Minimax Confidence Interval for Off-Policy Evaluation and Policy Optimization

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Abstract
We study minimax methods for off-policy evaluation (OPE) using value-functions and marginalized importance weights. Despite that they hold promises of overcoming the exponential variance in traditional importance sampling, several key problems remain:

(1) They require function approximation and are generally biased. For the sake of trustworthy OPE, is there anyway to quantify the biases?

(2) They are split into two styles (“weight-learning” vs “value-learning”). Can we unify them?

In this paper we answer both questions positively. By slightly altering the derivation of previous methods (one from each style: Uehara et al., 2019), we unify them into a single confidence interval (CI) that automatically comes with a special type of double robustness: when either the value-function or importance weight class is well-specified, the CI is valid and its length quantifies the misspecification of the other class. We can also tell which class is misspecified, which provides useful diagnostic information for the design of function approximation. Our CI also provides a unified view of and new insights to some recent methods: for example, one side of the CI recovers a version of AlgaeDICE (Nachum et al., 2019b), and we show that the two sides need to be used together and either alone may incur doubled approximation error as a point estimate.

We further examine the potential of applying these bounds to two long-standing problems: off-policy policy optimization with poor data coverage (i.e., exploitation), and systematic exploration. With a well-specified value-function class, we show that optimizing the lower and the upper bounds lead to effective exploitation and exploration, respectively. Our results also suggest an interesting asymmetry between exploration and exploitation, that the former might require substantially weaker realizability assumptions than the latter.

1. Introduction
A major barrier to applying reinforcement learning (RL) to many real-world applications is the difficulty of evaluation: how can we reliably evaluate a new policy before actually deploying it, possibly using historical data collected from a different policy? Known as off-policy evaluation (OPE), the problem is genuinely difficult as the variance of any unbiased estimator—including the popular importance sampling methods and their variants (Precup et al., 2000; Jiang and Li, 2016)—inevitably grows exponentially in horizon (Li et al., 2015).

To overcome this “curse of horizon”, the RL community has recently gained interest in a new family of algorithms (e.g., Liu et al., 2018), which require function approximation of value-functions and marginalized importance weights and provide accurate estimation when both function classes are well-specified. Despite that fast progress has been made to understand the nature of these methods, several key problems remain:
The methods are generally biased since they rely on function approximation. Is there anyway we can quantify the biases, which is important for trustworthy evaluation?

The original method by Liu et al. (2018) estimates the marginalized importance weights (“weight”) from minimax optimization with a discriminator class of value-functions (“value”). Later, Uehara et al. (2019) swap the roles of value-functions and important weights to learn a $Q$-function using weight discriminators. Not only we have two styles of methods now (“weight-learning” vs “value-learning”), each of them also ignores some important components of the data in their core optimization (see Section 3 for details). Can we have a unified method that makes effective use of all components of data?

In this paper we answer both questions positively. By modifying the derivation of one method from each style (Uehara et al., 2019), we unify them into a single confidence interval, which automatically comes with a special type of double robustness: when either the weight- or the value-class is well-specified, the CI is valid and its length quantifies the misspecification of the other class. We can also tell which class is misspecified, which provides useful diagnostic information for the design of function approximation. Each bound is computed from a single optimization program that uses all components of the data, which we show is generally tighter than naive CIs developed from previous methods.

Our derivation also unifies several recent OPE methods and reveals their surprisingly simple and direct connections; see Table 1. One side of our CI corresponds to (the unregularized version of) Frenchel AlgaeDICE (Nachum et al., 2019b), and we show that the two sides need to be used together and either alone fails to characterize the bias and may incur doubled approximation error as a point estimate (Remark 2).

We further examine the potential of applying these confidence bounds to two longstanding problems in RL: reliable off-policy policy optimization with poor data coverage (i.e., exploitation), and efficient exploration. When the data fails to cover the entire state space—which is highly likely in practice—the weight-class is poorly specified whatsoever. With a well-specified value-class, we show that optimizing the lower and the upper bounds lead to good exploitation and exploration, respectively, by connecting them to well-established algorithms such as Rmax (Brafman and Tennenholtz, 2003) in a tabular scenario and proving general guarantees in the function approximation setting.

On the term “confidence interval” Confidence interval (CI) often refers to the uncertainties in the estimates due to randomness of data. In this paper, however, our main goal is to quantify the biases, and our CI only captures approximation errors and ignores estimation errors (i.e., all expectations in our theory are exact). Despite that estimation errors are easier to handle in theory (by concentration inequalities and generalization bounds (Vapnik, 1998)), a careful characterization is important for the practical application of our methods (see e.g., Thomas et al., 2015, as an example), which we leave for future investigation.

1. Their discriminators are state-value functions and require knowledge of the behavior policy. In this paper we consider the most direct extension of their method to the behavior-agnostic setting, which is the MWL algorithm by Uehara et al. (2019). A more general version of MWL (with regularization) has been developed in parallel (GenDICE; Zhang et al. 2019a).
2. Preliminaries

2.1 Markov Decision Processes

An infinite-horizon discounted MDP is specified by \((\mathcal{S}, \mathcal{A}, P, R, \gamma, s_0)\), where \(\mathcal{S}\) is the state space, \(\mathcal{A}\) is the action space, \(P: \mathcal{S} \times \mathcal{A} \to \Delta(\mathcal{S})\) is the transition function (\(\Delta(\cdot)\) is probability simplex), \(R: \mathcal{S} \times \mathcal{A} \to \Delta([0, R_{\text{max}}])\) is the reward function, and \(s_0\) is a known and deterministic starting state, which is without loss of generality.\(^2\) For simplicity we assume \(\mathcal{S}\) and \(\mathcal{A}\) are finite and discrete but their cardinalities can be arbitrarily large. Any policy\(^3\) \(\pi: \mathcal{S} \to \mathcal{A}\) induces a distribution of the trajectory, \(s_0, a_0, r_0, s_1, a_1, r_1, \ldots\), where \(s_0\) is the starting state, and \(\forall t \geq 0\), \(a_t = \pi(s_t)\), \(r_t \sim R(s_t, a_t)\), \(s_{t+1} \sim P(s_t, a_t)\). The expected discounted return determines the performance of policy \(\pi\), which is defined as

\[
J(\pi) := \mathbb{E}[\sum_{t=0}^{\infty} \gamma^t r_t | \pi].
\]

It will be useful to define the discounted (state-action) occupancy of \(\pi\) as

\[
d^\pi(s, a) := \sum_{t=0}^{\infty} \gamma^t d_t^\pi(s, a),
\]

where \(d_t^\pi(\cdot, \cdot)\) is the marginal distribution of \((s_t, a_t)\) under policy \(\pi\). Note that \(d^\pi\) behaves like an unnormalized distribution (\(\|d^\pi\| = 1/(1 - \gamma)\)), and for notational convenience we still use it in expectations, with the understanding that for any function \(f\),

\[
\mathbb{E}_{d^\pi}[f(s, a, r, s')] := \sum_{s \in \mathcal{S}, a \in \mathcal{A}} d^\pi(s, a) \mathbb{E}_{r \sim R(s,a), s' \sim P(s,a)}[f(s, a, r, s')].
\]

With this notation, the discounted return can be also written as \(J(\pi) = \mathbb{E}_{d^\pi}[r]\). We also define the Q-value function \(Q^\pi\) via the Bellman equations: \(\forall s \in \mathcal{S}, a \in \mathcal{A}\),

\[
Q^\pi(s, a) = \mathbb{E}_{r \sim R(s,a), s' \sim P(s,a)}[r + \gamma Q^\pi(s', \pi)] =: (T^\pi Q^\pi)(s, a),
\]

where \(Q^\pi(s', \pi)\) is a shorthand for \(Q^\pi(s', \pi(s'))\) and \(T^\pi\) is the Bellman update operator. It will be also useful to keep in mind that

\[
J(\pi) = Q^\pi(s_0, \pi).
\]

2.2 Data and Marginalized Importance Weights

In off-policy RL, we are passively given a dataset and cannot interact with the environment to collect more data. The goal of OPE is to estimate \(J(\pi)\) for a given policy \(\pi\) using the dataset. We assume that the dataset consists of i.i.d. \((s, a, r, s')\) tuples, where \((s, a) \sim \mu, r \sim R(s, a), s' \sim P(s, a)\). \(\mu \in \Delta(\mathcal{S} \times \mathcal{A})\) is a distribution from which we draw \((s, a)\), which determines the exploratoriness of the dataset. We write \(\mathbb{E}_\mu[\cdot]\) as a shorthand for taking expectation w.r.t. this distribution. The strong i.i.d. assumption is only meant to simplify derivation and presentation, and we refer the readers to Uehara et al. (2019) for further discussions on this matter.

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\(^2\) When the initial state is drawn from a distribution \(d_0\), all our derivations hold if we simply replace any \(Q(s_0, \pi)\) term by \(\mathbb{E}_{s_0 \sim d_0}[Q(s_0, \pi)]\).

\(^3\) Our derivation also applies to stochastic policies.
A concept crucial to our discussions is the \textit{marginalized importance weights}. Given any $\pi$, if $\mu(s,a) > 0$ whenever $d^\pi(s,a) > 0$, define
\begin{equation}
w_{\pi/\mu}(s,a) := \frac{d^\pi(s,a)}{\mu(s,a)}.
\end{equation}
When there exists $(s,a)$ such that $\mu(s,a) = 0$ but $d^\pi(s,a) > 0$, we say that $w_{\pi/\mu}$ does not exist (and hence cannot be realized by any function class). When it does exist, the weighting function satisfies that $\forall f$,
\begin{equation}
\mathbb{E}_{d^\pi}[f(s,a,r,s')] = \mathbb{E}_{w_{\pi/\mu}}[f(s,a,r,s')] := \mathbb{E}_{\mu}[w_{\pi/\mu}(s,a)f(s,a,r,s')].
\end{equation}
Whenever we put an importance weighting function $w$ on the subscript, the expectation is always w.r.t. $\mu$ and weighted by $w$. In fact, if we knew $w_{\pi/\mu}$, OPE becomes easy as
\begin{equation}
J(\pi) = \mathbb{E}_{w_{\pi/\mu}}[r].
\end{equation}

2.3 Function Approximation
Throughout the paper, we assume access to two function classes $Q \subset (S \times A \rightarrow \mathbb{R})$ and $W \subset (S \times A \rightarrow \mathbb{R})$. To develop intuition, they are supposed to model $Q^\pi$ and $w_{\pi/\mu}$, respectively, though most of our main results are stated without assuming any kind of realizability. We use $\mathcal{C}(\cdot)$ to denote the convex hull of a set. We also make the following compactness assumption so that infima and suprema we introduce later are always attainable.

\textbf{Assumption 1.} We assume $Q$ and $W$ are compact subsets of $\mathbb{R}^{S \times A}$.

3. Related Work
\textbf{Minimax OPE} Liu et al. (2018) proposed the first minimax algorithm for learning marginalized importance weights. Under the assumption that the data distribution (e.g., our $\mu$) covers $d^\pi$ reasonably well, the method provides efficient estimation of $J(\pi)$ without incurring the exponential variance in horizon, a major drawback of traditional importance sampling methods (Precup et al., 2000; Li et al., 2015; Jiang and Li, 2016). Since then, the method has sparked a flurry of interest in the RL community (Xie et al., 2019; Nachum et al., 2019a; Liu et al., 2019a b; Rowland et al., 2019; Liao et al., 2019; Zhang et al., 2019a b).

While most of these methods solve for a weight function using value-function discriminators and plug into Eq.(7) to form the final estimate of $J(\pi)$, Uehara et al. (2019) recently show that one can flip the roles of weight- and value-functions to approximate $Q^\pi$, and plug it into Eq.(4). The two type of methods (“weight-learning” and “value-learning”) exhibit an interesting symmetry in terms of the guarantees and coincide with each other in some special cases (e.g., with two identical linear classes, both of them reduce to LSTDQ (Uehara et al., 2019)). As we will see, when we keep model-misspecification in mind and derive upper and lower bounds of $J(\pi)$ (as opposed to point estimates), the two types of methods merge into \textit{almost} the same confidence intervals—except that they are the reverse of each other, and only one of them is valid in general (Section 4.3).
Drawback of Existing Methods  One drawback of both types of methods is that some important components of the data are ignored in the core optimization. For example, “weight-learning” (e.g., Liu et al., 2018; Zhang et al., 2019a) completely ignores the rewards \( r \) in its loss function, and only uses it in the final plug-in step. Similarly, “value-learning” (MQL of Uehara et al., 2019) ignores the initial state \( s_0 \) until the final plug-in step (see also Feng et al., 2019). In contrast, each of our confidence bounds is computed from a single optimization program that uses all components of the data, and we show the advantage of unified optimization in Table 1 and Appendix B.

Double Robustness  Our CI is valid when either function class is well-specified, which can be viewed as a type of double robustness. This is related to but different from the usual notion of double robustness (Dud’ık et al., 2011; Jiang and Li, 2016; Kallus and Uehara, 2019; Tang et al., 2020): classical doubly robust methods are typically “meta”-estimators and require a value-function whose estimation procedure is unspecified, and the double robustness refers to the fact that the estimation is unbiased and/or enjoys reduced variance if the given value-function is accurate. In comparison, our double robustness gives weaker guarantees (valid CI, as opposed to accurate point estimates) but also requires much weaker assumptions (well-specified function class as opposed to an accurate function), so it is important not to confuse the two types of double robustness.

AlgaeDICE  Closest related to our work is the recently proposed AlgaeDICE for off-policy optimization (Nachum et al., 2019b). In fact, one side of our CI recovers a version of its policy evaluation component. Nachum et al. (2019b) derive the expression using Fenchel duality (see also Nachum and Dai, 2020), whereas we provide an alternative derivation using Fenchel duality (see also Nachum and Dai, 2020), whereas we provide an alternative derivation using

Table 1: Comparison of upper and lower bounds of \( J(\pi) \) obtained by different OPE methods. Row 1,2,4,5 are the minimax confidence bounds derived in this paper, and Row 3,6 (with ‘) are their naïve counterparts obtained by the approximation guarantees of previous methods, which are always looser (see Appendix B). \( \hat{w} \) (and \( \hat{q} \)) is the \( w \) (and \( q \)) that attains the infimum in the rest of the expression. The red terms highlight why the naïve bounds are loose. All expressions with subscript “\( w \)” are valid upper or lower bounds when \( \mathcal{C}(\mathcal{Q}) \) is realizable, and those with “\( q \)” are derived assuming realizable \( \mathcal{C}(\mathcal{W}) \).

| Expression | Remark |
|------------|--------|
| UB\(_{w}^{}\) | inf\(_{w}^{}\) sup\(_{q}^{}\) (\( E_{w}[r] + L_{w}(w,q) \)) |
| LB\(_{w}^{}\) | sup\(_{w}^{}\) inf\(_{q}^{}\) (\( E_{w}[r] + L_{w}(w,q) \)) |
| UB\(_{w}^{}\)' | \( E_{w}[r] \pm \inf_{w}^{\sup_{q}^{}\{L_{w}(w,q)\}} \) |
| LB\(_{w}^{}\)' | Frenchel AlgaeDICE (Nachum et al., 2019b) |
| UB\(_{q}^{}\) | inf\(_{q}^{}\) sup\(_{w}^{}\) (\( q(s_0, \pi) + L_{q}(w,q) \)) |
| LB\(_{q}^{}\) | sup\(_{q}^{}\) inf\(_{w}^{}\) (\( q(s_0, \pi) + L_{q}(w,q) \)) |
| UB\(_{q}^{}\)' | \( q(s_0, \pi) \pm \inf_{q}^{\sup_{w}^{}\{L_{q}(w,q)\}} \) |
| LB\(_{q}^{}\)' | MQL (Uehara et al., 2019) |

Our loss \( L(w,q) = E_{w}[r] + L_{w}(w,q) = q(s_0, \pi) + L_{q}(w,q) \).
basic telescoping properties such as Bellman equations (Lemmas 1 and 4). Our results also provide further justification for AlgaeDICE as an off-policy policy optimization algorithm (Section 5), and point out its weakness for OPE (Section 4) and how to address it.

4. The Minimax Confidence Intervals

In this section we derive the minimax confidence intervals by slightly altering the derivation of two recent methods (Uehara et al., 2019), one of “weight-learning” style (Section 4.1) and one of “value-learning” style (Section 4.2), and show that under certain conditions, they merge into a single unified confidence interval whose validity only relies on either \( Q \) or \( W \) being realizable (Section 4.3).

4.1 Confidence Interval for Realizable \( Q \) and Misspecified \( W \)

We start with a simple lemma that can be used to derive the “weight-learning” methods, such as the original algorithm by Liu et al. (2018) and its behavior-agnostic extension by Uehara et al. (2019). Our derivation assumes realizable \( Q \) but arbitrary \( W \).

**Lemma 1** (Evaluation Error Lemma for Importance Weights). For any \( w : S \times A \rightarrow \mathbb{R} \),

\[
J(\pi) - \mathbb{E}_w [r] = Q^\pi(s_0, \pi) + \mathbb{E}_w [r + \gamma Q^\pi(s', \pi) - Q^\pi(s, a)].
\]  

(8)

**Proof.** By moving terms, it suffices to show that \( J(\pi) - Q^\pi(s_0, \pi) = \mathbb{E}_w [r + \gamma Q^\pi(s', \pi) - Q^\pi(s, a)] \), which holds because both sides equal 0: The LHS is trivial. For the RHS, the expectation is zero when conditioned on any \((s, a)\) due to the Bellman equations for policy evaluation (Eq.(3)), and the weighting \( w \) is inconsequential.

“Weight-learning” in a nutshell  The “weight-learning” methods aim to learn a \( w \) such that \( J(\pi) \approx \mathbb{E}_w [r] \). By Lemma 1, we may simply find \( w \) that sets the RHS of Eq.(8) to 0. Of course, this expression depends on \( Q^\pi \), which is unknown. However, if we are given a function class \( Q \) that captures \( Q^\pi \), we can find \( w \) (over a class \( W \)) that minimizes

\[
\sup_{q \in Q} |L_w(w, q)|, \quad \text{where} \quad L_w(w, q) := q(s_0, \pi) + \mathbb{E}_w [r + \gamma q(s', \pi) - q(s, a)].
\]  

(9)

This derivation implicitly assumes that we can find \( w \) such that \( L_w(w, q) \approx 0 \ \forall q \in Q \), which is guaranteed when \( w_{\pi/\mu} \in W \). When \( W \) is misspecified, however, the estimate can be highly biased. Although such a bias can be somewhat quantified by the approximation guarantee of these methods (see Remark 3 for details), we show below that there is a more direct, elegant, and tighter approach.

**Derivation of the CI**  Again, suppose we are given a realizable \( Q \), that is, \( Q^\pi \in Q \).\(^4\) Then from Lemma 1,

\[
J(\pi) = Q^\pi(s_0, \pi) + \mathbb{E}_w [r + \gamma Q^\pi(s', \pi) - Q^\pi(s, a)] \\
\leq \sup_{q \in Q} \left\{ q(s_0, \pi) + \mathbb{E}_w [r + \gamma q(s', \pi) - q(s, a)] \right\}.
\]  

(10)

\(^4\) This condition can be relaxed to \( Q^\pi \in \mathcal{C}(Q) \) due to the affinity of \( L(w, \cdot) \).
For convenience, from now on we will use the shorthand

\[ L(w, q) := q(s_0, \pi) + \mathbb{E}_w[r + \gamma q(s', \pi) - q(s, a)], \] (11)

and the upper bound is then \( \sup_{q \in \mathcal{Q}} L(w, q) \). The lower bound is similar:

\[ J(\pi) \geq \inf_{q \in \mathcal{Q}} \left\{ q(s_0, \pi) + \mathbb{E}_w[r + \gamma q(s', \pi) - q(s, a)] \right\} = \inf_{q \in \mathcal{Q}} L(w, q). \] (12)

To recap, an arbitrary \( w \) will give us a valid confidence interval \([\inf_{q \in \mathcal{Q}} L(w, q), \sup_{q \in \mathcal{Q}} L(w, q)]\), and we may search over a class \( \mathcal{W} \) to find a tighter interval \(^5\) by taking the lowest upper bound and the highest lower bound:

\[ J(\pi) \leq \inf_{w \in \mathcal{W}} \sup_{q \in \mathcal{Q}} L(w, q) =: UB_w, \quad J(\pi) \geq \sup_{w \in \mathcal{W}} \inf_{q \in \mathcal{Q}} L(w, q) =: LB_w. \] (13)

It is worth keeping in mind that the above derivation assumes realizable \( \mathcal{Q} \). Without such an assumption, there is no guarantee that \( J(\pi) \leq UB_w, J(\pi) \geq LB_w \), or even \( LB_w \leq UB_w \). Below we establish the conditions under which the interval is valid (i.e., \( UB_w \leq J(\pi) \leq LB_w \)) and tight (i.e., \( UB_w - LB_w \) is small).

**Properties of the CI** Intuitively, if \( \mathcal{Q} \) is richer, we have a better chance of satisfying realizability and hence improving the CI’s validity. If we further make \( \mathcal{W} \) richer, the CI becomes tighter, as we are searching over a richer space to suppress the upper bound and raise the lower bound. We formalize these intuitions with the theoretical results below.

It is worth pointing out that, although the derivation above assumes exactly realizable \( \mathcal{Q} \) for developing intuitions, our main theorems do not require any of such explicit assumptions, which automatically make them agnostic.

**Theorem 2** (Validity). Define \( L_w(w, q) := q(s_0, \pi) + \mathbb{E}_w[r + \gamma q(s', \pi) - q(s, a)] \). We have

\[ UB_w - J(\pi) \geq \inf_{w \in \mathcal{W}} \sup_{q \in \mathcal{Q}} L_w(w, q - Q^\pi), \]

\[ J(\pi) - LB_w \geq \inf_{w \in \mathcal{W}} \sup_{q \in \mathcal{Q}} L_w(w, Q^\pi - q). \]

As a corollary, when \( Q^\pi \in \mathcal{C}(\mathcal{Q}) \), the CI is valid, i.e., \( UB_w \geq J(\pi) \geq LB_w \).

**Proof.** Let \( w_1 \) denote the \( w \) that attains the infimum in \( UB_w \).\(^6\)

\[ UB_w - J(\pi) = \sup_{q \in \mathcal{Q}} L(w_1, q) - L(w_1, Q^\pi) \quad \text{(Lemma 1: } \forall w, J(\pi) = L(w, Q^\pi)) \]

\[ \geq \inf_{w \in \mathcal{W}} \sup_{q \in \mathcal{Q}} \{ L(w, q) - L(w, Q^\pi) \} \]

\[ = \inf_{w \in \mathcal{W}} \sup_{q \in \mathcal{Q}} L_w(w, q - Q^\pi). \quad \text{ (} \mathbb{E}_w[r] \text{ terms cancel)} \]

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5. Note that we cannot search over the unrestricted (tabular) class in complex problems due to overfitting on finite sample.

6. Point-wise supremum is lower semi-continuous, i.e., \( \sup_{q \in \mathcal{Q}} L(w, q) \) is lower semi-continuous in \( w \) and hence the infimum is attainable.
Similarly, let \( w_2 \) denote the \( w \) that attains the supremum in \( \text{LB}_w \),

\[
J(\pi) - \text{LB}_w = L(w_2, Q^\pi) - \inf_{q \in Q} \sup_{w \in W} L(w, q) \geq \inf_{w \in W} \sup_{q \in Q} \{ L(w, Q^\pi) - L(w, q) \}.
\]

The corollary follows because \( \forall w \), both \( \sup_{q \in Q} \{ L(w, q) - L(w, Q^\pi) \} \) and \( \sup_{q \in Q} \{ L(w, Q^\pi) - L(w, q) \} \) are non-negative when \( Q^\pi \in \mathcal{C}(Q) \), noting that \( L(w, \cdot) \) is affine.

\( L_w(w, q - Q^\pi) \) and \( L_w(w, Q^\pi - q) \) can be viewed as a measure of difference between \( Q^\pi \) and \( q \), as they are essentially linear measurements of \( q - Q^\pi \) (note that \( L_w(w, \cdot) \) is linear) with the measurement vector determined by \( w \).

Even if valid, the CI may be useless if \( \text{UB}_w \gg \text{LB}_w \). Below we show that this can be prevented by having a well-specified \( W \).

**Theorem 3** (Tightness). \( \text{UB}_w - \text{LB}_w \leq 2 \inf_{w \in W} \sup_{q \in Q} |L_w(w, q)|. \) As a corollary, when \( w_{\pi/\mu} \in W \), we have \( \text{UB}_w \leq \text{LB}_w \).

**Proof.**

\[
\text{UB}_w - \text{LB}_w = \inf_{w \in W} \sup_{q \in Q} L(w, q) - \sup_{w \in W} \inf_{q \in Q} L(w, q) = \inf_{w, w' \in W} \left\{ \sup_{q \in Q} L(w, q) - \inf_{q \in Q} L(w', q) \right\} \leq \inf_{w \in W} \left\{ \sup_{q \in Q} L(w, q) - \inf_{q \in Q} L(w, q) \right\} \quad \text{(constraining } w = w' \text{)}
\]

Noting that \( L(w, q) = \mathbb{E}_w[r] + L_w(w, q) \),

\[
\sup_{q \in Q} L(w, q) - \inf_{q \in Q} L(w, q) = \sup_{q \in Q} L_w(w, q) - \inf_{q \in Q} L_w(w, q) \leq 2 \sup_{q \in Q} |L_w(w, q)|.
\]

When \( w_{\pi/\mu} \in W \), \( \text{UB}_w \leq \text{LB}_w \) follows from the fact that \( L_w(w_{\pi/\mu}, q) \equiv 0, \forall q \).

**Remark 1** (Interpretation of Theorem 3). At the first glance, the theorem might give the impression that the CI collapses to a point (i.e., \( \text{UB}_w = \text{LB}_w \)) if \( w_{\pi/\mu} \in W \) as \( \text{UB}_w \leq \text{LB}_w \), which is not true. Recall that without realizable \( Q \), it is possible that \( \text{UB}_w < \text{LB}_w \), and even if \( w_{\pi/\mu} \in W \), \( \text{UB}_w \) can be arbitrarily below \( J(\pi) \) and \( \text{LB}_w \) arbitrarily above. Therefore, a CI that is both tight and valid can only be implied from Theorems 2 and 3 together, when both \( W \) and \( Q \) are well-specified (e.g., realizable \( W \) and \( Q \) implies \( \text{UB}_w = \text{LB}_w = J(\pi) \)).

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7. Familiar readers may wonder why the approximation error of \( Q \) is characterized as \( \inf_{w} \sup_{q} L_w(\cdot, \cdot) \) instead of \( \sup_{q} \inf_{w} L_w(\cdot, \cdot) \), as the latter requires a global approximation of \( Q^\pi \) with small errors under all \( w \in W \). In fact, both work and our version is tighter (\( \inf_{w} \sup_{q} L_w(\cdot, \cdot) \)) and equal with convex \( Q \) and \( W \). Another possible confusion is that \( L_w(w, q - Q^\pi) \geq 0 \) as long as \( q \) is a uniform upper bound on \( Q^\pi \) (e.g., \( q \equiv R_{\max}/(1 - \gamma) \)). This would hold if the linear coefficients induced by \( w \) were non-negative, which in general is not true—even if \( w \) itself is non-negative—due to the \(- q(s, a)\) term in \( L_w(\cdot, \cdot) \).
Remark 2 (Point estimate). If a point estimate is desired, we may output $\frac{1}{2}(\text{UB}_w + \text{LB}_w)$, and under $Q^* \in C(Q)$ we can assert that its error is bounded by $\inf_{w \in W} \sup_{q \in Q} |L_w(w, q)|$. This coincides with the approximation error bound of MWL under the same assumption (Uehara et al., 2019, Theorem 2). Furthermore, if we simply output UB$_w$ or LB$_w$ (with the latter being the policy evaluation component of AlgaeDICE (Nachum et al., 2019b)), the approximation guarantee will be twice as large since they only incur one-sided errors.

Remark 3 (Naïve CI). As we alluded to earlier, the approximation guarantee of Uehara et al. (2019, Theorem 2) (see also Liu et al., 2018, Theorem 7) can be used to derive a CI that is also valid under realizable $Q$: for example, for MWL, the CI will be the point estimate of $J(\pi)$ plus-minus $\inf_{w \in W} \sup_{q \in Q} |L_w(w, q)|$ (UB$_w'$ and LB$_w'$ in Table 1). As Theorem 3 shows, such a naïve CI is never tighter than ours. Further discussions on this comparison can be found in Appendix B, where we show that our CI is always fully contained in the naïve CI with realizable $C(Q)$; this is stronger than Theorem 3 which only compares the lengths of the two CIs.

4.2 Confidence Interval for Realizable $W$ and Misspecified $Q$

Similar to Section 4.1, we now derive the CI for the other case where $W$ is realizable. We also base our entire derivation on the following simple lemma, which can be used to derive the “value-learning” method.

Lemma 4 (Evaluation Error Lemma for Value Functions). For any $q : S \times A \to \mathbb{R}$,

$$J(\pi) - q(s_0, \pi) = \mathbb{E}_d[r + \gamma q(s', \pi) - q(s, a)].$$

(14)

Proof. The lemma follows by observing tht $J(\pi) = \mathbb{E}_d[r]$, and $\mathbb{E}_d[q(s, a) - \gamma q(s', \pi)] = q(s_0, \pi)$. □

“Value-learning” in a nutshell MQL (Uehara et al., 2019) seeks to find $q$ such that $q(s_0, \pi) \approx J(\pi)$. Using Lemma 4, this can be achieved by finding $q$ that sets the RHS of Eq.(14) to 0, and we can search over a class $W$ that realizes $w_{\pi/\mu}$ to overcome the difficulty of unknown $d^{\pi}$, similar to how we handle the unknown $Q^*$ in Section 4.1. While the method gives accurate estimate when both $Q$ and $W$ are well-specified, below we show how to derive a CI to quantify the bias when only $W$ is realizable and $Q$ is not.

Derivation of the CI If we are given $W \subset (S \times A \to \mathbb{R})$ such that $w_{\pi/\mu} \in W$, then

$$J(\pi) \leq q(s_0, \pi) + \sup_{w \in W} \mathbb{E}_w[r + \gamma q(s', \pi) - q(s, a)] = \sup_{w \in W} L(w, q).$$

(15)

$$J(\pi) \geq q(s_0, \pi) + \inf_{w \in W} \mathbb{E}_w[r + \gamma q(s', \pi) - q(s, a)] = \inf_{w \in W} L(w, q).$$

(16)

Again, an arbitrary $q$ will give us a valid confidence interval, and we may search over a class $Q$ to tighten it:

$$J(\pi) \leq \inf_{q \in Q} \sup_{w \in W} L(w, q) =: \text{UB}_q,$$

$$J(\pi) \geq \sup_{q \in Q} \inf_{w \in W} L(w, q) =: \text{LB}_q.$$

(17)

8. This condition can be relaxed to $w_{\pi/\mu} \in C(W)$. 

9
Properties of the CI  We characterize the validity and the tightness of the CI below, with proofs deferred to Appendix A.

**Theorem 5** (Validity). Define \( L_q(w, q) := \mathbb{E}_w[r + \gamma q(s', \pi) - q(s, a)] \).

\[
\begin{align*}
UB_q - J(\pi) & \geq \inf_{q \in \mathcal{Q}} \sup_{w \in \mathcal{W}} L_q(w - w_{\pi/\mu}, q), \\
J(\pi) - LB_q & \geq \inf_{q \in \mathcal{Q}} \sup_{w \in \mathcal{W}} L_q(w_{\pi/\mu} - w, q).
\end{align*}
\]

As a corollary, when \( w_{\pi/\mu} \in \mathcal{C}(\mathcal{W}) \), the CI is valid, i.e., \( UB_w \geq J(\pi) \geq LB_w \).

Again, the validity of the CI is controlled by the realizability of \( \mathcal{C}(\mathcal{W}) \), defined as the best approximation of \( w_{\pi/\mu} \in \mathcal{W} \) where the difference between \( w_{\pi/\mu} \) and any \( w \) is measured by \( L_q(w - w_{\pi/\mu}, q) \) and \( L_q(w_{\pi/\mu} - w, q) \) (which are linear measurements of \( w - w_{\pi/\mu} \)).

**Theorem 6** (Tightness). \( UB_q - LB_q \leq 2 \inf_{q \in \mathcal{Q}} \sup_{w \in \mathcal{W}} |L_q(w, q)| \). As a corollary, when \( w_{\pi/\mu} \in \mathcal{W} \), we have \( UB_q \leq LB_q \).

4.3 Unification

So far we have obtained two confidence intervals:

\[
\begin{align*}
\mathcal{Q} \text{ realizable:} & \quad \{ UB_w = \inf_w \sup_q L(w, q), \quad LB_w = \sup_w \inf_q L(w, q) \}, \\
\mathcal{W} \text{ realizable:} & \quad \{ UB_q = \inf_q \sup_w L(w, q), \quad LB_q = \sup_q \inf_w L(w, q) \},
\end{align*}
\]

where \( L(w, q) := q(s_0, \pi) + \mathbb{E}_w[r + \gamma q(s', \pi) - q(s, a)] \). Taking a closer look, we can see that \( UB_w \) and \( LB_q \) are almost the same and only differ in the order of optimizing \( q \) and \( w \), and so are \( UB_q \) and \( LB_w \). It turns out that if \( \mathcal{W} \) and \( \mathcal{Q} \) are convex, these two confidence intervals are precisely the reverse of each other.

**Theorem 7.** If \( \mathcal{W} \) and \( \mathcal{Q} \) are compact and convex sets, we have

\[
UB_w = LB_q, \quad UB_q = LB_w.
\]

*Proof.* Since \( L(w, q) \) is bi-affine—which implies that it is convex-concave—by the minimax theorem (Neumann, 1928; Sion et al., 1958), the order of inf and sup are exchangeable. \( \square \)

This result implies that we do not need to separately consider these two intervals. Neither do we need to know which one of \( \mathcal{Q} \) and \( \mathcal{W} \) is (approximately) realizable. We just need to do the obvious thing, which is to compute \( UB_w (= LB_q) \) and \( UB_q (= LB_w) \), and let the smaller number be the lower bound and the greater be the upper bound. **This way we get a single CI that is valid when either \( \mathcal{Q} \) or \( \mathcal{W} \) is realizable (Theorems 2 and 5), and tight when both are.** Furthermore, by looking at which value is lower than the other, we can tell which class is misspecified (assuming one of them is well-specified), and this piece of information may provide guidance to the design of function approximation. We envision that a practical application of the minimax OPE methods may involve an iterative procedure—which we leave for future investigation—where we start with simple function classes, and gradually increase their capacities based on the outcomes of the algorithm.

---

9. For non-convex classes, we may search over their convex hulls so that the equivalence still holds, although this may pose additional challenges in optimization and sample efficiency.
4.4 Experiments

We provide preliminary empirical evidence that supports the theoretical predictions. The experiment is conducted in the CartPole environment, with the target policies being softmax policies over a pre-trained Q-function with different temperature parameters $\tau$ (behavior policy is $\tau = 1.0$). We compare the new interval $(\text{LB}_q$ and $\text{UB}_q)$ to the na"ıve interval $(\text{LB}_q'$ and $\text{UB}_q')$. The $Q$ and $W$ classes are constructed using multilayer perceptrons, and we optimize the objectives using stochastic gradient descent ascent (SGDA):$^{10}$ see Appendix C for further details. Figure 1 shows the learning curves for two different target policies: (1) in the top figure, we see that $\text{UB}_q > \text{LB}_q$ and the new interval is significantly tighter than the na"ıve interval. (2) in the bottom figure, a target policy with $\tau = 3.0$—which is significantly different from the behavior policy—is considered, and realizing $w_\pi/\mu$ is challenging. In this scenario, we observe a reversed interval ($\text{UB}_q < \text{LB}_q$) as predicted by theory.

5. On Policy Optimization with Insufficient Data Coverage

OPE is not only useful as an evaluation method, but can also serve as a crucial component for off-policy policy optimization: if we can estimate the return $J(\pi)$ for a class of policies $\pi \in \Pi$, then in principle we may use $\max_{\pi \in \Pi} J(\pi)$ to find the best policy in class. However, our CI gives two estimations of $J(\pi)$, an upper bound and a lower bound. Which one should we optimize? Traditional wisdom in robust MDP literature (e.g., Nilim and El Ghaoui, 2005) suggests pessimism, i.e., optimizing the lower bound for the best worst-case guarantees. But this only begs the next question: which side of the CI is the lower bound?

**RL with Insufficient Data Coverage** As Section 4 indicates, both $\text{UB}_w (= \text{LB}_q)$ and $\text{UB}_q (= \text{LB}_w)$ might be the lower bound, depending on the realizability of $Q$ and $W$. Which one of the function classes is more likely to be misspecified?

We note that even if $W$ and $Q$ are carefully chosen to incorporate domain knowledge and/or be sufficiently rich, the realizability of $W$ faces one additional and crucial challenge compared to $Q$: recall that $W$ needs to realize $w_\pi/\mu$, the importance weights between $d^\pi$ and $\mu$. If the data distribution $\mu$ itself does not fully cover the state space, then $w_\pi/\mu$ may not even exist and hence $W$ will be poorly specified whatsoever (see Section 2.2). Since the historical dataset in real applications are given passively to RL practitioners with no exploratory guarantees, this scenario is highly likely and remains as a crucial challenge to the application of RL, yet is surprisingly understudied especially in the function approximation setting (with a few exceptions; Fujimoto et al., 2019; Liu et al., 2019b).

In this section we analyze the algorithms that optimize the upper and the lower bounds when $W$ is poorly specified. For convenience we will call them$^{11}$

\[
\text{MUB-PO: } \max_{\pi \in \Pi} \text{UB}^\pi_w, \quad \text{MLB-PO: } \max_{\pi \in \Pi} \text{LB}^\pi_w, \quad (18)
\]

$^{10}$ Neural nets induce non-convex function classes, and the equivalence ($\text{UB}_q = \text{LB}_w$ and $\text{UB}_w = \text{LB}_q$) does not necessarily hold. However, since SGDA is symmetric w.r.t. $w$ and $q$, the two bounds computed by the algorithm can be viewed as heuristic approximations of $\text{UB}_q\&\text{LB}_w$ and $\text{UB}_w\&\text{LB}_q$, respectively.

$^{11}$ We make the dependence of $\text{UB}_w$ and $\text{LB}_w$ on $\pi$ explicit since we are concerned with multiple policies in this section.
Figure 1: Training curves averaged over 10 seeds. Error bars show twice the standard errors. The curves have been smoothed with a window size corresponding to 20 $q$-$w$ alternations. **Top**: The difference between behavior policy and target policy is relatively small, and $UB_q > LB_q$. The interval $[LB_q, UB_q]$ is significantly tighter than $[LB_q', UB_q']$. **Bottom**: Target policy is significantly different from the behavior policy, and realizing the importance weight is challenging. In this case, a reversed interval is observed, i.e. $UB_q < LB_q$.

where MUB-PO/MLB-PO stand for minimax upper (lower) bound policy optimization. MLB-PO is essentially Frenchel AlgaeDICE without regularization (Nachum et al., 2019b), so our results provide further justification for applying the method to off-policy policy optimization. On the other hand, while MUB-PO may not be appropriate for exploitation when data coverage is poor, it exercises *optimism* and may be better applied to induce exploration, that is, the policy computed by MUB-PO can be used to further interact with the environment and obtain new data to expand data coverage.\(^{12}\) Furthermore, our analyses show that exploration might be *easier* than exploitation, as MUB-PO’s guarantee requires significantly weaker realizability assumption on $Q$ than MLB-PO.

\(^{12}\) It should be noted, however, that a complete algorithm for systematic exploration usually involves multiple iterations of back-and-forth between data collection and policy re-computation, and we only show that MUB-PO performs one such iteration effectively. There are further design choices to be made to complete MUB-PO into a full algorithm (e.g., how much data to collect in each iteration and how to combine old and new datasets), which we leave for future investigation.
5.1 Case Study: Exploration and Exploitation in a Tabular Scenario

To substantiate the claim that MUB-PO/MLB-PO induce effective exploration/exploitation, we first consider a scenario where the solution concepts for exploration and exploitation are clearly understood, and show that MUB-PO/MLB-PO reduce to familiar algorithms.

Setup Consider the setting where the MDP has finite and discrete state and action spaces. Let \( \tilde{S} \subset S \) be a subset of the state space, and \( s_0 \in \tilde{S} \). Suppose the dataset contains \( n \) transition samples from each \( s \in \tilde{S}, a \in A \) with \( n \to \infty \) (i.e., the transitions and rewards in \( \tilde{S} \) are fully known), and 0 samples from \( s \notin \tilde{S} \).

Known Solution Concepts In such a simplified setting, effective exploration can be achieved by (the episodic version of) the well-known Rmax algorithm (Brafman and Tennenholtz, 2003; Kakade, 2003), which computes the optimal policy of the Rmax-MDP \( M_{\max} \), defined as \((S,A,P_{\max},R_{\max},\gamma,s_0)\), where

\[
P_{\max}(s,a) = \begin{cases} P(s,a), & \text{if } s \in \tilde{S} \\ \mathbb{I}[s' = s], & \text{if } s \notin \tilde{S} \end{cases}, \quad R_{\max}(s,a) = \begin{cases} R(s,a), & \text{if } s \in \tilde{S} \\ R_{\max}, & \text{if } s \notin \tilde{S}. \end{cases}
\]

In words, \( M_{\max} \) is the same as the true MDP \( M \) on states with sufficient data, and the remaining “unknown” states are assumed to have self-loops with \( R_{\max} \) immediate rewards, making them appealing to visit and thus encouraging exploration. The theoretical guarantee for the policy computed by Rmax is an optimal-or-explore statement (see e.g., Jiang, 2018), that either the optimal policy of \( M_{\max} \) is near-optimal in true \( M \), or its occupancy measure must visit states outside \( \tilde{S} \), with a mass proportional to its suboptimality. Similarly, when the goal is to exploit, that is, to output a policy with the best worst-case guarantee, one simply needs to change the \( R_{\max} \) in the Rmax-MDP to the minimally possible reward value (which is 0 in our setting), and we call this MDP \( M_{\min} \).

Below we present the central result of Section 5.1, that MUB-PO and MLB-PO in this setting precisely correspond to the Rmax and the Rmin algorithms, respectively.

**Proposition 8.** Consider the MDP and the dataset described above. Let \( W = [0, \frac{\tilde{S} \times A}{1 - \gamma}]^{S \times A} \) and \( Q = [0, R_{\max}/(1 - \gamma)]^{S \times A} \). In this case, MUB-PO reduces to Rmax, and MLB-PO reduces to Rmin.

Proof. Let \( \mathcal{M} \) be the space of all MDPs that are consistent with the given dataset. Let \( M_{\max} \) and \( M_{\min} \) be the Rmax and Rmin MDPs, respectively, and it is clear that \( M_{\max}, M_{\min} \in \mathcal{M} \).

To show that MLB-PO reduces to Rmin, it suffices to prove that for every \( \pi : S \to A \), \( LB_{w}^{\pi} = J_{\min}(\pi) \). Since \( Q \) is the tabular function space and always realizable (regardless of the true MDP \( M \)), \( LB_{w}^{\pi} \) is a valid lower bound, i.e., \( LB_{w}^{\pi} \leq J(\pi) \). Since all MDPs in \( M \) could be the true \( M \), it must hold that \( LB_{w}^{\pi} \leq J_{\min}(\pi) \). It suffices to show that \( LB_{w}^{\pi} \geq J_{\min}(\pi) \).

Recall that

\[
LB_{w}^{\pi} = \sup_{w \in W} \inf_{q \in Q} \left\{ q(s_0, \pi) + \mathbb{E}_w[r + \gamma q(s', \pi) - q(s, a)] \right\}.
\]

13. With a slight abuse of notations, in this section we treat \( R : S \times A \to [0, R_{\max}] \) as a deterministic reward function for convenience.
Since $\mathcal{Q}$ is the unrestricted tabular function space, we may represent $q \in \mathcal{Q}$ as a $|\mathcal{S} \times \mathcal{A}|$ vector where each coordinate $q(s, a)$ can take values between $[0, R_{\text{max}}/(1-\gamma)]$ independently. Now note that for any $\gamma q(s', \pi)$ term in the objective and can never appear as $q(s_0, \pi)$ or $-q(s, a)$. Since $\mathcal{W}$ only contains non-negative functions, $L(w, q)$ is non-decreasing in $q(s', \pi)$, and $\inf_{q \in \mathcal{Q}}$ can always be attained when $q(s', a') = 0$, $\forall s' \notin \mathcal{S}, a' \in \mathcal{A}$. For any $w \in \mathcal{W}$, let $q_w$ denote such a $q \in \mathcal{Q}$ that achieves the inner infimum, and

$$LB_w^\pi = \sup_{w \in \mathcal{W}} \{q_w(s_0, \pi) + E_w[r + \gamma q_w(s', \pi) - q_w(s, a)]\}.$$ 

Next, consider the discounted occupancy of $\pi$ in $M_{\text{min}}$, denoted as $d_{M_{\text{min}}}^\pi$. Define

$$w_0(s, a) := \mathbb{I}[s \in \mathcal{S}] d_{M_{\text{min}}}^\pi(s, a) / |\mathcal{S} \times \mathcal{A}|.$$ 

Let $q_0 = q_{w_0}$. Now, since $w_0 \in \mathcal{W}$,

$$LB_w^\pi \geq q_0(s_0, \pi) + E_{w_0}[r + \gamma q_0(s', \pi) - q_0(s, a)]$$

$$= q_0(s_0, \pi) + \frac{1}{|\mathcal{S} \times \mathcal{A}|} \sum_{s \in \mathcal{S}, a \in \mathcal{A}} w_0(s, a)(R(s, a) + \gamma E_{s' \sim P(s, a)}[q_0(s', \pi)] - q_0(s, a))$$

$$= q_0(s_0, \pi) + \sum_{s \in \mathcal{S}, a \in \mathcal{A}} d_{M_{\text{min}}}^\pi(s, a)(R(s, a) + \gamma E_{s' \sim P(s, a)}[q_0(s', \pi)] - q_0(s, a))$$

$$= \sum_{s \in \mathcal{S}, a \in \mathcal{A}} \nu(s, a)q_0(s, a),$$

where

$$\nu(s, a) := \mathbb{I}[s = s_0, a = \pi(s_0)] + \gamma \sum_{s' \in \mathcal{S}, a' \in \mathcal{A}} d_{M_{\text{min}}}^\pi(s', a')P(s|s', a') - \mathbb{I}[s \in \mathcal{S}] d_{M_{\text{min}}}^\pi(s, a).$$

Note that

$$\sum_{s \in \mathcal{S}, a \in \mathcal{A}} d_{M_{\text{min}}}^\pi(s, a)R(s, a) = \sum_{s \in \mathcal{S}, a \in \mathcal{A}} d_{M_{\text{min}}}^\pi(s, a)R(s, a) + \sum_{s \notin \mathcal{S}, a \in \mathcal{A}} d_{M_{\text{min}}}^\pi(s, a) \cdot 0 = J_{M_{\text{min}}}^\pi(\pi),$$

so it suffices to show that $\sum_{s \in \mathcal{S}, a \in \mathcal{A}} \nu(s, a)q_0(s, a) = 0$, which we establish in the rest of this proof.

Recall that $q_0(s, a) = 0$ for any $s \notin \mathcal{S}$. So $\sum_{s \in \mathcal{S}, a \in \mathcal{A}} \nu(s, a)q_0(s, a) = \sum_{s \notin \mathcal{S}, a \in \mathcal{A}} \nu'(s, a)q_0(s, a)$, where

$$\nu'(s, a) := \mathbb{I}[s = s_0, a = \pi(s_0)] + \gamma \sum_{s' \in \mathcal{S}, a' \in \mathcal{A}} d_{M_{\text{min}}}^\pi(s', a')P_{M_{\text{min}}}(s|s', a') - d_{M_{\text{min}}}^\pi(s, a).$$

This is because $\nu$ and $\nu'$ exactly agree on the value in $s \in \mathcal{S}$, and only differ on $s \notin \mathcal{S}$. To see this, consider any $s \in \mathcal{S}, a \in \mathcal{A}$. $\nu$ and $\nu'$ agree on the first and the last terms. They also agree on the second term for the summation variables $s' \in \mathcal{S}, a' \in \mathcal{A}$, as $P(s|s', a') = 0$. Thus,
\(P_{M_{\text{min}}}(s|s',a')\) (the MDP \(M_{\text{min}}\) has the true transition probabilities on states with sufficient data). So the only difference is

\[
\gamma \sum_{s' \not\in \tilde{S}, a' \in A} d_{M_{\text{min}}}^\pi(s', a') P_{M_{\text{min}}}(s'|s, a').
\]

However, this term must be zero, because for any \(s \in \tilde{S}, s' \not\in \tilde{S}, P_{M_{\text{min}}}(s'|s, a') = 0\), as the construction of \(M_{\text{min}}\) guarantees that no states outside \(\tilde{S}\) will ever transition back to \(\tilde{S}\). Now that we conclude \(\nu(s, a)q_0(s, a) = \nu'(s, a)q_0(s, a)\), the fact that it is zero is obvious: \(\nu' \equiv 0\), which follows directly from the Bellman equation for discounted occupancy in MDP \(M_{\text{min}}\). This completes the proof of \(\text{LB}_{\pi}^w = J_{M_{\text{min}}}^\pi(\pi)\), and the proof for \(\text{UB}_{\pi}^w = J_{M_{\text{max}}}^\pi(\pi)\) is similar and hence omitted.

**Remark 4.** In the simplified setting above, the states outside \(\tilde{S}\) receive no data at all. In the more general case where \(\tilde{S}\) is still under-explored but every state receives any least 1 data point, it is not difficult to show that both MUB-PO and MLB-PO reduce to the certainty-equivalent solution, and can overfit to the poor estimation of transitions and rewards in states with few data points. Such a degenerate behavior may be prevented by regularizing \(w\) and prohibiting any highly spiked \(w\) (e.g., regularizing with \(E_{\mu}[w^2]\), which measures the effective sample size of importance weighted estimate induced by \(w\), or by bootstrapping and taking data randomness into consideration during policy optimization.

### 5.2 Guarantees in the Function Approximation Setting

We give more general guarantees of MUB-PO and MLB-PO in the function approximation setting. For simplicity we still assume exact expectations and optimization, and incorporating estimation and/or optimization errors in such analyses is routine (see e.g., Munos and Szepesvári, 2008; Farahmand et al. 2010; Chen and Jiang, 2019).

Perhaps surprisingly, we show that effective exploitation with MLB-PO and exploration with MUB-PO require different realizability assumptions on \(Q\): MLB-PO requires \(Q^\pi \in \mathcal{C}(Q)\) for all \(\pi \in \Pi\) quite as expected, but MUB-PO only requires the existence of one good policy \(\pi \in \Pi\) such that \(Q^\pi \in \mathcal{C}(Q)\), suggesting some interesting asymmetry between exploration and exploitation in the function approximation setting.

**Exploitation with Well-specified \(Q\)** We start with the guarantee of MLB-PO.

**Proposition 9** (MLB-PO: to see is to get). Let \(\Pi\) be a policy class, and assume \(Q^\pi \in \mathcal{C}(Q)\) \(\forall \pi \in \Pi\). Let \(\hat{\pi} = \arg \max_{\pi \in \Pi} \text{LB}_{w}^\pi\). Then, for any \(\pi \in \Pi\),

\[
J(\hat{\pi}) \geq \text{LB}_{w}^\pi.
\]

As a corollary, for any \(\pi\) such that \(w_{\pi/\mu} \in \mathcal{W}\), we have \(J(\hat{\pi}) \geq J(\pi)\), that is, we compete with any policy whose importance weight is realized by \(\mathcal{W}\).

**Proof.** It suffices to show that \(J(\hat{\pi}) \geq \text{LB}_{w}^\hat{\pi}\) which follows directly from Theorem 2. \(\text{LB}_{w}^\pi\) is a valid lower bound for any \(\pi \in \Pi\) due to the realizability of \(Q\). The corollary holds because for \(\pi\) with \(w_{\pi/\mu}\) realized by \(\mathcal{W}\), Theorems 2 and 3 guarantee that \(J(\pi) = \text{LB}_{w}^\pi\). \(\square\)
Remark 5. Proposition 9 shows that MLB-PO puts the heavy expressivity burden on $Q$ and is agnostic against misspecified $W$. When data has sufficient coverage and $W$ is highly expressive, we can similarly show that optimizing $\text{LB}_q^\pi$ performs robust exploitation and is agnostic against misspecified $Q$.

**Proposition 10** (Exploitation with expressive $W$). Let $\Pi$ be a policy class, and assume $w_{\pi/\mu} \in C(W) \forall \pi \in \Pi$. Let $\hat{\pi} = \arg\max_{\pi \in \Pi} \text{LB}_q^\pi$. Then, for any $\pi \in \Pi$,

$$J(\hat{\pi}) \geq \text{LB}_q^\pi.$$  

As a corollary, for any $\pi$ such that $Q^\pi \in Q$, we have $J(\hat{\pi}) \geq J(\pi)$, that is, we compete with any policy whose value function can be realized by $Q$.

**Proof.** The proof is similar to that of Proposition 9 and hence omitted. 

**Exploration with (Less) Well-specified $Q$** We then provide the exploration guarantee of MUB-PO. Similar to the tabular case discussed in Section 5.1, the guarantee is an “optimal-or-explore” statement, that either the obtained policy is near-optimal (defined in a very specific manner; see below), or it will induce effective exploration. Perhaps surprisingly, we show that MUB-PO applied to exploration is significantly more robust against misspecified $Q$ than MLB-PO applied to exploitation. As far as we have tried, it seems difficult to improve the analyses of MLB-PO to enjoy similar robustness, suggesting some kind of asymmetry between exploration and exploitation.

The key idea behind the agnostic result is the following: instead of competing with $\max_{\pi \in \Pi} J(\pi)$ as the optimal value under the assumption that $Q^\pi \in C(Q), \forall \pi \in \Pi$ (the same assumption as MLB-PO), we aim at a less ambitious notion of optimality under a substantially relaxed assumption; without any explicit assumption on $Q$, we directly compete with

$$\max_{\pi \in \Pi: Q^\pi \in C(Q)} J(\pi).$$  \hfill (19)

In words, we compete with any policy whose Q-function is realized by $C(Q)$. When all policies satisfy this condition, we compete with $\max_{\pi \in \Pi} J(\pi)$ as usual.\footnote{Note that $Q^\pi \in C(Q), \forall \pi \in \Pi$ is only a sufficient but not necessary condition for competing with $\pi^*_{\Pi} := \arg\max_{\pi} J(\pi)$. To compete with $\pi^*_{\Pi}$, all we need is $Q^\pi_{\Pi} \in C(Q)$.} However, even if some (or most) policies’ Q-functions elude $C(Q)$, we can still compete with whichever policy whose Q-function is captured by $C(Q)$, making the algorithm much more robust against misspecified $C(Q)$. A similar definition of optimal value has been used by Jiang et al. (2017) in PAC-exploration with function approximation, and indeed their algorithm is closely related to MUB-PO, and we will discuss the detailed connections later.

We now state the exploration guarantee of MUB-PO.

**Proposition 11** (MUB-PO: optimal-or-explore). Let $\Pi$ be a policy class. Let $\hat{\pi} = \arg\max_{\pi \in \Pi} \text{UB}_w^\pi$. Then, for any $w \in W$,

$$\text{IPM}(w \cdot \mu, d^\hat{\pi}; F) \geq \max_{\pi \in \Pi: Q^\pi \in C(Q)} J(\pi) - J(\hat{\pi}),$$

where
15. Note that $w \cdot \mu$ may be unnormalized, but this does not affect our results.

Proof of Proposition 11

As a corollary, if we further assume $\|q\|_\infty \leq R_{\text{max}}/(1 - \gamma), \forall q \in Q$, 
\[
\|w \cdot \mu - d^\pi\|_1 \geq \frac{(1 - \gamma) \left( \max_{\pi \in \Pi} \max_{q \in C(Q)} J(\pi) - J(\hat{\pi}) \right)}{2R_{\text{max}}}
\]

To interpret the result, recall that $w \in W$ is supposed to model an importance weight function that coverts the data distribution to the occupancy measure of some policy, e.g., $w_{\pi/\mu} \cdot \mu = d^\pi$. The proposition states that either $\hat{\pi}$ is near-optimal w.r.t. Eq.(19), or it will induce an occupancy measure that cannot be accurately modeled by any importance weights in $W$ when applied on the current data distribution $\mu$. The distance\(^{15}\) between the two distributions $d^\pi$ and $w \cdot \mu$ is measured by the Integral Probability Metric (Müller, 1997) defined w.r.t. a discriminator class $F$, and can be relaxed to the looser but simpler $\ell_1$ distance. Therefore, if we have a rich $W$ class that models all distributions covered by $\mu$, then $\hat{\pi}$ must visit new areas in the state-action space or it must be near-optimal.

Below we give the proof of Proposition 11, which reuses many results established in Section 4.

**Proof of Proposition 11**. Fixing any $\pi \in \Pi$ such that $Q^\pi \in C(Q)$:
\[
J(\pi) - J(\hat{\pi}) \leq UB^\pi_w - J(\hat{\pi}) \quad (\text{UB}_w \text{ is valid upper bound as } Q^\pi \text{ realized by } C(Q))
\]
\[
\leq UB^\pi_w - J(\hat{\pi}). \quad (\hat{\pi} \text{ optimizes } UB^\pi_w)
\]

Recall that $UB^\pi_w = \inf_{w \in W} \sup_{q \in Q} L(w, q; \hat{\pi})$, so for any $w \in W$, $UB^\pi_w \leq \sup_{q \in Q} L(w, q; \hat{\pi})$. On the other hand, for any $q$, $J(\hat{\pi}) = L(w_{\hat{\pi}/\mu}, q)$. Now let $q_w := \arg\max_{q \in Q} L(w, q; \hat{\pi})$. For any $w \in W$,
\[
\max_{\pi \in \Pi} \frac{J(\pi) - J(\hat{\pi})}{UB^\pi_w - J(\hat{\pi})} \leq L(w, q_w; \hat{\pi}) - L(w_{\hat{\pi}/\mu}, q_w; \hat{\pi})
\]
\[
= \mathbb{E}_w[r + \gamma q_w(s', \hat{\pi}) - q_w(s, a)] - \mathbb{E}_{w_{\hat{\pi}/\mu}}[r + \gamma q_w(s', \hat{\pi}) - q_w(s, a)]
\]
\[
\leq |\mathbb{E}_w[\mathcal{T}^\pi q_w - q_w] - \mathbb{E}_{w_{\hat{\pi}/\mu}}[\mathcal{T}^\pi q_w - q_w]|.
\]

The main statement immediately follows by noticing that $\hat{\pi} \in \Pi, q_w \in Q$, hence $\mathcal{T}^\pi q_w - q_w \in F$. The $\ell_1$-distance corollary follows from relaxing IPM using Hölder’s inequality for the $\ell_1$ and $\ell_\infty$ pair. \qed

**Remark 6** (Full algorithm). As we have noted in Footnote 12, MUB-PO is not a full algorithm for exploration. While one can imagine a full algorithm that repeatedly collects new data using the policy computed by MUB-PO and merges it with data from previous rounds, it is difficult to analyze its theoretical properties: the realizability assumption of $W$
depends on $\mu$, but $\mu$ itself dynamically changes over the execution of the algorithm due to data pooling, and any realizability-type assumptions such as $w_\pi/\mu \in W$ are no longer static and cannot appear in an a priori guarantee.

One interesting way to avoid this difficulty is to use a special class of importance weights $W$: instead of $w$ that depends on $(s, a)$, consider $w$ that is $(s, a)$-independent and is indicator function of the identity of the dataset. That is, the $\sup_{w \in W}$ in $UB_\pi^w$ chooses among the datasets collected in different rounds, and takes expectation w.r.t. only one of them (without reweighting within the dataset), essentially avoiding data pooling. The resulting algorithm is very similar to a parameter-free variant\(^\text{16}\) of the OLIVER algorithm by Jiang et al. (2017, Algorithm 3), which has been shown to enjoy low-sample complexities in a wide range of low-rank environments.

6. Conclusion

We derive a minimax confidence interval for off-policy evaluation. The CI is valid as long as one of the weight- or value-function classes is realizable, and its length quantifies the misspecification error of the other class. When applied to off-policy policy optimization, we show that optimizing the lower and the upper bounds induce effective exploitation and exploration, respectively, and they reduce to familiar algorithms in the tabular setting. Our derivation also reveals connections between and produce new insights on existing methods.

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\(^{16}\) The original OLIVER algorithm requires the approximation error of $Q$ as an input, which can be avoided by replacing its constrained optimization step with an unconstrained one similar to MUB-PO.
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Appendix A. Remaining Proofs

Proof of Theorem 5. Let \( q_1 \) denote the \( q \) that attains the infimum in \( \text{UB}_q \).

\[
\text{UB}_q - J(\pi) = \sup_{w \in \mathcal{W}} L(w, q_1) - L(w_{\pi/\mu}, q_1) \quad (\forall q, J(\pi) = L(w_{\pi/\mu}, q))
\]

\[
\geq \inf_{q \in \mathcal{Q}} \sup_{w \in \mathcal{W}} \{ L(w, q) - L(w_{\pi/\mu}, q) \}.
\]

Similarly, let \( q_2 \) denote the \( q \) that attains the supremum in \( \text{LB}_q \),

\[
J(\pi) - \text{LB}_q = L(w_{\pi/\mu}, q_2) - \inf_{w \in \mathcal{W}} L(w, q_2) \geq \inf_{q \in \mathcal{Q}} \sup_{w \in \mathcal{W}} \{ L(w_{\pi/\mu}, q) - L(w, q) \}.
\]

The corollary follows because \( \forall q, \) both \( \sup_{w \in \mathcal{W}} \{ L(w, q) - L(w_{\pi/\mu}, q) \} \) and \( \sup_{w \in \mathcal{W}} \{ L(w_{\pi/\mu}, q) - L(w, q) \} \) are non-negative when \( w_{\pi/\mu} \in \mathcal{C}(\mathcal{W}) \).

Proof of Theorem 6.

\[
\text{UB}_q - \text{LB}_q = \inf_{q \in \mathcal{Q}} \sup_{w \in \mathcal{W}} L(w, q) - \sup_{q \in \mathcal{Q}} \inf_{w \in \mathcal{W}} L(w, q)
\]

\[
= \inf_{q, q' \in \mathcal{Q}} \left\{ \sup_{w \in \mathcal{W}} L(w, q) - \inf_{w \in \mathcal{W}} L(w, q') \right\}
\]

\[
\leq \inf_{q \in \mathcal{Q}} \left\{ \sup_{w \in \mathcal{W}} L(w, q) - \inf_{w \in \mathcal{W}} L(w, q) \right\}. \quad \text{(constraining } q = q')
\]

Note that \( L(w, q) = q(s_0, \pi) + L_q(w, q) \), therefore,

\[
\sup_{w \in \mathcal{W}} L(w, q) - \inf_{w \in \mathcal{W}} L(w, q) = \sup_{w \in \mathcal{W}} L_q(w, q) - \inf_{w \in \mathcal{W}} L_q(w, q) \leq 2 \sup_{w \in \mathcal{W}} |L_q(w, q)|.
\]

When \( w_{\pi/\mu} \in \mathcal{W} \), \( \text{UB}_q \leq \text{LB}_q \) follows from the fact that \( L_q(w, q) \equiv 0 \), \( \forall w \).

Appendix B. Comparison to Naïve CIs

We discuss in further details here why our upper and lower bounds are tighter than the naïve ones from Liu et al. (2018); Uehara et al. (2019) (see Table 1 and Remark 3). We compare \( \text{UB}_q \) and \( \text{UB}'_q \) as an example, and the situation for the other pairs of bounds are similar.

Recall that the upper bound derived from MQL (Uehara et al., 2019) is

\[
\text{UB}'_q = \hat{q}(s_0, \pi) + \inf_{q \in \mathcal{Q}} \sup_{w \in \mathcal{W}} \left| \mathbb{E}_w[L_q(w, q)] \right|,
\]

(20)

where \( L_q(w, q) := \mathbb{E}_w[r + \gamma q(s', \pi) - q(s, a)] \), and \( \hat{q} = \arg \min_{q \in \mathcal{Q}} \sup_{w \in \mathcal{W}} \left| L_q(w, q) \right| \). In comparison, our bound is

\[
\text{UB}_q = \inf_{q \in \mathcal{Q}} \sup_{w \in \mathcal{W}} \left( q(s_0, \pi) + L_q(w, q) \right).
\]

(21)

Both bounds are valid upper bounds with realizable \( \mathcal{Q} \). Below we show that our upper bound is never higher than its naïve counterpart (this result does not require realizable \( \mathcal{Q} \)).
Proposition 12. $\mathrm{UB}_q \leq \mathrm{UB}_q'$.

Proof.

\[
\begin{align*}
\mathrm{UB}_q &= \inf_{q \in \mathbb{Q}} \left( q(s_0, \pi) + \sup_{w \in \mathbb{W}} L_q(w, q) \right) \\
&\leq \hat{q}(s_0, \pi) + \sup_{w \in \mathbb{W}} L_q(w, \hat{q}) \\
&\leq \hat{q}(s_0, \pi) + \sup_{w \in \mathbb{W}} |L_q(w, \hat{q})| \\
&= \hat{q}(s_0, \pi) + \inf_{q \in \mathbb{Q}} \sup_{w \in \mathbb{W}} |L_q(w, q)| = \mathrm{UB}_q'.
\end{align*}
\]

Remark 7. As we can see, the tightness of $\mathrm{UB}_q$ comes from two sources: (1) that we perform a unified optimization and put $q(s_0, \pi)$ inside $\inf_{q \in \mathbb{Q}}$ (reflected in Eq.(22)), and (2) that we do not need the absolute value in our objective (reflected in Eq.(23)). On the other hand, if $\mathbb{W}$ is symmetric—that is, $-w \in \mathbb{W}, \forall w \in \mathbb{W}$—then we only enjoy the first kind of tightness.\(^{17}\)

Remark 8. $\mathrm{UB}_q = \mathrm{UB}_q'$ requires $\sup_{w \in \mathbb{W}} L_q(w, \hat{q}) = \sup_{w \in \mathbb{W}} |L_q(w, \hat{q})|$ as a necessary condition. Similarly, one can show that $\mathrm{LB}_q = \mathrm{LB}_q'$ requires $-\inf_{w \in \mathbb{W}} L_q(w, \hat{q}) = \sup_{w \in \mathbb{W}} |L_q(w, \hat{q})|$. Therefore, as long as

\[-\sup_{q \in \mathbb{Q}} \inf_{w \in \mathbb{W}} L_q(w, q) \neq \inf_{q \in \mathbb{Q}} \sup_{w \in \mathbb{W}} L_q(w, q),\]

at least one side of our CI will be strictly tighter than before.

Appendix C. Experiments

C.1 Environment and Behavior & Target Policies

We conduct experiments in the CartPole environment and we consider the infinite-horizon discounted case and set $\gamma = 0.99$. Following Uehara et al. (2019), we modify the reward function and add small Gaussian noise to transition dynamics to make OPE more challenging in this environment.\(^{18}\) To generate the behavior and the target policies, we apply softmax on a near-optimal $Q$-function trained via the open source code\(^{19}\) of DQN with an adjustable temperature parameter $\tau$:

\[
\pi(a | s) \propto \exp(\frac{Q(s,a)}{\tau}).
\]

The behavior policy $\pi_b$ is chosen as $\tau = 1.0$, and we use other values of $\tau$ for target policies. To collect the dataset, we truncate the generated trajectories at the 1000-th time step. For those terminated within 1000 steps, we pad the rest of the trajectories with the terminal states. We treat $\mu = d^\pi$ and approximate such a data distribution by weighting each data point $(s, a, r, s')$ with a weight $\gamma^t$, where $t$ is the time step $s$ is observed.

\(^{17}\) This is because $L_q(w, q)$ is linear in $w$, and Eq.(23) becomes an identity.

\(^{18}\) Many policies are indistinguishable under the original 0/1 reward function, so we define an angle-dependent reward function that takes numerical values. We also add random noise to make the transitions stochastic.

\(^{19}\) https://github.com/openai/baselines
C.2 Details of the Algorithms

We compare UB\(_q\) and LB\(_q\) to UB\(_q^\prime\) and LB\(_q^\prime\) in Table 1. We use Multilayer Perceptron (MLP) to construct \(Q\) and \(W\). The detailed specification of \(Q\) will be given later. For \(W\), the ideal choice denoted by \(W^\alpha\) is defined as:

\[
W^\alpha = \{ w(\cdot, \cdot) = \frac{\alpha |f(\cdot, \cdot)|}{E_\mu[|f|]} \mid f \in \text{MLP} \}.
\]

Note that normalizing with \(E_\mu[|f|]\) allows us to directly control the expectation of any \(w \in W\) to be \(\alpha\), which is a hyper-parameter. However, directly optimizing over \(W^\alpha\) is quite unstable, and we consider the following relaxation of our upper and lower bounds: fixing any \(q \in Q\), for any \(w \in W^\alpha\), we relax the \(E_w[r + \gamma q(s', \pi) - q(s, a)]\) term in UB\(_q\) as

\[
E_w[r + \gamma q(s', \pi) - q(s, a)] = E_\mu[(r + \gamma q(s', \pi) - q(s, a)) \frac{\alpha |f|}{E_\mu[|f|]}] \\
\leq E_\mu[(r + \gamma q(s', \pi) - q(s, a)) \frac{\alpha |f|}{E_\mu[|f|]}] \\
= E_\mu[(r + \gamma q(s', \pi) - q(s, a)) I[r + \gamma q(s', \pi) - q(s, a) > 0] \frac{\alpha |f|}{E_\mu[|f|]}] \\
\leq E_\mu[(r + \gamma q(s', \pi) - q(s, a)) \frac{\alpha |f[I[r + \gamma q(s', \pi) - q(s, a) > 0]|}{E_\mu[|f[I[r + \gamma q(s', \pi) - q(s, a) > 0]|]}].
\]

So essentially we turn each \(f\) into a weighting function \(w\) that evaluates to \(\frac{\alpha |f[I[r + \gamma q(s', \pi) - q(s, a) > 0]|}{E_\mu[|f[I[r + \gamma q(s', \pi) - q(s, a) > 0]|]}\) on each data point \((s, a, r, s')\). Such a relaxation results in a (slightly) looser upper bound compared to UB\(_q\), which is still valid as long as UB\(_q\) is a valid upper bound. We similarly relax the lower bound by replacing \(I[r + \gamma q(s', \pi) - q(s, a) > 0]\) with \(I[r + \gamma q(s', \pi) - q(s, a) < 0]\), and again obtain a slightly looser lower bound.

In addition, although optimizing MQL loss with \(W^\alpha\) can converge, we find that using the same relaxation can further stabilize training and lead to better results. Therefore, we adopt this trick in the calculation of UB\(_q^\prime\) and LB\(_q^\prime\) as well.

We use a \(32 \times 32\) MLP (with tanh activation) to parameterize \(q\) and use a one-hidden-layer MLP with 32 units for \(f\) (which produces \(w\)). Moreover, we clip \(q\) in the interval \([\frac{R_{\min}}{1-\delta} \frac{R_{\max}}{1-\delta}]\), where \(R_{\min} = 0.0, R_{\max} = 3.0, \delta = 50\). We use stochastic gradient descent ascent (SGDA) with minimatches for optimization, and alternate between \(q\) and \(w\) every 500 iterations. The learning rates are both fixed as 0.005, and each minibatch consists of 500 transition tuples. The normalization factor in the relaxed objective is approximated on the minibatch. During the \(q\)-optimization phases, the weights \(w\) (which depends on \(q\) through the indicators) is treated as a constant and does not contribute to the gradients, but is re-computed every time \(q\) is updated.