', a') + \]

\[ - \int w(s', a') f(s', a') d_{\pi_b}(s', a') d\nu(s', a') + \int (1 - \gamma) d_0(s') \pi_e(a'|s') f(s', a') d\nu(a', s') \]

\[ = \int \delta(\tilde{g}, s', a') f(s', a') d\nu(s', a'), \]

where \( \tilde{g}(s, a) = d_{\pi_b}(s, a) w(s, a) \). Note that \( E_{d_{\pi_b}}[\cdot] \) means the expectation with respect to \( d_{\pi_b}(s, a) \pi_b(a|s) P(s'|s, a) \pi_b(a'|s'). \)

First statement

We prove that \( L_w(w_{\pi_e/\pi_b}, f) = 0 \forall f \in L^2(\mathcal{X}, \nu) \). This follows because

\[ L_w(w_{\pi_e/\pi_b}, f) = \int \delta(d_{\pi_e,\gamma}, s', a') f(s', a') d\nu(s', a') = 0. \]

Here, we have used Lemma 12; \( \delta(d_{\pi_e,\gamma}, s', a') = 0 \forall (s', a') \).

Second statement

We prove the uniqueness part. Assume \( L_w(w, f) = 0 \forall f \in L^2(\mathcal{X}, \nu) \) holds. Noting the

\[ L_w(w, f) = \langle \delta(\tilde{g}, s', a'), f(s', a') \rangle, \]

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where the inner product is for Hilbert space $L^2(\mathcal{X}, \nu)$, the Riesz representative of the functional $f \to L_w(w, f)$ is $\delta(\tilde{g}, s', a')$. From the Riesz representator theorem and the assumption $L_w(w, f) = 0 \forall f \in L^2(\mathcal{X}, \nu)$, the Riesz representative is uniquely determined as 0, that is, $\delta(\tilde{g}, s', a') = 0$.

From the assumption (b), this implies $\tilde{g} = d_{\pi_e, \gamma}$. From the assumption (a) and the definition of $\tilde{g}$, this implies $w = w_{\pi_e/\pi_b}$. This concludes the proof.

**Proof of Theorem 2.** We prove two lemmas; then prove the statement in the theorem.

**Lemma 14.**

$$L_w(w, f) = E_{d_{\pi_b}}[\{w_{\pi_e/\pi_b}(s, a) - w(s, a)\} \prod f(s, a)],$$

where $\prod f(s, a) = f(s, a) - \gamma E_{\pi_e \sim P(s, a)}[f(s', a')]$.

**Proof of Lemma 14.**

$$L_w(w, f) = L_w(w, f) - L_w(w_{\pi_e/\pi_b}, f)$$

$$= E_{d_{\pi_b}}[\{w(s, a) - w_{\pi_e/\pi_b}(s, a)\} \beta_{\pi_e/\pi_b}(a', s') f(a', s')]$$

$$- E_{d_{\pi_b}}[\{w(s, a) - w_{\pi_e/\pi_b}(s, a)\} f(s, a)]$$

$$= E_{d_{\pi_b}}[\{w_{\pi_e/\pi_b}(s, a) - w(s, a)\} \prod f(s, a)].$$

**Lemma 15.** Define

$$f_g(s, a) = E_{\pi_e} \left[ \sum_{t=0}^{\infty} \gamma^t g(s_t, a_t) \right] s_0 = s, a_0 = a.$$

Here, the expectation is taken with respect to the density $P(s_1|s_0, a_0)\pi_e(a_1|s_1)\pi_e(s_2|s_1, a_1) \cdots$. Then, $f = f_g$ is a solution to $g = \prod f$.

**Proof of Lemma 15.**

$$\prod f_g(s, a)$$

$$= f_g(s, a) - \gamma E_{s' \sim P(s, a), a' \sim \pi_{e}(s')}[f_g(s', a')]$$

$$= E_{\pi_e} \left[ \sum_{t=0}^{\infty} \gamma^t g(s_t, a_t) \right] s_0 = s, a_0 = a - E_{\pi_e} \left[ \sum_{t=0}^{\infty} \gamma^{t+1} g(s_{t+1}, a_{t+1}) \right] s_0 = s, a_0 = a$$

$$= E_{\pi_e} \left[ g(s_0, a_0) \right] s_0 = s, a_0 = a = g(s, a).$$

We go back to the main proof. Here, we have $L_w(w, Q^e) = R_{\pi_e} - R_w[w]$ since

$$L_w(w, Q^e) = E_{d_{\pi_b}}[\{w_{\pi_e/\pi_b}(s, a) - w(s, a)\} \prod Q^e(s, a)]$$

$$= E_{d_{\pi_b}}[\{w_{\pi_e/\pi_b}(s, a) - w(s, a)\} E[r|s, a] ]$$

$$= E_{d_{\pi_b}}[\{w_{\pi_e/\pi_b}(s, a) - w(s, a)\} r] = R_{\pi_e} - R_w[w].$$
In the first line, we have used Lemma 14. From the first line to the second line, we have used Lemma 15.
Therefore, if $Q^\pi_e \in \text{conv}(\mathcal{F})$, for any $w$,
$$|R_{\pi_e} - R_w[w]| = |L_w(w, Q^\pi_e)| \leq \max_{f \in \text{conv}(\mathcal{F})} |L_w(w, f)| = \max_{f \in \mathcal{F}} |L_w(w, f)|.$$
Here, we have used a fact that $\max_{f \in \text{conv}(\mathcal{F})} |L_w(w, f)| = \max_{f \in \mathcal{F}} |L_w(w, f)|$. This is proved as follows. First, $\max_{f \in \text{conv}(\mathcal{F})} |L_w(w, f)|$ is equal to $|L_w(w, f')|$ where $f' = \sum \lambda_i f_i$ and $\sum \lambda_i = 1$. Since $|L_w(w, f)| \leq \sum \lambda_i |L_w(w, f_i)| \leq \max_{f \in \mathcal{F}} |L_w(w, f)|$, we have
$$\max_{f \in \text{conv}(\mathcal{F})} |L_w(w, f)| \leq \max_{f \in \mathcal{F}} |L_w(w, f)|.$$
The reverse direction is obvious.
Finally, from the definition of $\tilde{w}$,
$$|R_{\pi_e} - R_w[\tilde{w}]| \leq \min_{w \in \mathcal{W}} \max_{f \in \mathcal{F}} |L_w(w, f)|. \quad \square$$

Proof of Lemma 3. We have
\begin{equation}
L_w(w, f)^2 = \left\{ \mathbb{E}_{d_{sb}}[\gamma w(s, a)E_{a' \sim \pi_e(s')}[f(s', a')] - w(s, a)f(s, a)] + (1 - \gamma)\mathbb{E}_{d_0 \times \pi_e}[f(s, a)] \right\}^2
\end{equation}
\begin{equation}
= \left\{ \mathbb{E}_{d_{sb}}[\gamma w(s, a)E_{a' \sim \pi_e(s')}[f(s', a')] - w(s, a)f(s, a)] + (1 - \gamma)\mathbb{E}_{d_0 \times \pi_e}[f(s, a)] \right\}^2
\end{equation}
\begin{equation}
= \langle f, f^* \rangle^2_{\mathcal{H}_K},
\end{equation}
where
$$f^*(\cdot) = \mathbb{E}_{d_{sb}}[\gamma w(s, a)E_{a' \sim \pi_e(s')}[K((s', a'), \cdot)] - w(s, a)f(s, a)] + (1 - \gamma)\mathbb{E}_{d_0 \times \pi_e}[K((s, a), \cdot)].$$
Here, from (10) to (11), we have used a reproducing property of RKHS; $f(s, a) = \langle f(\cdot), K((s, a), \cdot) \rangle$. From (11) to (12), we have used a linear property of the inner product.
Therefore,
$$\max_{f \in \mathcal{F}} L_w(w, f)^2 = \max_{f \in \mathcal{F}} \langle f, f^* \rangle^2_{\mathcal{H}_K} = \langle f^*, f^* \rangle^2_{\mathcal{H}_K},$$
from Cauchy-Schwarz inequality. This is equal to
$$\max_{f \in \mathcal{F}} L_w(w, f)^2 = \mathbb{E}_{d_{sb}}[\gamma^2 w(s, a)w(\tilde{s}, \tilde{a})E_{a' \sim \pi_e(s'), \tilde{a}' \sim \pi_e(s')}\gamma w(s, a)E_{a' \sim \pi_e(s')}[K((s', a'), (s', \tilde{a}'))] +$$
$$+ \mathbb{E}_{d_{sb}}[w(s, a)w(\tilde{s}, \tilde{a})K((s, a), (\tilde{s}, \tilde{a}))]$$
$$+ (1 - \gamma)^2 \mathbb{E}_{d_0 \times \pi_e}[\gamma w(\tilde{s}, \tilde{a})K((s, a), (\tilde{s}, \tilde{a}))]$$
$$- 2\gamma(1 - \gamma)\mathbb{E}_{d_{sb}}[w(\tilde{s}, \tilde{a})E_{a' \sim \pi_e(s')}[\gamma w(s, a)E_{a' \sim \pi_e(s')}[K((s', a'), (\tilde{s}, \tilde{a}))]]$$
$$- 2(1 - \gamma)\mathbb{E}_{d_{sb}}[w(\tilde{s}, \tilde{a})E_{a' \sim \pi_e(s')}[w(s, a)w(\tilde{s}, \tilde{a})K((s, a), (\tilde{s}, \tilde{a}))]],$$
\end{equation}
where the first expectation is taken with respect to the density $d_{\pi_0}(s, a, s')d_{\pi_0}(\tilde{s}, \tilde{a}, \tilde{s}')$.

For example, the term $(1 - \gamma)^2 E_{d_0 \times \pi_a}[K((s, a), (\tilde{s}, \tilde{a}))]$ is derived by
\[
(1 - \gamma)^2 E_{d_0 \times \pi_a}[K((s, a), (\tilde{s}, \tilde{a}))] = (1 - \gamma)^2 \int K((s, a), \cdot) d_0(s) \pi(a|s) \nu(a, s) \int K((\tilde{s}, \tilde{a}), \cdot) d_0(\tilde{s}) \pi(\tilde{a}|\tilde{s}) \nu(\tilde{a}, \tilde{s}) \mathcal{H}_K
\]

Other terms are derived in a similar manner. Here, we have used a kernel property
\[
(K((s, a), \cdot), K((\tilde{s}, \tilde{a}), \cdot)) \mathcal{H}_K = K((s, a), (\tilde{s}, \tilde{a})). \square
\]

Next we show the result mentioned in the main text, that the minimizer of $\max_{f \in \mathcal{F}} L_w(w, f)$ is unique when $\mathcal{F}$ corresponds to an ISPD kernel.

**Theorem 16.** Assume $W$ is realizable, i.e., $w_{\pi_0/\pi_b} \in \mathcal{W}$ and conditions (a), (b) in Lemma 13. Then for $\mathcal{F} = L^2(\mathcal{X}, \nu)$, $w(s, a) = w_{\pi_0/\pi_b}(s, a)$ is the unique minimizer of $\max_{f \in \mathcal{F}} L_w(w, f)$. The same result holds when $\mathcal{F}$ is a RKHS associated with an integrally strictly positive definite (ISPD) kernel $K(\cdot, \cdot)$ (Sriperumbudur et al., 2010).

**Proof of Theorem 16.** The first statement is obvious from Lemma 13 and the proof is omitted, and here we prove the second statement on the ISPD kernel case. If we can prove Lemma 13 when replacing $L^2(\mathcal{X}, \nu)$ with RKHS associated with an ISPD kernel $K(\cdot, \cdot)$, the statement is concluded. More specifically, what we have to prove is

**Lemma 17.** Assume conditions in Theorem 16. Then, $L_w(w; f) = 0, \forall f \in \mathcal{F}$ holds if and only if $w(s, a) = w_{\pi_0/\pi_b}(s, a)$.

This is proved by Mercer’s theorem (Mohri et al., 2012). From Mercer’s theorem, there exist an orthonormal basis $(\phi_j)_{j=1}^{\infty}$ of $L^2(\mathcal{X}, \nu)$ such that RKHS is represented as
\[
\mathcal{F} = \left\{ f = \sum_{j=1}^{\infty} b_j \phi_j; (b_j)_{j=1}^{\infty} \in l^2(\mathbb{N}) \text{ with } \sum_{j=1}^{\infty} \frac{b_j^2}{\mu_j} < \infty \right\},
\]
where each $\mu_j$ is a positive value since kernel is ISPD. Suppose there exists $w(s, a) \neq w_{\pi_0/\pi_b}(s, a)$ in $w(s, a) \in \mathcal{W}$ satisfying $L_w(w, f) = 0, \forall f \in \mathcal{F}$. Then, by taking $b_j = 1$ ($j = j'$), $b_j = 1$ ($j \neq j'$), for any $j' \in \mathbb{N}$, we have $L_w(w, \phi_{j'}) = 0$. This implies $L_w(w, f) = 0, \forall f \in L^2(\mathcal{X}, \nu) = 0$. This contradicts the original Lemma 13. Then, Lemma 17 is concluded. \square

**B.1 Connection to Dual DICE (Nachum et al., 2019)**

Nachum et al. (2019) proposes an extension of Liu et al. (2018) without the knowledge of the behavior policy, which shares the same goal with our MWL in Section 4. In fact, there is an interesting connection between our work and theirs, as our key lemma (13) can be obtained if we take the functional gradient of their loss function. (Ideal) DualDICE with the chi-squared divergence $f(x) = 0.5x^2$ is described as follows;
• Estimate \( \nu(s, a) \):

\[
\min_{\nu} 0.5 \mathbb{E}_{d_{a_b}} [\{\nu(s, a) - (B\nu)(s, a)\}^2] - (1 - \gamma)\mathbb{E}_{d_0 \times \pi_e}[\nu(s, a)],
\]  

(13)

where \((B\nu)(s, a) = \gamma \mathbb{E}_{s' \sim P(s, a), a' \sim \pi_e(s')}[\nu(s', a')]\).

• Estimate the ratio as \(\nu(s, a) - (B\nu)(s, a)\).

Because this objective function includes an integral in \((B\nu)(s, a)\), the Monte-Carlo approximation is required. However, even if we take an Monte-Carlo sample for the approximation, it is biased. Therefore, they further modify this objective function into a more complex minimax form. See (11) in Nachum et al. (2019).

Here, we take a functional derivative of (13)(Gateaux derivative) with respect to \(\nu\). The functional derivative at \(\nu(s, a)\) is

\[
f(s, a) \to \mathbb{E}_{d_{a_b}} [\{\nu(s, a) - (B\nu)(s, a)\} f(s, a) - (Bf)(s, a)] - (1 - \gamma)\mathbb{E}_{d_0 \times \pi_e}[f(s, a)].
\]

The first order condition exactly corresponds to our Lemma 13:

\[
-L(w, f) = \mathbb{E}_{d_{a_b}} [w(s, a) f(s, a) - \gamma \mathbb{E}_{s' \sim P(s, a), a' \sim \pi_e(s')}[f(s', a')]] + (1 - \gamma)\mathbb{E}_{d_0 \times \pi_e}[f(s, a)] = 0 \\
\iff \mathbb{E}_{d_{a_b}} [w(s, a) f(s, a) - \gamma \mathbb{E}_{a' \sim \pi_e(s')}[f(s', a')]] + (1 - \gamma)\mathbb{E}_{d_0 \times \pi_e}[f(s, a)] = 0.
\]

where \(w(s, a) = \nu(s, a) - (B\nu)(s, a)\). Our proposed method with RKHS enables us to directly estimate \(w(s, a)\) in one step, and in contrast their approach requires two additional steps: estimating \((B\nu)(s, a)\) in the loss function, estimating \(\nu(s, a)\) by minimizing the loss function, and taking the difference \(\nu(s, a) - (B\nu)(s, a)\).

### B.2 Connection between MSWL (Liu et al., 2018) and Off-policy LSTD

Just as our methods become LSTDQ using linear function classes (Examples 2 and 7), here we show that the method of Liu et al. (2018) (which we call MSWL for easy reference) corresponds to off-policy LSTD. Under our notations, their method is

\[
\arg\min_{w \in \mathcal{W}^S} \max_{f \in \mathcal{F}^S} \left\{ \mathbb{E}_{d_{sb}} \left[ \left( \gamma w(s) f(s') \frac{\pi_e(a|s)}{\pi_b(a|s)} - w(s)f(s) \right) \right] + (1 - \gamma)\mathbb{E}_{d_0}[f(s)] \right\}^2.
\]

(14)

We call this method MSWL (minimax state weight learning) for easy reference. A slightly different but closely related estimator is

\[
\arg\min_{w \in \mathcal{W}^S} \max_{f \in \mathcal{F}^S} \left\{ \mathbb{E}_{d_{sb}} \left[ \frac{\pi_e(a|s)}{\pi_b(a|s)} (\gamma w(s) f(s') - w(s)f(s)) \right] + (1 - \gamma)\mathbb{E}_{d_0}[f(s)] \right\}^2.
\]

(15)

Although the two objectives are equal in expectation, under empirical approximations the two estimators are different. In fact, Eq.(15) corresponds to the most common form of off-policy LSTD (Bertsekas and Yu, 2009) when both \(\mathcal{W}^S\) and \(\mathcal{F}^S\) are linear (similar to Example 2). In the same linear setting, Eq.(14) corresponds to another type of off-policy LSTD discussed by Dann et al. (2014). In the tabular setting, we show that cannot achieve the semiparametric lower bound in Appendix E.
Appendix C. Proofs and Additional Results of Section 5

Proof of Lemma 4. First statement
We prove $L_q(Q_{\pi^e}, g) = 0 \forall g \in L^2(\mathcal{X}, \nu)$. The function $Q_{\pi^e}$ satisfies the following Bellman equation;

$$E_{r \sim \mathcal{R}(s,a), s' \sim P(s,a)}[r + \gamma Q_{\pi^e}(s', \pi^e) - Q_{\pi^e}(s, a)] = 0. \quad (16)$$

Then, $\forall g \in L^2(\mathcal{X}, \nu),$

$$0 = \int \left\{ E_{r \sim \mathcal{R}(s,a), s' \sim P(s,a)}[r + \gamma Q_{\pi^e}(s', \pi^e) - Q_{\pi^e}(s, a)] \right\} g(s, a) d\pi_b(s, a) d\nu(s, a)$$

$$= L_q(Q_{\pi^e}, g).$$

Second statement
We prove the uniqueness part. Recall that $Q_{\pi^e}$ is uniquely characterized as (Bertsekas, 2012): $\forall (s,a),$

$$E_{r \sim \mathcal{R}(s,a), s' \sim P(s,a)}[r + \gamma q(s', \pi^e) - q(s, a)] = 0. \quad (17)$$

Assume

$$E_{(s,a,r,s') \sim d_{\pi^e}}[\{r + \gamma q(s', \pi^e) - q(s, a)\}g(s, a)] = 0, \forall g(s, a) \in L^2(\mathcal{X}, \nu) \quad (18)$$

Note that the left hand side term is seen as

$$L_q(g, g) = \langle \{ E_{r \sim \mathcal{R}(s,a)}[r] + E_{s' \sim P(s,a)}[\gamma q(s', \pi^e)] - q(s, a) \} d\pi(s, b), g(s, a) \rangle$$

where the inner product $\langle \cdot, \cdot \rangle$ is for Hilbert space $L^2(\mathcal{X}, \nu)$ and the representator of the functional $g \to L_q(g, g)$ is $\{ E[r|s, a] + \gamma q(s', \pi^e) - q(s, a) \} d\pi_b(s, a)$. From Riesz representation theorem and the assumption (18), the representator of the linear bounded functional $g \to L_q(g, g)$ is uniquely determined as 0. Since we also assume $d\pi_b(s, a) > 0 \forall (s, a)$, we have $\forall (s, a),$

$$E_{r \sim \mathcal{R}(s,a), s' \sim P(s,a)}[r + \gamma q(s', \pi^e) - q(s, a)] = 0. \quad (19)$$

From (17), such $q$ is $Q_{\pi^e}$. \qed

Proof of Theorem 5. We prove the first statement. For fixed any $q$, we have

$$|R_{\pi^e} - R_q[q]| = |(1 - \gamma)E_{d_0 \times \pi^e}(q(s,a)) - R_{\pi^e}|$$

$$= |E_{d_{\pi^e}}[-\gamma w_{\pi^e/\pi_b}(s,a)v(s') + w_{\pi^e/\pi_b}(s,a)q(s,a)] - E_{d_{\pi^e}}[w_{\pi^e/\pi_b}(s,a)r]|$$

$$= |E_{d_{\pi^e}}[w_{\pi^e/\pi_b}(s,a)\{r + \gamma v(s') - q(s,a)\}]|$$

$$\leq \max_{g \in \text{conv}(\mathcal{G})} |L_q(g, g)| = \max_{g \in \mathcal{G}} |L_q(g, g)|.$$

From the first line to the second line, we use Lemma 13 choosing $f(s,a)$ as $q(s,a)$. From second line to the third line, we use $w_{\pi^e/\pi_b} \in \text{conv}(\mathcal{G})$.

Then, the second statement follows immediately based on the definition of $\hat{q}$. \qed
Proof of Lemma 6. We have
\[
\max_{g \in \mathcal{G}} L_q(g, g) = \max_{g \in \mathcal{G}} E_{d_{sb}}[g(s, a)(r + \gamma v(s') - q(s, a))]^2 \\
= \max_{g \in \mathcal{G}} E_{d_{sb}}[(g, K((s, a), \cdot))_{\mathcal{H}_K}(r + \gamma v(s') - q(s, a))]^2 \\
= \max_{g \in \mathcal{G}} E_{d_{sb}}[K((s, a), \cdot)(r + \gamma v(s') - q(s, a))]_{\mathcal{H}_K}^2 \\
= \max_{g \in \mathcal{G}} \langle g, g \rangle_{\mathcal{H}_K} = \langle g^*, g^* \rangle_{\mathcal{H}_K}
\]
where
\[g^*(\cdot) = E_{d_{sb}}[K((s, a), \cdot)(r + \gamma v(s') - q(s, a))].\]

From the first line to the second line, we use a reproducing property of RKHS; \(g(s, a) = (g(\cdot), K((s, a), \cdot))_{\mathcal{H}_K}.\) From the second line to the third line, we use a linear property of the inner product. From third line to the fourth line, we use a Cauchy–Schwarz inequality since \(\mathcal{G} = \{g; g, g)_{\mathcal{H}_K} \leq 1\}.

Then, the last expression \(\langle g^*, g^* \rangle_{\mathcal{H}_K}\) is equal to
\[
\langle E_{d_{sb}}[K((s, a), \cdot)(r + \gamma v(s') - q(s, a))], E_{d_{sb}}[K((s, a), \cdot)(r + \gamma v(s') - q(s, a))] \rangle_{\mathcal{H}_K} \\
= \langle E_{d_{sb}}[K((s, a), \cdot)(r + \gamma v(s') - q(s, a))], E_{d_{sb}}[K((s, a), \cdot)(r + \gamma v(s') - q(s, a))] \rangle_{\mathcal{H}_K} \\
= E_{d_{sb}}[K((\tilde{s}, \tilde{a}), \cdot)(E_{t \sim R(s, a)}[r] + E_{s' \sim P(s, a)}[\gamma v(s')] - q(s, a)))] \\
= E_{d_{sb}}[\Delta^q(q; s, a, r, s')\Delta^q(q; \tilde{s}, \tilde{a}, \tilde{r}, \tilde{s'})K((s, a), (\tilde{s}, \tilde{a}))]
\]
where \(\Delta^q(q; s, a, r, s') = r + \gamma v(s') - q(s, a)\) and the expectation is taken with respect to the density \(d_{sb}(s, a, r, s')d_{sb}(\tilde{s}, \tilde{a}, \tilde{r}, \tilde{s'}).\)

Proof of Theorem 18. Assume \(Q^\pi_e\) is included in \(Q\) and \(d_{sb}(s, a) > 0 \forall (s, a).\) Then, if \(\mathcal{G}\) is \(L^2(\mathcal{X}, \nu), \hat{q} = Q^\pi_e.\) Also if \(\mathcal{G}\) is a RKHS associated with an ISPD kernel, \(\hat{q} = Q^\pi_e.

Proof of Theorem 18. The first statement is obvious from Lemma 4. The second statement is proved similarly as Theorem 16.

Appendix D. Proofs of Section 6

Proof of Lemma 7. We have
\[
R[w, q] - R^\pi_e \\
= R[w, q] - R[w_{\pi_e/\pi_0}(s, a), Q^\pi_e(s, a)] \\
= E_{d_{sb}}[\{w(s, a) - w_{\pi_e/\pi_0}(s, a)\}{r - Q^\pi_e(s, a) + \gamma V^\pi_e(s')} + (1 - \gamma)E_{d_{sb}}[v(s) - V^\pi_e(s)] + E_{d_{sb}}[\{w(s, a) - w_{\pi_e/\pi_0}(s, a)\}{Q^\pi_e(s, a) - q(s, a) + \gamma v(s') - V^\pi_e(s')} + E_{d_{sb}}[\{w(s, a) - w_{\pi_e/\pi_0}(s, a)\}{Q^\pi_e(s, a) - q(s, a) + \gamma v(s') - V^\pi_e(s')}].
\]

From (20) to (21), this is just by algebra following the definition of \(R[\cdot, \cdot].\) From (21) to (22), we use the following lemma.
Lemma 19.

\[ 0 = \mathbb{E}_{d_{vb}}[w_{\pi_e/\pi_b}(s,a)\{Q^{\pi_e}(s,a) - q(s,a) + \gamma v(s') - \gamma V^{\pi_e}(s')\}] + (1 - \gamma)\mathbb{E}_{d_{vb}}[v(s) - V^{\pi_e}(s)], \]

\[ 0 = \mathbb{E}_{d_{vb}}[\{w(s,a) - w_{\pi_e/\pi_b}(s,a)\}\{r - Q^{\pi_e}(s,a) + \gamma V^{\pi_e}(s')\}]. \]

Proof. The first equation comes from Lemma 13 with \( f(s,a) = q(s,a) - Q^\pi(s,a) \). The second equation comes from Lemma 4 with \( g(s,a) = w(s,a) - w_{\pi_e/\pi_b}(s,a) \).

This concludes the proof of Lemma 7.

Proof of Theorem 8. We begin with the second statement, which is easier to prove from Lemma 7:

\[ R[w', q] - R_{\pi_e} = \mathbb{E}_{d_{vb}}[\{w'(s,a) - w_{\pi_e/\pi_b}(s,a)\}\{-\gamma V^{\pi_e}(s') - \gamma q(s', \pi_e) + \gamma v(s') + Q^{\pi_e}(s,a)\}] \]
\[ = L_q(q, w' - w_{\pi_e/\pi_b}) - L_q(Q^{\pi_e}, w' - w_{\pi_e/\pi_b}) \]
\[ = -L_q(q, w_{\pi_e/\pi_b} - w') - 0. \]  

(Lemma 4)

Thus, if \( (w_{\pi_e/\pi_b} - w') \in \text{conv}(\mathcal{G}) \)

\[ |R[w', q] - R_{\pi_e}| \leq \max_{g \in \text{conv}(\mathcal{G})} |L_q(q, g)| = \max_{g \in \mathcal{G}} |L_q(q, g)|. \]

Next, we prove the first statement. From Lemma 7,

\[ R[w, q'] - R_{\pi_e} = \mathbb{E}_{d_{vb}}[\{w(s,a) - w_{\pi_e/\pi_b}(s,a)\}\{-\gamma V^{\pi_e}(s') - \gamma q'(s', \pi_e) + \gamma v(s') + Q^{\pi_e}(s,a)\}] \]
\[ = L_w(w, q' - Q^{\pi_e}) - L_w(w_{\pi_e/\pi_b}, q' - Q^{\pi_e}) \]
\[ = -L_w(w, Q^{\pi_e} - q') - 0. \]  

(Lemma 13)

Then, if \( (Q^{\pi_e} - q') \in \text{conv}(\mathcal{F}) \),

\[ |R[w, q'] - R_{\pi_e}| \leq \max_{f \in \text{conv}(\mathcal{F})} |L_w(w, f)| = \max_{f \in \mathcal{F}} |L_w(w, f)|. \]

Finally, from the definition of \( \hat{w} \) and \( \hat{q} \), we also have

\[ |R[\hat{w}, q'] - R_{\pi_e}| \leq \min_{w \in \mathcal{W}} \max_{f \in \mathcal{F}} |L_w(w, f)|, \]
\[ |R[w', \hat{q}] - R_{\pi_e}| \leq \min_{q \in \mathcal{Q}} \max_{g \in \mathcal{G}} |L_q(q, g)|. \]

Proof of Theorem 9. We prove the first statement. The second statement is proved in the same way. We have

\[ |R[\hat{w}_n, q'] - R_{\pi_e}| \]
\[ \leq \max_{f \in \mathcal{F}} |L_w(\hat{w}_n, f)| \]
\[ = \max_{f \in \mathcal{F}} |L_w(\hat{w}_n, f)| - \max_{f \in \mathcal{F}} |L_{w,n}(\hat{w}_n, f)| + \max_{f \in \mathcal{F}} |L_{w,n}(\hat{w}_n, f)| - \max_{f \in \mathcal{F}} |L_w(\hat{w}, f)| + \max_{f \in \mathcal{F}} |L_w(\hat{w}, f)| \]
\[ \leq \max_{f \in \mathcal{F}} |L_w(\hat{w}_n, f)| - \max_{f \in \mathcal{F}} |L_{w,n}(\hat{w}_n, f)| + \max_{f \in \mathcal{F}} |L_{w,n}(\hat{w}_n, f)| - \max_{f \in \mathcal{F}} |L_w(\hat{w}, f)| + \max_{f \in \mathcal{F}} |L_w(\hat{w}, f)| \]
\[ \leq 2 \max_{f \in \mathcal{F}, w \in \mathcal{W}} \max_{f \in \mathcal{F}} |L_w(w, f)| - |L_w(w, f)| + \min \max_{w \in \mathcal{W}} |L_w(w, f)|. \]  

(23)
The remaining task is to bound term \( \max_{f \in \mathcal{F}, w \in \mathcal{W}} ||L_{w,n}(w,f)| - |L_w(w,f)||. \) This is bounded as follows;

\[
\max_{f \in \mathcal{F}, w \in \mathcal{W}} ||L_{w,n}(w,f)| - |L_w(w,f)|| \leq \mathcal{R}_n'(\mathcal{F}, \mathcal{W}) + C_fC_w \sqrt{\log(1/\delta)/n}. \tag{24}
\]

where \( \mathcal{R}_n'(\mathcal{F}, \mathcal{W}) \) is the Rademacher complexity of the function class

\[
\{(s,a,s') \mapsto |w(s,a)(\gamma f(s',\pi_e) - f(s,a))| : w \in \mathcal{W}, f \in \mathcal{F}\}.
\]

Here, we just used an uniform law of large number based on the Rademacher complexity noting \(|(w(s,a)(\gamma f(s',\pi_e) - f(s,a)))|\) is uniformly bounded by \(C_fC_w\) up to some constant (Bartlett and Mendelson, 2003, Theorem 8). From the contraction property of the Rademacher complexity (Bartlett and Mendelson, 2003, Theorem 12),

\[
\mathcal{R}_n(\mathcal{F}, \mathcal{W}) \leq 2\mathcal{R}_n(\mathcal{F}, \mathcal{W})
\]

Finally, Combining (23), (24) and (25), the proof is concluded.

\[\square\]

**Proof of Corollary 10.** We can prove in the same way as for Theorem 9. The only difference is we use Theorem 2 (Mohri and Rostamizadeh, 2009) to bound the term \( \sup_{f \in \mathcal{F}, w \in \mathcal{W}} ||L_{w,n}(w,f)| - |L_w(w,f)||. \)

\[\square\]

**Appendix E. Statistical Efficiency in the Tabular Setting**

**E.1 Statistical efficiency of MWL and MQL**

As we already have seen in Example 7, when \( \mathcal{W}, \mathcal{F}, Q, G \) are the same linear class, MWL, MQL, and LSTDQ give the same OPE estimator. These methods are also equivalent in the tabular setting—as tabular is a special case of linear representation (with indicator features)—which also coincides with the model-based (or certainty-equivalent) solution. Below we prove that this tabular estimator can achieve the semiparametric lower bound for infinite horizon OPE (Kallus and Uehara, 2019b).

This variance matches the semiparametric lower bound for OPE given by Kallus and Uehara (2019b, Theorem 5).

\[\square\]

**Theorem 20** (Restatement of Theorem 11). Assume the whole data set \( \{(s,a,r,s')\} \) is geometrically Ergodic. Then, in the tabular setting, \( \sqrt{n}(R_{w,n}[\hat{w}_n] - R_{\pi_e}) \) and \( \sqrt{n}(R_{q,n}[\hat{q}_n] - R_{\pi_e}) \) weakly converge to the normal distribution with mean 0 and variance

\[
E_{d_{\pi_e}}[w_{\pi_e/(a,s)}(r + \gamma V_{\pi_e}(s') - Q_{\pi_e}(s,a))^2].
\]

This variance matches the semiparametric lower bound for OPE given by Kallus and Uehara (2019b, Theorem 5).

\[\square\]

14. Semiparametric lower bound is the non–parametric extension of Cramer–Rao lower bound (Bickel et al. 1998). It is the lower bound of asymptotic MSE among regular estimators (van der Vaart 1998).

15. Regarding the definition, refer to Meyn and Tweedie (2009).
Table 3: Summary of the connections between several OPE methods and LSTD, and their optimality in the tabular setting.

Two remarks are in order:

1. Theorem 20 could be also extended to the continuous sample space case in a non-parametric manner, i.e., replacing \( \phi(s,a) \) with some basis functions for \( L^2 \)-space and assuming that its dimension grows with some rate related to \( n \) and the data-generating process has some smoothness condition (Newey and McFadden, 1994). The proof is not obvious and we leave it to future work.

2. In the contextual bandit setting, it is widely known that the importance sampling estimator with plug-in weight from the empirical distribution and the model-based approach can achieve the semiparametric lower bound (Hahn, 1998; Hirano et al., 2003). Our findings are consistent with this fact and is novel in the MDP setting to the best of our knowledge.

E.2 Statistical inefficiency of MSWL and MVL for OPE

Here, we compare the statistical efficiency of MWL, MQL with MSWL, MVL in the tabular setting. First, we show that MSWL, MVL positing the linear class is the same as the off-policy LSTD (Bertsekas and Yu, 2009; Dann et al., 2014). Then, we calculate the asymptotic MSE of these estimators in the tabular case and show that this is larger than the ones of MWL and MQL.

Equivalence of MSWL, MVL with linear models and off-policy LSTD

By slightly modifying Liu et al. (2018, Theorem 4), MSWL is introduced based on the following relation:

\[
\mathbb{E}_{d\pi_e} \left[ \frac{\pi_e(a|s)}{\pi_b(a|s)} \left( \gamma \frac{d_{x_e,\gamma}(s)}{d_{\pi_b}(s)} f(s') - \frac{d_{x_e}(s)}{d_{\pi_b}(s)} f(s) \right) \right] + (1 - \gamma)\mathbb{E}_{d_0}[f(s)] = 0 \forall f \in L^2(S,\nu).
\]

Then, the estimator for \( \frac{d_{x_e}(s)}{d_{\pi_b}(s)} \) is given as

\[
\hat{\alpha} = (1 - \gamma)\mathbb{E}_n \left[ \frac{\pi_e(a|s)}{\pi_b(a|s)} \left\{ -\gamma \phi(s') + \phi(s) \right\} \phi^\top(s) \right]^{-1} \mathbb{E}_{d_0}[\phi(s)].
\]
Then, the final estimator for $R_{\pi_e}$ is
\[
(D_{v_1})^T D_{v_2}^{-1} D_{v_3},
\]
where
\[
D_{v_1} = (1 - \gamma)E_{d_b}[\phi(s)],
D_{v_2} = E_n \left[ \frac{\pi_e(a|s)}{\pi_b(a|s)} \phi(s) \left\{ -\gamma \phi^T(s') + \phi^T(s) \right\} \right],
D_{v_3} = E_n \left[ \frac{\pi_e(a|s)}{\pi_b(a|s)} \phi(s) \right].
\]

In MVL, the estimator for $V^{\pi_e}(s)$ is constructed based on the relation;
\[
E_{d_{e_b}} \left[ \frac{\pi_e(a|s)}{\pi_b(a|s)} \{ r + \gamma V^{\pi_e}(s') - V^{\pi_e}(s) \} g(s) \right] = 0 \forall g \in L^2(S, \nu).
\]
Then, the estimator for $V^{\pi_e}(s)$ is given by
\[
\min_{v \in \mathcal{V}} \max_{g \in G^3} E_{d_{e_b}} \left[ \frac{\pi_e(a|s)}{\pi_b(a|s)} \{ r + \gamma v(s') - v(s) \} g(s) \right]^{2}.
\]
As in Example 7, in the linear model case, let $v(s) = \phi(s)^T \beta$ where $\phi(s) \in \mathbb{R}^d$ is some basis function and $\beta$ is the parameters. Then, the resulting estimator for $V^{\pi_e}(s)$ is
\[
\hat{\beta} = E_n \left[ \frac{\pi_e(a|s)}{\pi_b(a|s)} \phi(s) \left\{ -\gamma \phi^T(s') + \phi^T(s) \right\} \right]^{-1} E_n \left[ \frac{\pi_e(a|s)}{\pi_b(a|s)} \phi(s) \right].
\]
Then, the final estimator for $R_{\pi_e}$ is still $(D_{v_1})^T D_{v_2}^{-1} D_{v_3}$. This is exactly the same as the estimator obtained by off-policy LSTD (Bertsekas and Yu, 2009).

Another formulation of MSWL and MVL According to Liu et al. (2018, Theorem 4), we have
\[
E_{d_{e_b}} \left[ \left( \gamma \frac{d_{e,\gamma}(s)}{d_{\pi_b}(s)} \frac{\pi_e(a|s)}{\pi_b(a|s)} - \frac{d_{e,\gamma}(s')}{d_{\pi_b}(s')} \right) f(s') \right] + (1 - \gamma)E_{d_0}[f(s)] = 0 \forall f \in L^2(S, \nu).
\]
They construct an estimator for $\frac{d_{e,\gamma}(s)}{d_{\pi_b}(s)}$ as;
\[
\min_{w \in \mathcal{W}} \max_{f \in \mathcal{F}^3} E_{d_{e_b}} \left[ \left( \gamma w(s)f(s') \frac{\pi_e(a|s)}{\pi_b(a|s)} - w(s)f(s) \right) \right] + (1 - \gamma)E_{d_0}[f(s)] \biggr]^{2}.
\]
Note that compared with the previous case (26), the position of the importance weight $\pi_e/\pi_b$ is different. In the same way, MVL is constructed base on the relation;
\[
E_{d_{e_b}} \left[ \left\{ \frac{\pi_e(a|s)}{\pi_b(a|s)} \{ r + \gamma V^{\pi_e}(s') \} - V^{\pi_e}(s) \right\} g(s) \right] = 0 \forall g \in L^2(S, \nu).
\]
The estimator for $V^{\pi_e}(s)$ is given by

$$\min_{\nu \in \nu_b} \max_{g \in \mathcal{G}} \mathbb{E}_{\pi_b} \left[ \left( \frac{\pi_e(a|s)}{\pi_b(a|s)} \{ r + \gamma v(s') \} - v(s) \right) g(s) \right]^2.$$  

When positing linear models, in both cases, the final estimator for $R_{\pi_e}$ is

$$D_{v_1}^\top \{D_{v_4}^{-1}D_{v_3} - R_{\pi_e} \},$$

where

$$D_{v_4} = \mathbb{E}_{\pi_b} \left[ \frac{\phi(s) \left\{ -\gamma \frac{\pi_e(a|s)}{\pi_b(a|s)} \phi(s') + \phi(s) \right\}}{\pi_e(a|s)} \right].$$

This is exactly the same as the another type of off-policy LSTD (Dann et al., 2014).

**Statistical inefficiency of MSWL, MVL and off-policy LSTD** Next, we calculate the asymptotic variance of $D_{v_1}D_{v_2}^{-1}D_{v_3}$ and $D_{v_1}D_{v_4}^{-1}D_{v_3}$ in the tabular setting. It is shown that these methods cannot achieve the semiparametric lower bound (Kallus and Uehara, 2019b). These results show that these methods are statistically inefficient. Note that this implication is also brought to the general continuous sample space case since the asymptotic MSE is generally the same even in the continuous sample space case with some smoothness conditions.

**Theorem 21.** Assume the whole data is geometrically Ergodic. In the tabular setting, $\sqrt{n}(D_{v_1}D_{v_2}^{-1}D_{v_3} - R_{\pi_e})$ weakly converges to the normal distribution with mean 0 and variance:

$$\mathbb{E}_{d_{\pi_b}} \left[ \left\{ \frac{d_{\pi_e,\gamma}(s)}{d_{\pi_b}(s)} \right\}^2 \var_{d_{\pi_b}} \left[ \frac{\pi_e(a|s)}{\pi_b(a|s)} \{ r + V^{\pi_e}(s') - V^{\pi_e}(s) \} | s \right] \right].$$

This is larger than the semiparametric lower bound.

**Theorem 22.** Assume the whole data is geometrically Ergodic. In the tabular setting, $\sqrt{n}(D_{v_1}D_{v_4}^{-1}D_{v_3} - R_{\pi_e})$ weakly converges to the normal distribution with mean 0 and variance:

$$\mathbb{E}_{d_{\pi_b}} \left[ \left\{ \frac{d_{\pi_e,\gamma}(s)}{d_{\pi_b}(s)} \right\}^2 \var_{d_{\pi_b}} \left[ \frac{\pi_e(a|s)}{\pi_b(a|s)} \{ r + V^{\pi_e}(s') \} | s \right] \right].$$

This is larger than the semiparametric lower bound.

**E.3 Details of the Experiments**

We show some empirical results that back up the theoretical discussions in this section. We conduct experiments in the Taxi environment (Dietterich, 2000), which has 20000 states and 6 actions; see Liu et al. (2018, Section 5) for more details. We compare three methods, all using the tabular representation: MSWL with exact $\pi_e$, MSWL with estimated $\pi_e$ (“plug-in”), and MWL (same as MQL). As we have mentioned earlier, this comparison is essentially among off-policy LSTD, plug-in off-policy LSTD, and LSTDQ.
We choose the target policy \( \pi_e \) to be the one obtained after running Q-learning for 1000 iterations, and choose another policy \( \pi_+ \) after 150 iterations. The behavior policy is \( \pi_b = \alpha \pi_e + (1 - \alpha) \pi_+ \). We report the results for \( \alpha \in \{0.2, 0.4\} \). The discount factor is \( \gamma = 0.98 \).

We use a single trajectory and vary the truncation size \( T \) as \([5, 10, 20, 40] \times 10^4\). For each case, by making 200 replications, we report the Monte Carlo MSE of each estimator with their 95% interval in Figure 1.

It is observed that MWL is significantly better than MSWL and MWL is slightly better than plug-in MSWL. This is because MWL is statistically efficient and MSWL is statistically inefficient as we have shown earlier in this section. The reason why plug-in MSWL is superior to the original MSWL is that the plug-in based on MLE with a well specified model can be viewed as a form of control variates (Henmi and Eguchi, 2004; Hanna et al., 2019). Whether the plug-in MSWL can achieve the semiparametric lower bound remains as future work.

\[ E.4 \text{ Proofs of Theorems 20, 21, and 22} \]

**Proof of Theorem 20.** Recall that the estimator is written as \( D_{q1}^T D_{q2}^{-1} D_{q3} \), where

\[
\begin{align*}
D_{q1} &= (1 - \gamma) E_{d_0 \times \pi_e} [\phi(s,a)] \\
D_{q2} &= E_{n} [-\gamma \phi(s,a) \phi^\top(s', \pi_e) + \phi(s,a) \phi(s,a)^\top] \\
D_{q3} &= E_{n} [\gamma \phi(s,a)]
\end{align*}
\]

Recall that \( D_{q2}^{-1} D_{q3} = \hat{\beta} \) is seen as Z-estimator with a parametric model \( q(s,a; \beta) = \beta^\top \phi(s,a) \). More specifically, the estimator \( \hat{\beta} \) is given as a solution to

\[
E_{n} [(r + \gamma q(s, \pi_e; \beta) - q(s,a; \beta)) \phi(s,a)] = 0.
\]

Following the standard theory of Z-estimator (van der Vaart, 1998), the asymptotic MSE of \( \beta \) is calculated as a sandwich estimator;

\[
\sqrt{n}(\hat{\beta} - \beta_0) \xrightarrow{d} \mathcal{N}(0, D_1^{-1} D_2 D_1^{-1\top})
\]

where \( \beta_0^\top \phi(s,a) = Q^\pi_e(s,a) \) and

\[
\begin{align*}
D_1 &= E_{d_{\pi_b}} [\phi(s,a) \{-\gamma \phi(s', \pi_e) + \phi(s,a)\}^\top]_{\beta_0}, \\
D_2 &= \text{var}_{d_{\pi_b}} \left[ (r + \gamma q(s, \pi_e; \beta) - q(s,a; \beta)) \phi(s,a) \right]_{\beta_0} \\
&= E_{d_{\pi_b}} [\text{var}_{d_{\pi_b}} [r + \gamma V^\pi_e(s') - Q^\pi_e(s,a)|s,a] \phi(s,a) \phi^\top(s,a)] \\
&+ \text{var}_{d_{\pi_b}} [E_{d_{\pi_b}} [r + \gamma V^\pi_e(s') - Q^\pi_e(s,a)|s,a] \phi(s,a) \phi^\top(s,a)] \\
&= E_{d_{\pi_b}} [\text{var}_{d_{\pi_b}} [r + \gamma V^\pi_e(s') - Q^\pi_e(s,a)|s,a] \phi(s,a) \phi^\top(s,a)].
\end{align*}
\]

Here, we use a variance decomposition to simplify \( D_2 \) from (27) to (28). We use a relation \( E_{d_{\pi_b}} [r + \gamma V^\pi_e(s') - Q^\pi_e(s,a)|s,a] = 0 \) from (28) to (29). Then, by delta method,

\[
\sqrt{n}(D_{q1}^T D_{q2}^{-1} D_{q3} - R_{\pi_e}) \xrightarrow{d} \mathcal{N}(0, D_{q1}^T D_{q2}^{-1} D_{q3} D_{q2}^{-1\top} D_{q1}).
\]
From now on, we simplify the expression $D_q^1D_1^{-1}D_2D_1^{-1\top}D_q$. First, we observe
\[
[D_q]|_{S_{i1}+i_2} = (1 - \gamma)d_0(S_{i1})\pi_e(A_{i2}|S_{i1}),
\]
where $[D_q]|_{S_{i1}+i_2}$ is a element corresponding $(S_{i1}, A_{i2})$ of $D_q$. In addition,
\[
D_1^{-1} = E_{d_{nb}}[\phi(s, a)(-\gamma\phi(s', \pi_e) + \phi(s, a))\top]^{-1}
\]
\[
= E_{d_{nb}}[\phi(s, a)\phi\top(s, a)(-\gammaP^\pi_e + I)\top]^{-1}
\]
\[
= \{(-\gammaP^\pi_e + I)^{-1}\top}E_{d_{nb}}[\phi(s, a)\phi\top(s, a)]^{-1}.
\]
where $P^\pi_e$ is a transition matrix between $(s, a)$ and $(s', a')$, and $I$ is an identity matrix.

Therefore, by defining $g(s, a) = \text{var}_{d_{nb}}[r + \gamma V^\pi_e(s') - Q^\pi_e(s, a)|s, a]$ and $(I - \gamma P^\pi_e)^{-1}D_q = D_3$ the asymptotic variance is
\[
D_3^\top E_{d_{nb}}[\phi(s, a)\phi\top(s, a)]^{-1}E_{d_{nb}}[g(s, a)\phi(s, a)\phi\top(s, a)]E_{d_{nb}}[\phi(s, a)\phi\top(s, a)]^{-1}D_3
\]
\[
= \sum_{\tilde{s} \in S, \tilde{a} \in A} \{d_{nb}(\tilde{s}, \tilde{a})\}^{-1}g(\tilde{s}, \tilde{a})\{D_3^\top I_{\tilde{s}, \tilde{a}}\}^2
\]
where $I_{\tilde{s}, \tilde{a}}$ is a $|S||A|$-dimensional vector, which the element corresponding $(\tilde{s}, \tilde{a}) = 1$ and other elements are 0. Noting $D_3^\top I_{\tilde{s}, \tilde{a}} = d_{\pi_e, \gamma}(\tilde{s}, \tilde{a})$, the asymptotic variance is
\[
\sum_{\tilde{s} \in S, \tilde{a} \in A} \{d_{nb}(\tilde{s}, \tilde{a})\}^{-1}g(\tilde{s}, \tilde{a})d_{\pi_e, \gamma}^2(\tilde{s}, \tilde{a})
\]
\[
= E_{d_{nb}}[w_{\pi_e/\pi_b}^2(s, a)\text{var}_{d_{nb}}[r + \gamma V^\pi_e(s') - Q^\pi_e(s, a)|s, a]]
\]
\[
= E_{d_{nb}}[w_{\pi_e/\pi_b}^2(s, a)(r + \gamma V^\pi_e(s') - Q^\pi_e(s, a))^2].
\]
This concludes the proof.

**Proof of Theorem 21.** Recall that $D_2^{-1}D_{v3} = \hat{\beta}$ is seen as $Z$-estimator with a parametric model $v(s; \beta) = \beta^\top \phi(s)$. More specifically, the estimator $\hat{\beta}$ is given as a solution to
\[
E_n \left[ \begin{array}{c} \pi_e(a|s) \\ \pi_b(a|s) \end{array} \right] \{r + v(s'; \beta) - v(s; \beta)\} \phi(s) = 0.
\]

Following the standard theory of $Z$-estimator (van der Vaart, 1998), the asymptotic variance of $\beta$ is calculated as a sandwich estimator;
\[
\sqrt{n}(\hat{\beta} - \beta_0)^{\top} \overset{d}{\rightarrow} \mathcal{N}(0, D_1^{-1}D_2(D_1^{-1})^{\top}),
\]
where $\beta_0^{\top} \phi(s) = V^\pi_e(s)$ and
\[
D_1 = E_{d_{nb}}[\phi(s)\{-\gamma\phi(s') + \phi(s)\}]\]
\[
D_2 = \text{var}_{d_{nb}} \left[ \begin{array}{c} \pi_e(a|s) \\ \pi_b(a|s) \end{array} \right] \{r + v(s'; \beta) - v(s; \beta)\} \phi(s) |_{\beta_0}
\]
\[
= E_{d_{nb}} \left[ \text{var}_{d_{nb}} \left[ \begin{array}{c} \pi_e(a|s) \\ \pi_b(a|s) \end{array} \right] \{r + \gamma V^\pi_e(s'; \beta) - V^\pi_e(s)\} | s \right] \phi(s) \phi^\top(s).
\]
Then, by delta method,
\[
\sqrt{n}(D_{v1}^{-1}D_{v2}^{-1}D_{v3} - R_e) \xrightarrow{d} \mathcal{N}(0, D_{v1}^{-1}D_2(D_{v1}^{-1})^\top D_{v1}).
\]

From now on, we simplify the expression \(D_{v1}^{-1}S_1^{-1}S_2(S_1^{-1})^\top D_{v1}\). First, we observe
\[
[D_{v1}]_i = (1 - \gamma)d_0(S_i),
\]
where \([D_{v1}]_i\) is \(i\)-th element. In addition,
\[
D_1^{-1} = E_{\Delta b}[\phi(s)\{-\gamma\phi(s') + \phi(s)\}]^{-1}
\]
\[
= E_{\Delta b}[\phi(s)\phi^\top(s)\{-\gamma P_e^\pi + I\}]^{-1}
\]
\[
= (-\gamma P_e^\pi + I)^{-1}E_{\Delta b}[\phi(s)\phi^\top(s)]^{-1},
\]
where \(P_e^\pi\) is a transition matrix from the current state to the next state.

Therefore, by defining \(g(s) = \text{var}_{\Delta b}\left[\frac{\pi_e(a|s)}{\pi_b(a|s)}(r + V_e^\pi(s') - V_e^\pi(s))|s\right]\) and \(\{-\gamma P_e^\pi + I\}^{-1}D_{v1} = D_3\), the asymptotic variance is
\[
\sum_{\tilde{s}\in S} d_{\tilde{s}}^{-1}g(\tilde{s})d_{\tilde{s}}^2(\tilde{s}) = E_{\Delta b}\left[\left\{\frac{d_{\tilde{s}}}{d_{\tilde{s}}^2}\right\}^2\text{var}_{\Delta b}\left[\frac{\pi_e(a|s)}{\pi_b(a|s)}(r + \gamma V_e^\pi(s') - V_e^\pi(s))|s\right]\right].
\]

Finally, we show this is larger than the semiparametric lower bound. This is seen as
\[
E_{\Delta b}\left[\left\{\frac{d_{\tilde{s}}}{d_{\tilde{s}}^2}\right\}^2\text{var}_{\Delta b}\left[\frac{\pi_e(a|s)}{\pi_b(a|s)}(r + \gamma V_e^\pi(s') - V_e^\pi(s))|s\right]\right]
\]
\[
\geq E_{\Delta b}\left[\left\{\frac{d_{\tilde{s}}}{d_{\tilde{s}}^2}\right\}^2\text{var}_{\Delta b}\left[\frac{\pi_e(a|s)}{\pi_b(a|s)}(r + \gamma V_e^\pi(s') - V_e^\pi(s))|s, a\right]\right]
\]
\[
= E_{\Delta b}\left[w^2_{\pi_e/a}r + \gamma V_e^\pi(s') - Q_e^\pi(s, a)|s, a\right].
\]

Here, from the first line to the second line, we use a general inequality \(\text{var}[x] = \text{var}[E[x|y]] + E[\text{var}[x|y]] \geq E[\text{var}[x|y]]\).

**Proof of Theorem 22.** By refining \(g(s) = \text{var}\left[\frac{\pi_e(a|s)}{\pi_b(a|s)}(r + V_e^\pi(s))|s\right]\) in the proof of Theorem 21, the asymptotic variance is
\[
\sum_{\tilde{s}\in S} d_{\tilde{s}}^{-1}g(\tilde{s})d_{\tilde{s}}^2(\tilde{s}) = E_{\Delta b}\left[\left\{\frac{d_{\tilde{s}}}{d_{\tilde{s}}^2}\right\}^2\text{var}_{\Delta b}\left[\frac{\pi_e(a|s)}{\pi_b(a|s)}(r + \gamma V_e^\pi(s'))|s\right]\right].
\]
Then, we show this is larger than the semiparamatric lower bound. This is seen as

\[
\sum_{s \in S} d^{-1}_{\pi_b(s)} g(s) d^2_{\pi_c,\gamma}(s) = E_{d_{\pi_b}} \left[ \left\{ \frac{d_{\pi_c,\gamma}(s)}{d_{\pi_b}(s)} \right\}^2 \text{var}_{d_{\pi_b}} \left[ \frac{\pi_c(a|s)}{\pi_b(a|s)} \{r + \gamma V_{\pi_c}(s')\} \right] \right]
\geq E_{d_{\pi_b}} \left[ \left\{ \frac{d_{\pi_c,\gamma}(s)}{d_{\pi_b}(s)} \right\}^2 E_{\pi_b} \left[ \text{var}_{d_{\pi_b}} \left[ \frac{\pi_c(a|s)}{\pi_b(a|s)} \{r + \gamma V_{\pi_c}(s')\} | s, a \right] \right] \right]
= E_{d_{\pi_b}} \left[ w^2_{\pi_c/\pi_b}(s, a) \text{var}[r + \gamma V_{\pi_c}(s') - Q_{\pi_c}(s, a)| s, a] \right].
\]