A Theoretical Framework of
Almost Hyperparameter-free Hyperparameter Selection Methods for
Offline Policy Evaluation

Kohei Miyaguchi
IBM Research - Tokyo
miyaguchi@ibm.com

Abstract
We are concerned with the problem of hyperparameter selection of offline policy evaluation (OPE). OPE is a key component of offline reinforcement learning, which is a core technology for data-driven decision optimization without environment simulators. However, the current state-of-the-art OPE methods are not hyperparameter-free, which undermines their utility in real-life applications. We address this issue by introducing a new approximate hyperparameter selection (AHS) framework for OPE, which defines a notion of optimality (called selection criteria) in a quantitative and interpretable manner without hyperparameters. We then derive four AHS methods each of which has different characteristics such as convergence rate and time complexity. Finally, we verify effectiveness and limitation of these methods with a preliminary experiment.

1 Introduction
Offline policy evaluation (OPE) is an indispensable component of the offline reinforcement learning (RL), which is a variant of reinforcement learning with special emphasis on cost-sensitive real-life applications (Levine et al. 2020), such as autonomous vehicles, finance, healthcare and molecular discovery.

Almost all the offline RL algorithms involve their own hyperparameters. For example, if we employ neural networks in policy learning, we have to at least decide the network topology (e.g., number of neurons and layers), to use the residual connection or not, to use the dense connection or the convolution), the activation functions, regularization weights and the optimizers (e.g., SGD or Adam with their own hyperparameter choices). The choice of the models such as neural network is also considered to be a hyperparameters. OPE allows us optimize or validate the choices over these hyperparameters based only on offline datasets. This is especially useful if test run in the target environment is expensive.

However, with the current form of OPE, we end up with another hyperparameter selection problem (Paine et al. 2020). Note that one must employ a higher-order hyperparameter selection scheme to resolve it and there is no apparent reason to expect such a higher-order problem to be easier than that of the lower-order problem, i.e., offline RL.

In this paper, we seek for the OPE methods that requires no hyperparameter. In particular, we consider a class of OPE algorithms generalizing Fitted Q Evaluation (FQE) (Le, Voloshin, and Yue 2019) and derive four hyperparameter selection methods (Table 1) for it based on a newly introduced framework called approximate hyperparameter selection (AHS). Differences in their characteristics of consistency and computational time are investigated theoretically and empirically.

In Section 2, we formally introduce the notion of OPE, FQE and hyperparameter selection for FQE. Then, in Section 3, we present the main results, namely the AHS framework and its instantiations. We empirically demonstrate effectiveness and limitation of the proposed methods in Section 4. Finally, we discuss previous result in the literature in Section 5 and present some concluding remarks in Section 6.

All the proofs of the propositions in this paper is given in the appendix.

2 Preliminary
Let \( P(\mathcal{X}) \) denote the space of probability distributions on \( \mathcal{X} \), where \( \mathcal{X} \) is an arbitrary measure space. The order notation \( \mathcal{O}(\cdot) \) is used to hide universal multiplicative constants in the limit of \( n \to \infty \), where \( n \) is the data size. Let \( \| \cdot \|_p \) denotes the \( L^p(\mu) \)-norm of functions defined over \( S \times A \), where \( \mu \), \( S \) and \( A \) are defined in Section 2.1. We assume \( S \times A \) is a compact measurable space and \( \text{supp}(\mu) = S \times A \).

2.1 Offline Policy Evaluation (OPE)

The goal of OPE is to estimate the value of given policy \( \pi \), \( J(\pi) \), with respect to the sequential decision making in the environment of interest \( \mathcal{M} \).

The policy value \( J(\pi) \) quantifies the expected rewards obtained within some time horizon by sequentially taking action according to policy \( \pi \). It is formally defined as

\[
J(\pi) := \mathbb{E}^{\pi} \left[ \sum_{h=1}^{H} \gamma^{h-1} r_h \right],
\]

where \( H \geq 1 \) and \( \gamma \in [0, 1] \) respectively denote the time horizon parameter and the discounting factor that determine
how far in the future the rewards are taken into account as the value. The sequence \( \{r_h\}_{h \geq 1} \) denotes the rewards generated with the policy \( \pi \) and the environment \( \mathcal{M} \). The symbol \( E^\pi \) represents the expectation operator, highlighting the dependency on \( \pi \). Let \( S \) and \( A \) be the suitably-defined state space and action space, respectively. We assume the policy is identified with a state-conditional action distribution \( \mathcal{S} \ni s \mapsto (s, a) \in \mathcal{P}(A) \) and the environment is a Markov decision process (MDP) \( \mathcal{M} \equiv (S_1, R, T) \), where \( S_1 \in \mathcal{P}(S) \), \( R(s, a) \in \mathcal{P}([0, 1]) \) and \( T(s, a, t) \in \mathcal{P}(S) \) respectively denote the initial state distribution, the conditional reward distribution and the conditional succeeding-state distribution given state-action pair \((s, a) \in S \times A\). Thus, the rewards are subject to the following chain of distributional equations, \( s_1 \sim S_1, a_h \sim \pi(s_h), r_h \sim R(s_h, a_h), s_{h+1} \sim T(s_h, a_h), h \geq 1 \).

The major constraint of OPE is that the environmental parameters \((T, R)\) are unknown and \( J(\pi) \) must be inferred with an offline dataset \( D \). We assume the dataset consists of \( n \) transition tuples \( D \equiv \{(s_i, a_i, r_i, s_{i+1})\}_{i=1}^n \) sampled with an unknown query distributions \( \mu \) such that \((s_i, a_i) \sim \mu, r_i \sim R(s_i, a_i), s_{i+1} \sim T(s_i, a_i), 1 \leq i \leq n \). We sometimes abuse the notation and write \((s_i, a_i, r_i, s_{i+1}) \sim \mu \) and \( D \sim \mu^n \).

Finally, we introduce a common assumption of OPE, the condition of sufficient exploration.

\textbf{Assumption 1 (Sufficient exploration).} For \( 1 \leq h \leq H \), the distribution of \((s_h, a_h)\) is absolutely continuous with respect to \( \mu \), where the Radon–Nikodym derivative is denoted by \( \rho_h(s, a) \).

In other words, it is guaranteed the data distribution \( \mu \) has positive measure on any measurable events \( E \subset S \times A \) that can be happened to the target state-action pairs \((s_h, a_h)\) at some time steps \( 1 \leq h \leq H \). Note that this assumption is significantly relaxed if we know a parametric model of MDPs that contains the environment \( \mathcal{M} \), such as linear MDPs (e.g., Assumption 1 in [Duan, Jia, and Wang 2020]). However, we do not assume we know such models in the present study as our goal is to select the best model from data, not from domain knowledge.

\subsection{2.2 Fitted Q-Evaluation (FQE)}

The fitted Q-evaluation is a simple OPE algorithm proposed by [Le, Voloshin, and Yue 2019]. It solves a slightly more general problem than OPE, the estimation of the action-value function. The action-value function \( Q^\pi(s, a) \) quantifies the value of taking given action \( a \in A \) at given state \( s \in S \) and then following the policy \( \pi \) to make all the subsequent decisions. It is formally defined as

\[ Q^\pi(s, a) := E^\pi \left[ \sum_{h=1}^{H} \gamma^{h-1} r_h \bigg| s_1 = s, a_1 = a \right]. \]

Note that the policy value \( J(\pi) \) is computable with \( Q^\pi \),

\[ J(\pi) = \bar{J}(Q^\pi) := E[Q^\pi(s_1, \pi(s_1))]. \]

FQE is derived from the recursive property of \( Q^\pi \). More specifically, the action-value function \( Q^\pi \) is known to be satisfying the Bellman equation, \( Q_{h}^\pi = B_{h}Q_{h-1}^\pi, h \geq 1 \), where \( Q_{h}^\pi \) is the action-value function with the time horizon set to \( H = h \) and \( B_{h} \) is the Bellman operator given by

\[ (B_{h}f)(s, a) := E[R(s, a) + \gamma f(s', \pi(s')) | s' \sim T(s, a)], \]

for \( f : S \times A \rightarrow \mathbb{R}, s \in S \) and \( a \in A \). This implies by induction

\[ Q^\pi = Q_{H}^\pi = B_{H}0 = B_{H}(B_{H-1}0) = \cdots = B_{H}(B_{H-1}0). \]

Therefore, a natural idea to estimate \( Q^\pi \) is to construct an approximate Bellman operator \( X \approx B_{e} \) and then apply it to the zero function \( H \) times to obtain the action-value function estimate \( X^{H}0 \approx Q^\pi \). We refer to this abstract procedure as MetaFQE (Algorithm 1). FQE is derived with one of the most natural implementations of \( X \), the least-squares regression operator,

\[ X_{\text{FQE}}(\pi, D; Q) : f \mapsto \arg\min_{\theta \in Q} \sum_{(s, a, r, s') \in D} \left| r + \gamma f(s', \pi(s')) - g(s, a) \right|^2. \]
Algorithm 1: Meta Fitted Q-Evaluation (MetaFQE)

Input: Approximate Bellman operator $X$.
Output: Action value function estimate $Q^X$.
1: $Q^X_0 = 0$.
2: for $h = 1, 2, ..., H$ do
3: $Q^X_h := XQ^X_{h-1}$
4: Return $Q^X := Q^X_H$.

with $Q$ being a hypothetical set of action-value functions.

Note that FQE has a hyperparameter $Q$ that heavily influences the output of the algorithm. It is usually given as a parametric model of functions such as linear functions and neural networks. Moreover, practical implementations of the FQE operator often involve a number of hyperparameters other than $Q$ such as regularization terms and optimizers.

### 2.3 Hyperparameter Selection for MetaFQE

Observe that a single hyperparameter configuration of FQE is corresponding to a single operator $X$. Hence, the hyperparameter selection of FQE is equivalent to select the best operator $X_*$ from given candidates of operators $X$. Generalizing this idea, we first introduce the scope of operators $\Omega$ from which the candidate sets $X$ are taken.

**Definition 1** (Range-bounded operators). Let $C := \sum_{h=1}^{H} \gamma^{h-1}$. Let $\Omega$ denote the set of all the operators on $[0, C]$-valued functions over $S \times A$.

$$\Omega := \{ X : [0, C]^{S \times A} \rightarrow [0, C]^{S \times A} \} .$$

The restriction on the range boundedness is justified since the true action-value functions $Q_h^X$, $1 \leq h \leq H$, are all bounded to $[0, C]^{S \times A}$. Note that one can modify any $X$ to satisfy the boundedness by composing it with a clipping function, $\hat{X} = \text{clip} \circ X$, where $\text{clip}(f)(s, a) := \max\{0, \min\{C, f(s, a)\}\}$, $s \in S, a \in A$.

Our goal is formally defined as solving the following problem.

**Problem 1** (Ideal hyperparameter selection for FQE). Given $\pi, D$ and $X \subset \Omega$ with $|X| < \infty$, find $X_* \in X$ such that

$$|\Delta J(Q^{X_*})| = \min_{X \in \Omega} |\Delta J(Q^X)| ,$$

where $Q^X := X^H Q$ is the $Q$-function and $\Delta J(Q^X) := J(Q^X) - J(\pi)$ is the OPE error associated with $X \in \Omega$.

Without loss of generality, we assume each $X \in X$ is independent of $D$. Although the operators are often learned from the dataset as in FQE, the independence is guaranteed with the training-validation split $D = D_{\text{train}} + D_{\text{valid}}$. The subsequent analyses and discussions are also applicable to this setting simply by replacing $D$ with $D_{\text{valid}}$.

### 3 Method

#### 3.1 Approximate Hyperparameter Selection Framework

Problem 1 cannot be always solved since the OPE error $|\Delta J(Q^X)|$ is difficult to estimate in general. As such, we introduce a relaxation of Problem 1 namely the approximate hyperparameter selection (AHS) problem. To this end, we first present the notions of the selection criteria and the optimality of choices.

**Definition 2** (Selection criterion). A function $C : \Omega \rightarrow \mathbb{R}$ is said to be a selection criterion when the following conditions are met.

1. For all $X \in \Omega$, $|\Delta J(Q^X)| \leq C(X)$.
2. $C(B_\pi) = 0$.

**Definition 3** ($C$-optimal choice). Let $X \subset \Omega$ be a set of candidate operators and $C$ be any selection criterion. Let $X = X(\pi, D) \in X$ represent a possibly random choice from $X$, i.e., an $X$-valued random variable. We say a choice $\hat{X} \in X$ is optimal with respect to $C$, or $C$-optimal, if

$$|\Delta J(Q^{\hat{X}})| \leq \min_{X \in \Omega} C(X) + o_P(1),$$

where $o_P(1)$ denotes a diminishing term, $\mathbb{P}\{|o_P(1)| > \epsilon\} \rightarrow 0$ for all $\epsilon > 0$. Equivalently, $\hat{X}$ is $C$-optimal if it achieves asymptotically zero $C$-suboptimality in probability,

Subopt($\hat{X}; X, C$) $\rightarrow P$ 0, where the suboptimality is defined as

Subopt($\hat{X}; X, C$) := max $\left\{ 0, |\Delta J(Q^{\hat{X}})| - \min_{X \in \Omega} C(X) \right\}$.

Now, we are ready to define a relaxation of Problem 1.

**Problem 2** ($C$-approximate hyperparameter selection (C-AHS)). Let $C$ be a given selection criterion. For given $\pi, D$ and $X$ with $|X| < \infty$, find a $C$-optimal choice $\hat{X} = X(\pi, D) \in X$.

A few remarks follow in order. Firstly, C-AHS is in fact a relaxation of Problem 1. This is seen from that, in [2], we have weakened the solution condition replacing the RHS of [2] with a probabilistic upper bound, $\min_{X \in \Omega} |\Delta J(Q^X)| \leq \min_{X \in \Omega} C(X) + o_P(1)$. Specifically, all the solutions $X_*$ of Problem 1 have zero $C$-suboptimality with any $C$.

Secondly, the solutions of C-AHS are asymptotically consistent. If the candidate set $X$ happens to contain the true operator $B_\pi$ and $\hat{X}$ is $C$-optimal, we have $|\Delta J(Q^{\hat{X}})| \rightarrow 0$ in probability. Moreover, the OPE error of $\hat{X}$ is exactly characterized by the $C$-suboptimality, $|\Delta J(Q^{\hat{X}})| = \text{Subopt}($$\hat{X}; X, C$).

Thirdly, if $X$ does not contain the true operator, the quality of the solutions depends on the tightness of the criterion $C$ as a function. As a tightest example, suppose we have a selection criterion $C^{\text{tight}}$ such that $C^{\text{tight}}(X) \leq c |\Delta J(Q^X)|$, where $1 \leq c < \infty$ is a constant measuring the tightness. Then it is easily seen $|\Delta J(Q^{\hat{X}})| \leq c |\Delta J(Q^{X^{\pi}})| + o_P(1)$, which implies Problem 1 is solved asymptotically with a constant approximation rate. On the other hand, the loosest possible criterion is given as $C^{\text{loose}}(X) := C^* I(X \neq B_\pi) + o_P(1)$. It gives no information on the goodness of $X$ if $X$ does not contain the true operator $B_\pi$. Generally speaking, if $C(X) \leq C^*(X)$ for all $X \in \Omega$, a solution to C-AHS is also a solution to C-AHS. Accordingly, solving $C^{\text{loose}}$-AHS
is easier than solving \( \mathcal{C}_{\text{tight}} \)-AHS. However, neither of these extreme cases is plausible in practice; the solutions of \( \mathcal{C}_{\text{tight}} \) is rarely tractable without domain knowledge and \( \mathcal{C}_{\text{loose}} \) is useless if \( B_\pi \not\subset \mathcal{X} \), which is likely the case in most practical scenarios. Thus, we construct criteria \( \mathcal{C} \) with tightness somewhere in between these extrema.

Finally, the values of criteria \( \mathcal{C}(X) \) themselves are not necessarily tractable. The minimum requirement is that we have an algorithm that choose \( \hat{X} \in \mathcal{X} \) that satisfies the optimality \( \mathcal{C} \). In fact, all the algorithms presented in this paper minimize computationally intractable criteria.

### 3.2 OPE Error Characterization

**Error Identity.** By Definition 2 the selection criteria should be upper bounds on the OPE error \( \Delta J(Q^X) \). It is desirable for the tractability of AHS (Problem 2) that the upper bounds are in some sense minimizable based on \( \mathcal{D} \). As such, understanding the relationship between \( \Delta J(Q^X) \) and \( X \) is useful to design such criteria. The following proposition characterizes the relationship.

**Proposition 1 (Error identity).** Let \( \Delta X := X - B_n \) be the Bellman residual operator of \( X \in \Omega \). Then, for all \( X \in \Omega \),

\[
\Delta J(Q^X) = \sum_{h=1}^H \gamma^{h-1} \mathbb{E} \left[ \| \Delta X Q_{h-1}^X \|_{\mathcal{F}_*} \right],
\]

where \( \{Q_h^X\}_{h=0}^H \) is defined by Algorithm 1.

**Proof.** See Section A.1.

It can be seen as a generalization of the telescoping lemma of model-based RL (Lemma 4.3 of Luo et al. 2019, Lemma 4.1 of Yu et al. 2020). As opposed to these results, Proposition 1 allows the approximate operator \( X \) to be those that admit no model-based interpretation.

**Error Bound.** Proposition 1 can be utilized to obtain a spectrum of upper bounds on \( \Delta J(Q^X) \). In particular, the following upper bounds are indexed with error-measuring Banach spaces \( \mathcal{F} \).

**Proposition 2 (Error bound).** Let \( \mathcal{F} \) be a dense Banach subspace of \( L^1(\mu) \). Then, under Assumption 2, we have

\[
|\Delta J(Q^X)| \leq \varphi_{\mathcal{F}} \left( \sum_{h=1}^H \gamma^{H-h} \| \Delta X Q_{h-1}^X \|_{\mathcal{F}_*} \right)
\]

for all \( X \in \Omega \). Here, \( \varphi_{\mathcal{F}} : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0} \) is a function called the link function of \( \mathcal{F} \), which is nonnegative, continuous, nondecreasing, concave and satisfying \( \varphi(0) = 0 \). \( \| \cdot \|_{\mathcal{F}_*} \) denotes the dual norm of \( \mathcal{F} \), given by

\[
\| g \|_{\mathcal{F}_*} := \sup_{\| f \|_{\mathcal{F}} \leq 1} \mathbb{E}_{(s,a)\sim \mu} [f(s,a)g(s,a)],
\]

where \( g : S \times A \to \mathbb{R} \).

**Proof.** See Section A.2.

Proposition 2 suggests the RHS of (4) can be used as a selection criterion. In particular, although the link function itself is intractable, its argument can be used to minimize the OPE error owing to the monotonicity. We refer to the argument of the link function,

\[
\tilde{C}_\pi(X) := \sum_{h=1}^H \gamma^{H-h} \| \Delta X Q_{h-1}^X \|_{\mathcal{F}_*},
\]

as the precriterion of \( X \) with respect to \( \mathcal{F} \). Note that minimizing the RHS of (4) is equivalent to minimizing the precriterion. Moreover, we have zero OPE error if \( \mathcal{C}_\pi(X) = 0 \) thanks to the boundary condition \( \varphi_{\mathcal{F}}(0) = 0 \). In other words, \( \mathcal{C} = \varphi_{\mathcal{F}} \circ \tilde{C}_\pi \) is a selection criterion and its minimization is possible if the minimization of the precriterion is.

Thus, to solve \( \mathcal{C} \)-AHS, we confine our focus to the construction of upper bounds on the precriterion.

### 3.3 Algorithms

Proposition 2 suggests a spectrum of OPE error bounds corresponding to different error-measuring Banach spaces \( \mathcal{F} \).

In general, there is a trade-off in the choice of \( \mathcal{F} \). If \( \mathcal{F} \) is more expressive, the link function \( \varphi_{\mathcal{F}} \) is smaller but the precriterion is larger. To see this, consider two Banach spaces \( \mathcal{F} \) and \( \mathcal{G} \) such that \( \| \cdot \|_{\mathcal{F}} \geq \| \cdot \|_{\mathcal{G}} \) (i.e., \( \mathcal{G} \) is more expressive than \( \mathcal{F} \)). Then, we have \( \tilde{C}_\pi(X) \leq \tilde{C}_\pi(X) \) for all \( X \in \Omega \) by the definition of the dual norm and \( \varphi_{\mathcal{F}}(y) \geq \varphi_{\mathcal{G}}(y) \) for all \( y \geq 0 \) by definition (see the proof of Proposition 2). Below, we discuss the algorithms induced by typical choices on \( \mathcal{F} \).

**A Failed Attempt.** The most trivial and most expressive choice of \( \mathcal{F} = L^1(\mu) \). In this case, the link function is explicitly calculated as \( \varphi_{L^1(\mu)}(y) = y \) for \( y \geq 0 \). However, the precriterion \( \tilde{C}_{L^1(\mu)} \) is difficult to estimate or minimize since the corresponding dual norms \( \| \Delta X Q_{h-1}^X \|_{\infty} \) are essential suprema.

**Regret Minimization (RM).** A slightly less expressive space is \( \mathcal{F} = L^2(\mu) \). Note that \( L^2(\mu) \) is dense in \( L^1(\mu) \). In this case, the dual space is itself, \( \mathcal{F}^* = \mathcal{F} \), and the precriterion is the sum of the \( L^2(\mu) \)-norms \( \| \Delta X Q_{h-1}^X \|_2 \). As shown below, the norms are simplified using the empirical Bellman residual, which is given by

\[
\hat{L}_{2,\mathcal{D}}^\pi(X; f) := \frac{1}{n} \sum_{(s,a,r,s',a') \in \mathcal{D}_\pi} (r + \gamma f(s', a') - (X(f)(s,a))^2,
\]

where \( \mathcal{D}_\pi := \{(s_i, a_i, r_i, s'_i, a'_i)\}_{i=1}^n \) denotes the \( \pi \)-enriched data, \( a'_i \sim \pi(s'_i), 1 \leq i \leq n \).

**Proposition 3 (Residual representation of \( L^2(\mu) \) precriterion).** For any \( f : S \times A \to \mathbb{R} \), we have

\[
\| \Delta X f \|_2^2 = \mathbb{E} \left[ \hat{L}_{2,\mathcal{D}}^\pi(X; f) - \hat{L}_{2,\mathcal{D}}^\pi(B_x; f) \right].
\]

**Proof.** See Section A.3.
Algorithm 2: FQE with Regret Minimization (FQE-RM)

**Input:** Enriched data \( D_e \), operator candidates \( \mathcal{X} \).

**Output:** Action-value estimate \( \hat{Q} \).

1. for \( k = 1, \ldots, |\mathcal{X}| \) do
2. \((\hat{Q}^k, \text{BRS}_k) := \text{MetaFQE-BRS}(\mathcal{X}, k, D_e)\);
3. \(k^* := \arg\min_{1 \leq k \leq |\mathcal{X}|} \text{BRS}_k\);
4. Return \( \hat{Q}^{k^*} \).

Note that the identity \([5]\) cannot be used directly to evaluate the precriterion \( C_{L^2(\mu)}(X, \mathcal{X}) \) since we have the true Bellman operator \( B_\pi \) on the RHS, which is unknown. Instead, we introduce a proxy loss called the Bellman regret,

\[
\text{Regret}^2_{\pi}(X; \mathcal{X}, f) := \hat{L}_{\pi, D}^2(X; f) - \min_{A \in \mathcal{X}} \hat{L}_{\pi, D}^2(A; f),
\]

which substitutes \( B_\pi \) with the best approximate operator in \( \mathcal{X} \). The Bellman regret is then used to compute the Bellman regret sum (BRS).

\[
\text{BRS}_{\pi}^2(X; \mathcal{X}) := \sum_{h=1}^{H} \gamma^{H-h} \sqrt{\text{Regret}^2_{\pi}(X; \mathcal{X}, Q_h^{X_{h-1}})},
\]

which approximate the precriterion \( C_{L^2(\mu)}(X) \). We refer to the minimization of BRS as Regret Minimization (RM). In fact, RM is shown to be optimal with a selection criterion

\[
C_2(X) := \varphi_{L^2(\mu)}(3C_2e_2(X)),
\]

where \( e_2(X) := \sup_{f \in [0,1]} \| \Delta f \|_2 \).

**Proposition 4** (Optimality of RM). Let \( \hat{X}_{\text{RM}} := \arg\min_{X \in \mathcal{X}} \text{BRS}_{\pi}^2(X; \mathcal{X}) \). Then, \( \hat{X}_{\text{RM}} \) is \( C_2 \)-optimal. The suboptimality is bounded by

\[
\text{Subopt}(\hat{X}_{\text{RM}}; \mathcal{X}, C_2) \leq \varphi_{L^2(\mu)} \left( 2C(1 + \gamma C) \left( \frac{2 \ln(2H|\mathcal{X}|^2/\delta)}{n} \right)^{1/4} \right) = O \left( C^2 \max_{1 \leq k \leq H} \| \rho_k \|_2 \left( \frac{\ln(2H|\mathcal{X}|^2/\delta)}{n} \right)^{1/4} \right),
\]

with probability \( 1 - \delta \), where \( \delta \in (0, 1) \).

**Proof.** See Section A.4.

Algorithm 2 (with Algorithm 3 as a subroutine) shows the OPE algorithm based on RM, which requires no hyperparameter other than the candidate set of operators \( \mathcal{X} \). Note that the computational complexity of RM is \( O(nHK^2) \), where \( n \) is the size of \( D \), \( H \) is the time horizon, and \( K \) is the cardinality of \( \mathcal{X} \) (i.e., the size of the hyperparameter grid).

**Dynamic Regret Minimization (DRM).** We also present a variant of Regret Minimization to achieve lower computational complexity in exchange with slower suboptimality convergence. The goal is the same as RM, i.e., the minimization of BRS, but we relax the domain of the minimization from static operators \( X \in \mathcal{X} \) to dynamic ones, denoted by \( X \). A dynamic operator \( X \) is identified with a sequence of operators \( X := (X_1, \ldots, X_H) \in \mathcal{X}^H \) and acts as \( X_h \) in the \( h \)-th iteration of MetaFQE. Consequently, the MetaFQE with \( X \) computes the cascading application of \( F \) on \( 0, \text{MetaFQE}(X) = Q_X \). Note that static operators \( X \in \mathcal{X} \) can be seen as constant dynamic operators \( X := (X, \ldots, X) \in \mathcal{X}^H \), hence it is relaxation.

The relaxation allows us to compute the regret minimizer \( \hat{X}_{\text{DRM}} := \arg\min_{X \in \mathcal{X}^H} \text{BRS}_{\pi}^2(X; \mathcal{X}) \) in \( O(nHK) \) time by a greedy algorithm (Algorithm 4). We refer to this algorithm as Dynamic Regret Minimization (DRM). In fact, DRM is shown to be \( C_2 \)-optimal.

**Proposition 5** (Optimality of DRM). Let \( \hat{X}_{\text{DRM}} = (X_{k,1}, \ldots, X_{k,H}) \) be the dynamic operator chosen by DRM. Then, \( \hat{X}_{\text{DRM}} \) is \( C_2 \)-optimal. The suboptimality is bounded by

\[
\text{Subopt}(\hat{X}_{\text{DRM}}; \mathcal{X}, C_2) \leq \varphi_{L^2(\mu)} \left( 2C(1 + \gamma C) \left( \frac{2 \ln(2H|\mathcal{X}|^2/\delta)}{n} \right)^{1/4} \right) = O \left( C^2 \max_{1 \leq k \leq H} \| \rho_k \|_2 \left( \frac{\ln(2H|\mathcal{X}|^2/\delta)}{n} \right)^{1/4} \right),
\]

with probability \( 1 - \delta \), where \( \delta \in (0, 1) \) and \( \| X \| := 1 + \sum_{h=1}^{H-1} \| X_h \neq X_{h+1} \| \) denotes the number of change points in \( X \).

**Proof.** See Section A.5.

Note that the convergence rate of the suboptimality is worsen by a factor of \( 1 \leq \| \hat{X}_{\text{DRM}} \| \leq H \), the number of change points in \( \hat{X}_{\text{DRM}} \).

**Kernel Loss Minimization (KLM).** As an even less expressive example, we take \( \mathcal{F} \) as the reproducing kernel Hilbert space (RKHS). An RKHS is dense in \( L^1(\mu) \) if the corresponding kernel \( k(\cdot, \cdot) \) is universal, e.g., Gaussian kernels. The following proposition gives a useful identity of the RKHS precriterion based on the kernel.
Algorithm 4: FQE with Dynamic Regret Minimization (FQE-DRM)

Input: Enriched data $D_e$, operator candidates $\mathcal{X} = \{X_k\}_{k=1}^K$.

Output: Action-value estimate $\hat{Q}$.
1: $Q_0 := 0$;
2: for $h = 1, ..., H$ do
3: $y_i := r_i + \gamma Q_{h-1}(s_i', \tilde{a}_i')$, $1 \leq i \leq n$;
4: for $k = 1, ..., K$ do
5: $f^k_h := \frac{1}{n} \sum_{i=1}^{n} (y_i - f_i^k(s_i, \tilde{a}_i))^2$;
6: $k^*_h := \arg\min_{k \leq K} f^k_h$;
7: $Q_h := f_{k^*_h}$;
8: Return $Q_H$.

Assumption 2 (Kernel function). $\kappa : (\mathcal{S} \times \mathcal{A})^2 \to \mathbb{R}_{\geq 0}$ is a universal kernel function on $\mathcal{S} \times \mathcal{A}$ that is continuous, symmetric, positive definite and normalized, i.e., $\sup_{u \in \mathcal{S} \times \mathcal{A}} \kappa(u, u) \leq 1$.

Proposition 6 (Kernel representation of RKHS precriterion). Let $\mathcal{F}_\kappa$ be the RKHS generated by $\kappa$. Then, for any $f : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$, we have

$$\|f\|^2_{\mathcal{F}_\kappa} = \mathbb{E}_{u, \tilde{u} \sim \mu} \left[ \kappa(u, \tilde{u}) f(u) f(\tilde{u}) \right].$$

Proof. See Section $\alpha$.6

To approximate the dual norm on the RHS of $\phi_\kappa$ based on the data $D$, we introduce the operator kernel Bellman statistic,

$$\text{KBS}^\kappa_{\kappa, D}(X; f) := \frac{1}{n^2} \sum_{(u, r, u') \in D_e} \left[ \kappa(u, \tilde{u}) \times \right.$$

$$\left. (r + \gamma f(r') - X f(u')) \{\tilde{r} + \gamma f(\tilde{u}') - X f(\tilde{u})\} \right],$$

where $(u, r, u') \in D_e$ indicates $u$ is a state-action pair before transition in $D$, $r$ is the corresponding reward, and $u'$ is the pair of the state after transition and the action drawn from $\pi$. Summing up the kernel Bellman statistics, we have the kernel Bellman loss

$$\text{KBL}^\kappa_{\kappa, D}(X; \kappa) := \sum_{h=1}^{H} \gamma^{H-h} \sqrt{\text{KBS}^\kappa_{\kappa, D}(X; Q_{h-1}^X)}$$

as an approximation of $\hat{C}_\kappa(X)$. We refer to the minimization of KBL as Kernel Loss Minimization (KLM). In fact, KLM is optimal with respect to a criterion $C_\kappa(X) := \phi_\kappa \circ \hat{C}_\kappa(X)$.

Proposition 7 (Optimality of KLM). Let $\hat{X}_{\text{KLM}(\kappa)} := \arg\min_{X \in \mathcal{X}} \text{KBL}^\kappa_{\kappa, D}(X; \kappa)$. Then, $\hat{X}_{\text{KLM}(\kappa)}$ is $C_\kappa$-optimal.

Algorithm 5: FQE with Kernel Loss Minimization (FQE-KLM)

Input: Enriched data $D_e$, operator candidates $\mathcal{X} = \{X_k\}_{k=1}^K$.

Output: Action-value estimate $\hat{Q}$.
1: for $k = 1, ..., K$ do
2: $(Q^k, \text{KBL}_k) := \text{MetaFQE-KBL}(X_k, D_e, \kappa)$;
3: $k^* := \arg\min_{k \leq K} \text{KBL}_k$;
4: Return $Q^{k^*}$.

Algorithm 6: KBL computation (MetaFQE-KBL)

Input: Operator $X$, enriched data $D_e$, kernel $\kappa$.

Output: Action-value estimate $Q^{X_{k^*}}$, kernel Bellman loss $\text{KBL}^\kappa_{\kappa, D}(X_k; \kappa)$.
1: $Q_0 := 0$;
2: $\text{KBL}_0 := 0$;
3: $\kappa_{ij} := \kappa(s_i, \tilde{a}_i, (s_j, \tilde{a}_j))$, $1 \leq i, j \leq n$;
4: for $h = 1, ..., H$ do
5: $Q_h := XQ_{h-1}$;
6: $\epsilon_i := r_i + \gamma Q_{h-1}(s_i', \tilde{a}_i') - Q_h(s_i', \tilde{a}_i')$, $1 \leq i \leq n$;
7: $\text{KBL}_h := \text{KBL}_{h-1} + \gamma^{H-h} \frac{1}{n^2} \sum_{i, j=1}^{n} \epsilon_i \kappa_{ij}$;
8: Return $Q_H$ and $\text{KBL}_H$.

The suboptimality is bounded by

$$\text{Subopt}(\hat{X}_{\text{KLM}(\kappa)}; \mathcal{X}, C_\kappa) \leq \varphi_{\mathcal{F}_\kappa} \left( 2C(1 + \gamma C) \left( \frac{4 \ln(2H |\mathcal{X}| / \delta)}{n} \right)^{1/4} \right) = O \left( C^2 \max_{1 \leq h \leq H} \|\rho_h\|_{\mathcal{F}_\kappa} \left( \frac{\ln(H |\mathcal{X}| / \delta)}{n} \right)^{1/4} \right)$$

with probability $1 - \delta$, where $\delta \in (0, 1)$.

Proof. See Section $\alpha$.7

Algorithm 5 (with Algorithm 6 as a subroutine) shows the OPE algorithm based on KLM. It requires a universal kernel $\kappa$ as a hyperparameter. Note that the computational complexity of KLM is $O(n^2HK)$.

Kernel Loss Minimization over Q-Functions (KLM-\kappa).

Finally, we present a variant of KLM for infinite horizon case, $H = \infty$ and $\gamma < 1$. Note that none of FQE-RM, FQE-DRM and FQE-KLM cannot be applied to this setting since their number of the FQE iteration is equal to $H$.

Now observe that KLM only requires $X \in \mathcal{X}$ to be evaluated at $\{Q_{h-1}^X\}_{h=1}^{H}$, which is in contrast with RM or DRM evaluating $X$ on $\{Q_{h-1}^X : 1 \leq h \leq H, X' \in \mathcal{X}\}$. This implies that, FQE-KLM also accept the sequence of Q-functions $\{Q_{h}^X\}_{h=1}^{H}$ as a representation of $X$.

The idea is to further compress the representation by computing the kernel loss only on the last Q-function $Q_H^X$. This is justified if the sequence $\{Q_0^X, Q_1^X, Q_2^X, \ldots\}$ is converging since the kernel losses at the initial steps $h$ are discounted by factors of $\gamma^{H-h}$, which is zero if $H = \infty$.
**Algorithm 7: Kernel Loss Minimization over Q-Functions (KLMQ)** [Feng, Li, and Liu 2019]

**Input:** Enriched data $D_r$, Q-function candidates $\{Q_k\}_{k=1}^K$, kernel $\kappa$.

**Output:** Action-value estimate $\hat{Q}$.

1. $\kappa_{ij} := \kappa((s_i, a_i), (s_j, a_j))$, $1 \leq i, j \leq n$.
2. for $k = 1, ..., K$ do
3. $\epsilon_i := \tilde{r}_i + \gamma Q(\tilde{s}_i, \tilde{a}_i) - Q_k(\tilde{s}_i, \tilde{a}_i), 1 \leq i \leq n$;
4. KBSQ$_k$ := $\frac{1}{n} \sum_{i,j=1}^{n} \epsilon_k \kappa_{ij}$;
5. $k^* := \arg \min_{1 \leq k \leq K} \text{KBSQ}_k$;
6. Return $Q_{k^*}$.

Formally, we minimize the Q-function kernel Bellman statistics KBSQ$_{\kappa, D}(f)$ over $f \in \{Q^X : X \subset \mathcal{X}\}$, where

$$KBSQ_{\kappa, D}(f) := \frac{1}{n} \sum_{(u, \tilde{u}) \in D_r} \left[ \kappa(u, \tilde{u}) \times \{r + \gamma f(u') - f(u)\} \{\tilde{r} + \gamma f(\tilde{u'}) - f(\tilde{u})\} \right],$$

which is originally proposed by [Feng, Li, and Liu 2019] as the kernel Bellman V-statistic. We refer to this selection algorithm as Kernel Loss Minimization over Q-Functions (KLMQ). Algorithm 7 shows the OPE based on KLMQ. The following proposition shows the optimality of KLMQ.

**Proposition 8** (Optimality of KLMQ). Assume $H = \infty$ and $\gamma < 1$. Also assume $Q^X = Q^X = \lim_{t \to \infty} Q^X$ exists for all $X \in \mathcal{X}$. Let $\hat{X}_{\text{KLMQ}(\kappa)} := \arg \min_{X \subseteq \mathcal{X}} \text{KBSQ}_{\kappa, D}(Q^X)$. Then, $\hat{X}_{\text{KLMQ}(\kappa)}$ is $C_r$-optimal. The suboptimality is bounded by

$$\text{Subopt}(\hat{X}_{\text{KLMQ}(\kappa)}; \mathcal{X}, C_r) \leq \varphi_{C_r} \left(2C(1 + \gamma C) \left(4 \ln(2 |X| / \delta) \vee \frac{1}{n}\right)^{1/4} \right)$$

$$= O \left(C^2 \max_{1 \leq k \leq H} \|\rho_k\|_{F} \left(\ln(|X| / \delta) / n\right)^{1/4}\right)$$

with probability $1 - \delta$, where $\delta \in (0, 1)$.

**Proof.** See Section A.8

Note that, in practice, it is impossible to find the exact Q-function $Q^X = Q^X$ given $X$. Instead, one may employ the FQE with finite iterations $\hat{H} < \infty$ to get an approximation $Q_{\hat{H}}^X \approx Q^X$. However, as KLMQ requires $Q^X$ rather than $X$ itself as the representation of hyperparameters, one can include $\hat{H}$ as an additional hyperparameter and select the best combination of $(X, \hat{H})$ with KLMQ. Moreover, it is also possible to select among different Q-function estimation algorithms other than FQE.

**3.4 Comparison of Algorithms**

We have derived four hyperparameter selection algorithms for OPE, namely, RM, DRM, KLM and KLMQ. In this section, we discuss their properties in a comparative manner with different perspectives (see Table 1).

**Distribution-shift tolerance.** The first property is the distribution-shift tolerance. Specifically, the $L^2(\mu)$-type selection methods (RM and DRM) have better convergence guarantee on the suboptimality than those of the kernel type (KLM and KLMQ) if there is large mismatch between the state-action distributions of the target episode $\{(s_h, a_h) \sim \mu_h\}_{h=1}^H$ and the offline data $\{(\tilde{s}_i, \tilde{a}_i) \sim \mu_{\tilde{X}}\}_{i=1}^n$. This can be seen from the domination in the leading coefficients of the upper bounds, $\|\rho_h\|_2 \leq \|\rho_h\|_{\text{KBSQ}}$ (see the column of Suboptimality Bound in Table 1). For example, consider $\kappa$ as a Gaussian kernel with $S \times \mathcal{A}$ being a subset of a Euclidean space $\mathbb{R}^d$. Then, if the density ratio $\rho_h$ is bounded but discontinuous, we have $\|\rho_h\|_2$ finite but $\|\rho_h\|_{\text{KBSQ}}$ infinite. In general, there is significant difference in the convergence rate if $\rho_h = \rho_h / \mu$ is non-smooth for some $1 \leq h \leq H$. Note, however, that the suboptimalties of KLM and KLMQ do converge with arbitrary non-smooth $\rho_h$, albeit slowly.

**Operator-error tolerance.** The second property is the operator-error tolerance. Specifically, KLM and KLMQ are guaranteed to select the best $X \in \mathcal{X}$ in terms of the resulting Q-functions $(Q_X^X)_{h=1}^H$ (with KLM) and $Q^X$ (with KLMQ) even if $X$ is totally incorrect as a uniform approximation of $B_C$ as an operator. This is not the case with RM and DRM, in which the error of $X$ is measured through $\epsilon(X) = \sup_{f} \|X f - B_C f\|_2$ with $f$ ranging over all $[0, C]$-bounded functions of $\mathcal{S} \times \mathcal{A}$. See the column of Sufficient Stats. in Table 1. Summing up, the kernel-type methods have better guarantee than the $L^2(\mu)$-type when $X$ does not necessarily contains the true operator $B_C$.

**Time complexity.** For finite-horizon problems, RM and KLM have suboptimal time complexity of $O(nHK^2)$ and $O(n^2HK)$, respectively. On the other hand, DRM has the optimal time complexity $O(nHK)$. This makes DRM most handy in practice, but it may require more samples than necessary to obtain reliable results in the long time horizon problems due to the extra multiplicative factor $H^{1/4}$ in the suboptimality bound. For infinite horizon problems, only KLMQ out of four is applicable. KLMQ can be also used to partly complement the issue of DRM’s sample complexity with large $H$ since the OPE with long horizon is approximable with infinite horizon as long as $\gamma H < 1$.

**Hyperparameter.** The $L^2(\mu)$-type methods has no hyperparameter other than the candidate set $\mathcal{X}$. This is not the case with the kernel-type methods, requiring users to specify the kernel function $\kappa((s, a), (s', a'))$ satisfying Assumption 2. A typical choice of the kernel function is exponential type kernels for continuous state-action spaces,

$$\kappa(u, \tilde{u}) = \exp \left\{-\frac{|u - \tilde{u}|_p / \sigma}{\sigma}\right\},$$

where $|\cdot|_p$ is the $\ell^p$-norm of vectors. Note that there are hyperparameters: the shape parameter $1 \leq p < \infty$ and the scale parameter $\sigma > 0$.

**Interoperability.** While the $L^2(\mu)$-type methods require the full information of approximated Bellman operator $X$, the kernel-type methods only require the resulting Q-functions. This difference makes the kernel type more fa-
Figure 1: Mean absolute errors (MAE) of KLMQ with different kernels of three independent runs. The horizontal axis is corresponding to different target policies $\pi$ with different expert ratios. The three black dashed lines denote the maximum possible, mean and minimum possible MAEs on the given candidate set, respectively. The blue dashed line denote the MAE of DRM.

4 Experimental Results

We report the result of a preliminary experiment to verify the effectiveness of DRM and KLMQ, two most practical algorithms out of the four. To prepare an instance of OPE problem, we employ InvManagement-v1 from OR-Gym (Hubbs et al. 2020) as the environment and set $\gamma = 0.9$. The offline data $D$ of $n = 2700$ is sampled with a episode-wise mixture of the random agent and a expert agent. The target policy $\pi$ is then prepared as action-wise mixtures of the random and expert agents with the ratios in $\{0, 0.1, 0.2, ..., 1\}$. As the candidate set $X$, we prepared d3rlpy’s implementation (Seno and Imai 2021) of neural-network-based FQE with $n_{\text{steps}} \in \{1000, 2000, ..., 10000\}$ and $n_{\text{hidden layers}} \in \{1, 2, 3\}$, and a custom implementation of DRM over the gradient-boosting-tree-based FQEs (i.e., $|X| = 31$ candidates in total), trained on another dataset of $n = 2700$. Figure 1 shows the mean absolute errors of KLMQ with exponential-type kernel $[\tilde{\pi}]$, $p \in \{1, 2, \infty\}$, $\sigma \in \{0.01, 0.1, 1\}$.

\footnote{The data $(s_i, a_i)$ are normalized so that each feature dimension has zero mean and unit vector.}

It is seen the best hyperparameter is chosen regardless of the kernel parameters if $\pi$ is close to one of the two logging policies (i.e., random or expert), but otherwise the optimality of the choice is strongly affected by the kernel parameter, even if the near optimal OPE by DRM is given (the blue dashed line). This observation matches the analysis of the shift-intolerance of the kernel-type methods and the tolerance of $L^2(\mu)$-type methods (given a good operator candidates).

5 Related Work

To the best of our knowledge, this is the first to study the problem of hyperparameter selection for OPE from theoretical perspective. (Liu, Thomas, and Brunskill 2017) addressed a similar problem in their technical memo, in which the importance of the model selection and possible solutions are demonstrated with a toy example of five-state MDP.

One closely related topic is the loss-minimization formulation of OPE (Baird 1995; Feng, Li, and Liu 2019; Dai et al. 2018), in which OPE is formulated as ordinary optimization problems with objective functions. The objective functions are readily usable as hyperparameter selection criteria (e.g., KLM is originally proposed by (Feng, Li, and Liu 2019)), but there have been no study known to date applying them to OPE with theoretical treatment. Moreover, these objective functions are either inconsistent (unable to select the true operator $B_\pi$, e.g., (Baird 1995)) or have hyperparameter by themselves (e.g., (Feng, Li, and Liu 2019; Dai et al. 2018)).

6 Conclusion

We have proposed the framework of approximate hyperparameter selection (AHS) to address the issue of the hyperparameter selection of OPE. We have then derived four AHS methods based on a new error bound for FQE-like algorithms. We also have drawn theoretical observations on these four methods and discussed different characteristics according to the selection criteria they conform. Finally, we have confirmed a part of these theoretical observations in a preliminary experiment.

Possible future directions include theoretical justification on a specific kernel choice and more time-efficient algorithms reducing the factor of $n^2$ for the kernel-type methods.

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A Proofs

A.1 Proof of Proposition 1

Proof. Let \( \hat{r}(s, a) := \mathbb{E}[R(s, a)] \) and let \( P_\pi \) be the state-transition operator such that \( (P_\pi f)(s, a) = \mathbb{E}[f(s', \pi(s')) | s' \sim T(s, a)] \) for \( f : S \times A \rightarrow \mathbb{R} \). Then, we have \( B_\pi f = \hat{r} + \gamma P_\pi f \) for all \( f : S \times A \rightarrow \mathbb{R} \) and therefore

\[
Q_\pi = B_\pi^0 = \sum_{h=1}^{\infty} (\gamma P_\pi)^{h-1} \hat{r}
\]

by the linearity of \( P_\pi \). Since \( P_\pi \) is linear, we can telescope the sum to get

\[
Q_\pi = Q_H^X - Q_0^X + \sum_{h=1}^{H} (\gamma P_\pi)^{h-1} \{ \hat{r} + \gamma P_\pi Q_H^X - Q_H^{X-h} \}.
\]

Note that \( \hat{r} + \gamma P_\pi Q_H^{X-h} - Q_H^{X-h+1} = -\Delta XQ_H^X \). Since we have \( Q_0^X = 0 \) and \( Q_H^X = Q_H^X \) by definition, we also get

\[
Q_H^X - Q_\pi = \sum_{h=1}^{H} (\gamma P_\pi)^{h-1} \Delta XQ_H^{X-h}.
\]

Taking expectation of both sides as in the definition of \( J(Q_\pi) \), we get

\[
\Delta \hat{J}(Q_\pi) = \sum_{h=1}^{H} \gamma^{h-1} \mathbb{E} \left[ (P_\pi)^{h-1} \Delta XQ_H^{X-h} (s_1, a_1) \right].
\]

Since \( \mathbb{E}[(P_\pi f)(s_h, a_h)] = \mathbb{E}[f(s_{h+1}, a_{h+1})] \) for \( h \geq 1 \) and \( f : S \times A \rightarrow \mathbb{R} \), we obtain the desired result by induction. \( \square \)

A.2 Proof of Proposition 2

Proof. Let \( \rho_h \in L^1(\mu) \) be the Radon-Nikodym derivative of \( (s_h, a_h) \)'s distribution with respect to \( \mu \) for \( 1 \leq h \leq H \). Note that they exist by the assumption of the absolute continuity. Let \( \varphi_h(x) := \inf_{\|f\|_{L^\infty} \leq \|x\|} \|\rho_h - f\|_1 \).

Now, by Proposition 1 we have

\[
|\Delta J(Q_\pi)| = \left| \sum_{h=1}^{H} \gamma^{h-1} \mathbb{E}_{(s,a) \sim \mu} \left[ \rho_h(s, a) \cdot (\Delta XQ_H^{X-h})(s, a) \right] \right|
\]

\[
= \left| \sum_{h=1}^{H} \gamma^{h-1} \mathbb{E}_{(s,a) \sim \mu} \left[ \rho_h(s, a) \cdot (\Delta XQ_H^{X-h})(s, a) \right] \right|
\]

Fix any \( x > 0 \) and \( f \in \mathcal{F} \) satisfying \( \|f\|_{L^\infty} \leq x \). Each summand is bounded as

\[
\left| \mathbb{E}_{(s,a) \sim \mu} \left[ \rho_h(s, a) \cdot (\Delta XQ_H^{X-h})(s, a) \right] \right|
\]

\[
= \left| \mathbb{E}_{(s,a) \sim \mu} \left[ \rho_h(s, a) \cdot (\Delta XQ_H^{X-h})(s, a) \right] \right|
\]

\[
\leq \|\Delta XQ_H^{X-h}\|_{L^\infty} \|\rho_h - f\|_1 + \|\mathbb{E}_{(s,a) \sim \mu} \left[ f(s, a) \cdot (\Delta XQ_H^{X-h})(s, a) \right] \|
\]

(Hölder's inequality)

\[
\leq C' \|\rho_h - f\|_1 + x \|\Delta XQ_H^{X-h}\|_{L^\infty},
\]

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where $C' := 1 + \gamma C$. The last inequality is owing to the boundedness of the range of $X \in \Omega$. Taking the infimum over $f$, we get

$$
\left[ E_{(s,a) \sim \mu} \left[ \rho_h(s,a) \cdot (\Delta X Q_H^X(s,a)) \right] \right] \\
\leq C' \varphi_h(x) + x \left\| \Delta X Q_H^X \right\|_{\infty},
$$

for all $x > 0$. Putting it back to the summation, we get

$$
\left| \Delta J(Q^X) \right| \leq \sum_{h=1}^{H} \gamma^{h-1} \left\{ C' \varphi_h(x) + x \left\| \Delta X Q_H^X \right\|_{\infty} \right\},
$$

$$
= C' \sum_{h=1}^{H} \gamma^{h-1} \varphi_h(x) + x \sum_{h=1}^{H} \gamma^{h-1} \left\| \Delta X Q_H^X \right\|_{\infty}.
$$

We get the desired result by taking the infimum over $x > 0$ and defining $\varphi(y) := \inf_{x > 0} \left\{ C' \sum_{h=1}^{H} \gamma^{h-1} \varphi_h(x) + xy \right\}$. The nonnegativity and monotonicity of $\varphi(y)$, $y \geq 0$, are trivial from the definition. Note that it is concave also by the definition, which implies the continuity except on the boundary $y = 0$. Therefore, it suffices to show the boundary condition $\lim_{y \to 0} \varphi(y) = \varphi(0) = 0$. In fact, it is a direct consequence of $\varphi_h(x) \to 0$ as $x \to \infty$, $1 \leq h \leq H$, which is the case since $F$ is dense in $L^1(\mu)$ and $\rho_h \in L^1(\mu)$ by the assumptions. \hfill $\square$

### A.3 Proof of Proposition 3

**Proof.** Let $\tilde{\varepsilon}(X, f) := \tilde{r}_i + \gamma f(\tilde{s}_i, \pi(\tilde{s}_i)) - (X f)(\tilde{s}_i, \tilde{a}_i)$, $m_i(X, f) := E \left[ \tilde{\varepsilon}(X, f) \right]$, $s_i(X, f) := \left\{ \{\tilde{r}_i + \gamma f(\tilde{s}_i, \pi(\tilde{s}_i))\} \right\} \frac{1}{2} \tilde{s}_i, \tilde{a}_i$, $1 \leq i \leq n$. Observe that $m_i^2(X, f) = -(\Delta X f)(\tilde{s}_i, \tilde{a}_i)$ and therefore $E[m_i^2(X, f)] = \left\| \Delta X f \right\|_2^2$ for $1 \leq i \leq n$. Thus,

$$
E \left[ \tilde{L}_2^\pi(D; f) \right] = E \left[ \frac{1}{n} \sum_{i=1}^{n} m_i^2(X, f) \right] \\
= E \left[ \tilde{z}_i^2(X, f) \right] \\
= E \left[ m_i^2(X, f) \right] + E \left\{ \tilde{\varepsilon}_1(X, f) - m_1(X, f) \right\}^2 \\
= \left\| \Delta X f \right\|_2^2 + E \left[ v_1^2(f) \right].
$$

In particular, we have

$$
E \left[ \tilde{L}_2^\pi(B^\pi; f) \right] = E \left[ v_1^2(f) \right]
$$

since $\Delta X = 0$ if $X = B_\pi$. Taking the difference of the above equations, we get the desired result. \hfill $\square$

### A.4 Proof of Proposition 4

First, we show the following lemma showing the Bellman regret sum (BRS) is a good estimate of the precritic $C_{L^2(\mu)}$ if the set $\mathcal{X}$ well approximates the true operator $B_\pi$ in a collective sense.

**Proposition 9.** Let $\delta \in (0, 1)$. For all $\mathcal{X} \subseteq \Omega$, we have

$$
\left| \tilde{C}_{L^2(\mu)}(X) - BRS_{\mathcal{X}}^n(X; \mathcal{X}) \right| \\
\leq C \left\{ \min_{\mathcal{X} \subseteq \Omega} \varepsilon_2(X) + (1 + \gamma C) \left( \frac{2 \ln(2|\mathcal{X}|^2/\delta)}{n} \right)^{1/4} \right\}
$$

with probability $1 - \delta$ for all $X \in \mathcal{X}$ simultaneously.

**Proof.** Let $f : S \times A \to [0, C]$. With Proposition 3 observe

$$
\left| \Delta X f \right|_2^2 - \text{Regret} \left[ \mathcal{X} \right] \\
\leq E \left[ \tilde{L}_2^\pi(D; f) \right] - \tilde{L}_2^\pi(D; f) + \\
\min_{A \in \mathcal{X}} \frac{\tilde{L}_2^\pi(D; f) - \min_{A \in \mathcal{X}} E \left[ \tilde{L}_2^\pi(A; f) \right]}{\min_{A \in \mathcal{X}} E \left[ \tilde{L}_2^\pi(A; f) - \tilde{L}_2^\pi(B\pi; f) \right]}
$$

By Hoeffding’s inequality, we have

$$
E \left[ \tilde{L}_2^\pi(B\pi; f) \right] - \tilde{L}_2^\pi(B\pi; f) \leq C' \sqrt{\frac{\ln(2\delta)}{2n}}
$$

with probability $1 - \delta$ for $X \in \mathcal{X}$, where $C' := 1 + \gamma C$. Thus, by taking union bound with $X \in \mathcal{X}$,

$$
(A) \leq C'^2 \sqrt{\frac{\ln(2K\delta)}{2n}}, \quad (B) \leq C'^2 \sqrt{\frac{\ln(2K\delta)}{2n}},
$$

with probability $1 - \delta$, where $K := |\mathcal{X}|$. As for (C), we have

$$
(C) = \min_{A \in \mathcal{X}} \left\| \Delta A f \right\|_2 \leq \min_{A \in \mathcal{X}} \varepsilon_2^2(A).
$$

by Proposition 3. Combining the upper bounds on (A), (B) and (C), we get

$$
\left| \Delta X f \right|_2^2 - \text{Regret} \left[ \mathcal{X} \right] \\
\leq \min_{A \in \mathcal{X}} \varepsilon_2^2(A) + 2C'^2 \sqrt{\frac{\ln(2K\delta)}{2n}}
$$

for all $X \in \mathcal{X}$ with probability $1 - \delta$. Finally, observe $|\sqrt{a} - \sqrt{b}| \leq \sqrt{|a - b|}$, $a, b \geq 0$, by the concavity of $x \mapsto \sqrt{x}$ and thus, taking union bound with $f \in \bigcup_{X \in \mathcal{X}} \{ Q_h^X \}_{h=1}^H$,

$$
\left| \tilde{C}_{L^2(\mu)}(X) - BRS_{\mathcal{X}}^n(X; \mathcal{X}) \right| \\
\leq \sum_{h=1}^{H} \gamma^{H-h} \left\| \Delta X Q_h^X \right\|_2^2 - \text{Regret} \left[ \mathcal{X} \right] \\
\leq C \sqrt{\min_{A \in \mathcal{X}} \varepsilon_2^2(A) + 2C'^2 \sqrt{\frac{\ln(2K^2H/\delta)}{2n}}}
$$

$$
\leq C \left\{ \min_{A \in \mathcal{X}} \varepsilon_2(A) + C' \left( \frac{2 \ln(2K^2H/\delta)}{n} \right)^{1/4} \right\}
$$

for all $X \in \mathcal{X}$ with probability $1 - \delta$. The last inequality follows again from the concavity of $x \mapsto \sqrt{x}$. \hfill $\square$

Now we are ready to prove Proposition 4.
Proof. By Proposition 3, 
\[
\tilde{c}_{L^2(\mu)}(\hat{X}_{BR}) - \min_{X \in \mathcal{X}} \tilde{c}_{L^2(\mu)}(X) \\
\leq BRS_D^T(\hat{X}_{BR}) - \min_{X \in \mathcal{X}} BRS_D^T(X) + \\
\left| \tilde{c}_{L^2(\mu)}(\hat{X}_{BR}) - BRS_D^T(\hat{X}_{BR}) \right| + \\
\left| \min_{X \in \mathcal{X}} BRS_D^T(X) - \min_{X \in \mathcal{X}} \tilde{c}_{L^2(\mu)}(X) \right|
\]
\[
\leq BRS_D^T(\hat{X}_{BR}) - \min_{X \in \mathcal{X}} BRS_D^T(X) + \\
2C \left\{ \min_{X \in \mathcal{X}} \varepsilon_2(X) + (1 + \gamma C) \left( \frac{2 \ln(2H |\mathcal{X}| / \delta)}{n} \right)^{1/4} \right\}
\]
\[
= 2C \left\{ \min_{X \in \mathcal{X}} \varepsilon_2(X) + (1 + \gamma C) \left( \frac{2 \ln(2H |\mathcal{X}| / \delta)}{n} \right)^{1/4} \right\},
\]
where the last equality is owing to the definition of \(\hat{X}_{RM}\).
Since \(\tilde{c}_{L^2(\mu)}(X) = \sum_{h=1}^{H} \gamma^{h-h} \| \Delta X Q_h X \|_2 \leq C \varepsilon_2(X)\) for \(X \in \Omega\), we have
\[
\min_{X \in \mathcal{X}} \tilde{c}_{L^2(\mu)}(X) \leq C \min_{X \in \mathcal{X}} \varepsilon_2(X).
\]
Combining the above, we get
\[
\tilde{c}_{L^2(\mu)}(\hat{X}_{BR}) \\
\leq C \left\{ 3 \min_{X \in \mathcal{X}} \varepsilon_2(X) + 2(1 + \gamma C) \left( \frac{2 \ln(2H |\mathcal{X}| / \delta)}{n} \right)^{1/4} \right\}
\]
with probability \(1 - \delta\). Applying \(\varphi_{L^2(\mu)}(\cdot)\) on both sides, we further get
\[
\Delta J(\tilde{X}_{RM}) \\
\leq \varphi_{L^2(\mu)}(\tilde{c}_{L^2(\mu)}(\hat{X}_{RM})) \\
\leq \varphi_{L^2(\mu)} \left( C \left\{ 3 \min_{X \in \mathcal{X}} \varepsilon_2(X) + \\
2(1 + \gamma C) \left( \frac{2 \ln(2H |\mathcal{X}| / \delta)}{n} \right)^{1/4} \right\} \right)
\]
\[
\leq \min_{X \in \mathcal{X}} \varphi_{L^2(\mu)} (3C \varepsilon_2(X)) + \\
\varphi_{L^2(\mu)} \left( 2C(1 + \gamma C) \left( \frac{2 \ln(2H |\mathcal{X}| / \delta)}{n} \right)^{1/4} \right)
\]
\[
= \min_{X \in \mathcal{X}} \varphi_{L^2(\mu)} (3C \varepsilon_2(X)) + o_P(1),
\]
where the last inequality follows from the monotonicity and the concavity of \(\varphi_{L^2(\mu)}\).
The simplified upper bound with the order notation is shown by the following inequality,
\[
\varphi_\mathcal{X}(y) \leq \max_{1 \leq h \leq H} \| \rho_h \|_\mathcal{X} y,
\]
which is directly seen by taking \(x = \max_{1 \leq h \leq H} \| \rho_h \|_\mathcal{X} \) in the definition of \(\varphi_\mathcal{X}\), which is given in the proof of Proposition 3.

A.5 Proof of Proposition 5

Proof. The proof is analogous to that of Proposition 4 as \(\tilde{X}_{DRM}\) is the regret minimizer on the relaxed domain implying \(BRS_D^T(\tilde{X}_{DRM}, X) \leq BRS_D^T(\hat{X}_{RM}, X)\). The difference is in the way we take the union bound. Since there are \(|\mathcal{X}|^H\) possible candidates of dynamic operators, the union bound with the naive uniform probability assignment yields
\[
\text{Subopt}(\tilde{X}_{DRM}, X, C_2) \\
\leq \varphi_{L^2(\mu)} \left( 2C (1 + \gamma C) \left( \frac{2 \ln(H |\mathcal{X}|)}{n} \right)^{1/4} \right),
\]
which have an additional dependency on \(H\) compared to \(\hat{X}_{RM}\).
Instead, we consider assigning the probability of \(P([X]) = \frac{1}{2} (H |\mathcal{X}|)^{-[X]}\) to each \(X \in \mathcal{X}^H\). This yields the desired result.

A.6 Proof of Proposition 6

Proof. It suffices to show the first identity. By Mercer’s theorem, there exist a orthonormal basis \(\{e_j\}_{j=1}^\infty\) of \(L^2(\mu)\) and a sequence of positive numbers \(\{\sigma_j\}_{j=1}^\infty\) such that
\[
\kappa(u, \hat{u}) = \sum_{j=1}^\infty \sigma_j e_j(u) e_j(\hat{u}), \quad u, \hat{u} \in S \times A, \quad (8)
\]
where the convergence is uniform. Observe that any \(f \in \mathcal{F}_\kappa\) is decomposed as
\[
f(u) = \sum_{m=1}^\infty \alpha_m \kappa(u, u_m), \quad u \in S \times A,
\]
for some \(\alpha_m \in \mathbb{R}\) and \(u_m \in S \times A (m = 1, 2, \ldots)\), which implies by (8)
\[
f(u) = \sum_{j=1}^\infty \beta_j e_j(u),
\]
where \(\beta_j := \sigma_j \sum_{m=1}^\infty \alpha_m e_j(u_m)\). The RKHS norm is accordingly decomposed
\[
\| f \|^2_{\mathcal{F}_\kappa} = \langle f, f \rangle_{\mathcal{F}_\kappa} \\
= \sum_{m=1}^\infty \sum_{\tilde{m}=1}^\infty \alpha_m \alpha_{\tilde{m}} \kappa(u_m, u_{\tilde{m}}) \\
= \sum_{j=1}^\infty \sum_{m=1}^\infty \sum_{\tilde{m}=1}^\infty \sigma_j e_j(u_m) e_j(u_{\tilde{m}}) \\
= \sum_{j=1}^\infty \sigma_j \left( \sum_{m=1}^\infty \alpha_m e_j(u_m) \right)^2 \\
= \sum_{j=1}^\infty \beta_j^2 \sigma_j.\]
Let $B := \{ \{ \beta_j \}_{j=1}^\infty : \sum_{j=1}^\infty \beta_j^2 / \sigma_j \leq 1 \}$ be the unit ball of the coefficients with respect to $F_\kappa$. Thus, the dual norm is written as
\[
\| g \|_{F_\kappa}^2 = \left( \sup_{\{ \beta_j \}_{j=1}^\infty \in B} \sum_{j=1}^\infty \beta_j \mathbb{E} [ e_j(u) g(u) ] \right)^2
\]
\[
= \sum_{j=1}^\infty \sigma_j \left( \mathbb{E}_{u \sim \mu} [ e_j(u) g(u) ] \right)^2
\]
\[
= \mathbb{E}_{u, \tilde{u} \sim \mu} \left[ \sum_{j=1}^\infty \sigma_j e_j(u) e_j(\tilde{u}) g(u) g(\tilde{u}) \right]
\]
\[
= \mathbb{E}_{u, \tilde{u} \sim \mu} [ \kappa(u, \tilde{u}) g(u) g(\tilde{u}) ].
\]

### A.7 Proof of Proposition 7

**Proof.** The concentration of the kernel Bellman loss is shown by the general result of $V$-statistics. In particular, (Feng et al. 2020) shows that, for any $f : \mathcal{S} \times \mathcal{A} \to [0, C]$,\[
\left| \text{KBS}^n_{\kappa, \mathcal{D}}(X; f) - \| \Delta X f \|_{F_\kappa}^2 \right| \leq 2(1 + \gamma C)^2 \sqrt{\frac{\ln 2/\delta \lor \frac{1}{n}}{n}}
\]
with probability $1 - \delta$. Thus, by the union bound,\[
\left| \text{KBL}^n_{\mathcal{D}}(X; \kappa) - \hat{C}_{\mathcal{F}_\kappa}(X) \right| \leq C(1 + \gamma C) \left( \frac{4 \ln(2 |\mathcal{X}| / \delta) \lor \frac{1}{n}}{n} \right)^{1/4}
\]
for simultaneously all $X \in \mathcal{X}$ with probability $1 - \delta$. This implies\[
\text{Subopt}(\hat{X}_{\text{KLM} (\kappa)}; \mathcal{X}, C_\kappa)
\]
\[
= \max \left\{ 0, \left| \Delta J(Q_{\text{KLM} (\kappa)}) \right| - \min_{X \in \mathcal{X}} C(X) \right\}
\]
\[
\leq \max \left\{ 0, C_\kappa(\hat{X}_{\text{KLM} (\kappa)}) - \min_{X \in \mathcal{X}} C_\kappa(X) \right\}
\]
\[
\leq \varphi_{\mathcal{F}_\kappa} \left( \max \left\{ 0, \hat{C}_{\mathcal{F}_\kappa}(\hat{X}_{\text{KLM} (\kappa)}) - \min_{X \in \mathcal{X}} \hat{C}_{\mathcal{F}_\kappa}(X) \right\} \right)
\]
\[
\leq \varphi_{\mathcal{F}_\kappa} \left( 2C(1 + \gamma C) \left( \frac{4 \ln(2 |\mathcal{X}| / \delta) \lor \frac{1}{n}}{n} \right)^{1/4} \right).
\]
The simplified upper bound with the order notation is shown in the same way as Proposition 4.

### A.8 Proof of Proposition 8

**Proof.** Observe that\[
\hat{C}_{\mathcal{F}_\kappa}(X) = \sum_{t=0}^\infty \gamma^t \| \Delta X Q^X \|_{F_\kappa}
\]
\[
= C \| B_n Q^X - Q^X \|_{F_\kappa},
\]
which implies\[
\left| \hat{C}_{\mathcal{F}_\kappa}(X) - \text{KBS}^n_{\kappa, \mathcal{D}}(Q^X) \right| \leq C(1 + \gamma C) \left( \frac{4 \ln(2 |\mathcal{X}| / \delta) \lor \frac{1}{n}}{n} \right)^{1/4}
\]
for simultaneously all $X \in \mathcal{X}$. The desired result is proved as in the proof of Proposition 7. \[\square\]