OFFLINE POLICY LEARNING FOR NONPARAMETRIC CONTEXTUAL BANDITS UNDER RELAXED COVERAGE

Anonymous authors
Paper under double-blind review

ABSTRACT

This paper is concerned with learning an optimal policy in a nonparametric contextual bandit from offline, and possibly adaptively collected data. Existing methods and analyses typically rely on i.i.d. offline data, and a uniform coverage condition on the behavior policy. In this work, similar to the single-policy concentrability coefficient, we propose a relaxed notion of coverage that measures how well the optimal action is covered by the behavior policy for the nonparametric bandits. Under this new notion, we develop a novel policy learning algorithm by combining the k-nearest neighbor method with the pessimism principle. The new algorithm has three notable properties. First and foremost, it achieves the minimax optimal suboptimality gap for any fixed coverage level (up to log factors). Second, this optimality is attained adaptively, without requiring prior knowledge of the coverage level of the offline data. Last but not least, it maintains these guarantees even with adaptively collected offline data.

1 INTRODUCTION

The contextual multi-armed bandit provides an elegant and powerful framework for modeling various sequential decision-making problems. In this setup, the learner engages with an environment in rounds: at each round, it observes contextual information, selects an action based on that context, and receives a reward corresponding to the chosen action. Notable advances in bandit algorithms over recent decades have led to successful applications in areas such as personalized medicine, online recommendation, and crowdsourcing (Kim et al., 2011; Li et al., 2010; Kittur et al., 2008).

The abundance of data from past deployments presents an opportunity to improve future decision-making via offline learning. This involves learning effective policies from batch datasets, a problem widely investigated in offline reinforcement learning (RL) (Lange et al., 2012; Levine et al., 2020; Chen & Jiang, 2019; Jin et al., 2021; Rashidinejad et al., 2021). Unlike online RL, which relies on active exploration, offline RL focuses on extracting insights from pre-collected data and has demonstrated effectiveness in high-stakes domains such as autonomous driving and healthcare (Bojarski, 2016; Yurtsever et al., 2020; Tang & Wiens, 2021).

Offline learning in the realm of contextual bandits has attracted growing attention in the past decade. Rashidinejad et al. (2021) studied the tabular case and Li et al. (2022); Zhu et al. (2023) subsequently considered offline learning in linear bandits. Another line of work (Swaminathan & Joachims, 2015; London & Sandler, 2019; Jin et al., 2022; Wang et al., 2024; Gabbianelli et al., 2024; Sakhi et al., 2024) advanced the understanding of parametric offline learning for contextual bandits by applying the importance-weighting method to learn a given policy class. While parametric offline learning has been extensively studied in the past literature, the problem of learning a policy from batch data under the nonparametric model remains underexplored.

The nonparametric contextual bandit is a classical personalized decision-making framework, where the expected reward for each action takes the form of a smooth function of the contexts (Yang & Zhu, 2002). For the online learning setting, the minimax rate of the cumulative regret has been established by (Perchet & Rigollet, 2013; Rigollet & Zeevi, 2010). Recent work Cai et al. (2024) initiated the study of nonparametric bandit learning with offline data. Their result displayed the ability of the offline dataset to improve the online learning regret. However, it imposed a uniform coverage condition on the offline dataset which says all actions need to be taken with sufficient probability by the behavior policy in order for the offline data to be useful. Such uniform coverage condition may not hold in many practical scenarios.

In this paper, we study the problem of nonparametric offline policy learning under a relaxed coverage condition. Similar to the single-policy concentrability coefficient (Rashidinejad et al., 2021), we propose a relaxed notion of coverage that describes how well the optimal action is covered by the behavior policy for the nonparametric bandits. Since the quality of the offline data is often unknown in reality, it would be desirable to develop an algorithm that can learn an optimal policy from the batch data without knowing the coverage level. To that end, we introduce policy learning algorithms that bridge techniques from nonparametric statistics and the pessimism principle from offline RL (Jin et al., 2021; Rashidinejad et al., 2021). We summarize our theoretical results as follows.

1.1 Main contributions

First, we establish the fundamental limits of policy learning for nonparametric bandits under a relaxed coverage condition. Let β be the smoothness parameter of the nonparametric reward functions (Assumption 2.1), and α be the margin parameter which measures the separation between the arms (Assumption 2.2). Denote by $C^\star$ the coefficient that reflects the coverage of the optimal action under the offline data (Definition 2.4), and denote by d the dimension of the covariates. We show the minimax optimal suboptimality gap of policy learning for nonparametric bandits is of order $(N/C^\star)^{-\frac{\beta(1+\alpha)}{2\beta+d}}$, where N is the size of the offline dataset. Intuitively, the coverage coefficient $C^\star$ controls the effective sample size of the offline data. When $C^\star$ becomes larger, the quality of the offline dataset degrades, and consequently the minimax rate of convergence decreases.

We introduce two nonparametric offline policy learning rules that nearly attain the optimal suboptimality gap. BIN-LCB (Algorithm 1) is based on splitting the continuous covariate space into smaller bins and applying the lower-confidence bound approach to each bin. By choosing the number of bins appropriately, we prove BIN-LCB achieves the optimal suboptimality up to log factors. A limitation of BIN-LCB is that the optimal binning parameter depends on the coverage coefficient $C^\star$, which is often unknown in practice.

To overcome this limitation, we propose KNN-LCB (Algorithm 2) that combines the k-nearest neighbor regression (Kpotufe, 2011; Chaudhuri & Dasgupta, 2014; Reeve et al., 2018) with the lower-confidence bound principle. The number of nearest neighbors considered at a covariate point is determined in a data-driven fashion, thereby allowing KNN-LCB to achieve the optimal suboptimality (up to log factors) without any knowledge of $C^\star$. Finally, in contrast to previous work that assume i.i.d. offline samples, our theoretical guarantees hold even when the batch dataset is generated by running adaptive algorithms.

1.2 Related work

Nonparametric contextual bandits. Since Woodroofe (1979) incorporated contextual information into the multi-armed bandits problem, there has been significant progress in the theory of contextual bandits. Auer (2002); Abbasi-Yadkori et al. (2011); Goldenshluger & Zeevi (2013); Bastani & Bayati (2020) adopted a parametric perspective and studied linear contextual bandits in both low and high dimensional settings. Meanwhile, modeling the reward function as a nonparametric function of the contexts was proposed by (Yang & Zhu, 2002). In the online learning setting, Rigollet & Zeevi (2010) developed a UCB-type algorithm that nearly achieves the optimal regret for nonparametric bandits and its results were further improved by (Perchet & Rigollet, 2013). Reeve et al. (2018) designed the k-Nearest Neighbor UCB algorithm that is able to utilize the low intrinsic dimensionality of the contexts. Cai et al. (2024) studied transfer learning for nonparametric bandits where the learner is given an offline dataset before starting to perform online learning. Additional insights in nonparametric bandits were developed in (Qian & Yang, 2016; Guan & Jiang, 2018; Hu et al., 2022; Suk & Kpotufe, 2021; Gur et al., 2022; Jiang & Ma, 2024).

Offline policy learning. Learning an optimal policy from batch data has received considerable attention in the past decade. Earlier works relied on the all-policy concentrability condition which requires the state-action pairs of all possible policies to be covered in the offline dataset (Munos & Szepesvári, 2008; Kallus, 2018; Chen & Jiang, 2019; Zhang et al., 2020; Xie & Jiang, 2021; Zhou et al., 2023). Nevertheless, such uniform coverage assumption can be violated in many practical applications. A line of work relaxed this requirement by using the principle of pessimism to optimize conservatively on the batch data (Jin et al., 2021; Rashidinejad et al., 2021; Uehara & Sun, 2021; Xie et al., 2021a; Zanette et al., 2021; Shi et al., 2022; Zhan et al., 2022; Li et al., 2024a). For contextual bandits, Li et al. (2022); Zhu et al. (2023) studied pessimistic offline learning in linear bandits; Swaminathan & Joachims (2015); London & Sandler (2019); Jin et al. (2022); Wang et al. (2024); Gabbianelli et al. (2024); Sakhi et al. (2024) obtained policy learning guarantees via the importance weighting method when given a policy class. The prevalence of adaptive online learning algorithms has made it important to analyze situations where the offline dataset is adaptively collected (Zhan et al., 2024; Jin et al., 2022; Bibaut et al., 2021). Using both offline and online data to reduce sample complexity has been explored in hybrid RL (Xie et al., 2021b; Song et al., 2022; Wagenmaker & Pacchiano, 2023; Yang et al., 2023; Li et al., 2024c; Nakamoto et al., 2024). Finally, off-policy evaluation is a task related to policy learning but its main goal is to estimate the value function of a target policy based on offline data, and has been widely studied in recent literature (Thomas & Brunskill, 2016; Jiang & Li, 2016; Wang et al., 2017; Duan et al., 2020; Jiang & Huang, 2020; Ma et al., 2022; Li et al., 2024b; Lee & Ma, 2024).

2 Problem setup

A K-armed nonparametric bandit instance is specified by a sequence of i.i.d. random vectors

$$(X_i, Y_i^{(1)}, \dots, Y_i^{(K)}), \quad 1 \le i \le N.$$

Here, each context X_i is assumed to be from $\mathcal{X} := [0,1]^d$, and is sampled from a distribution P_X. We assume P_X has a density (w.r.t. the Lebesgue measure) that is bounded below and above by some constants $\underline{c}, \bar{c} > 0$, respectively. In addition, $Y_i^{(a)}$ denotes the potential reward associated with choosing action a at the i-th round. Denote by $\mathcal{I} = [K]$ the set of arms. Given any $a \in \mathcal{I}$ and $i \ge 1$, we assume that $Y_i^{(a)} \in [0,1]$ and

$$\mathbb{E}[Y_i^{(a)} \mid X_i] = f_a(X_i),$$

where f_a is the unknown mean reward function for the arm a.

Suppose that we have access to an offline dataset $\mathcal{D}_{\text{off}} = \{(X_i, A_i, Y_i^{(A_i)})\}_{i=1}^N$ collected from a behavior policy $\mu = \{\mu_i\}_{i=1}^N$. More precisely, for $1 \le i \le N$, the action obeys $A_i \sim \mu_i(\cdot \mid X_i, \mathcal{F}_{i-1})$, where μ_i is the behavior policy at step i that can depend on the history $\mathcal{F}_{i-1} = \{X_1, A_1, Y_1, \dots, X_{i-1}, A_{i-1}, Y_{i-1}\}$.

Define the optimal arm at x to be

$$\pi^\star(x) \in \arg\max_{a \in \mathcal{I}} f_a(x),$$

with ties broken arbitrarily.

Our goal is to learn a policy $\pi : \mathcal{X} \to \mathcal{I}$ based on the batch dataset $\mathcal{D}_{\text{off}}$ that minimizes the expected suboptimality, which is defined as

$$\mathbb{E}\left[f_{\pi^\star(X)}(X) - f_{\pi(X)}(X)\right]. \tag{1}$$

2.1 Assumptions

We adopt the following assumptions that are standard in nonparametric bandits (Rigollet & Zeevi, 2010; Perchet & Rigollet, 2013). The first assumption says the reward functions of different arms are Hölder smooth.

Assumption 2.1 (Smoothness)**.** We assume that the reward function for each arm is (β, L)-smooth, that is, there exist $\beta \in (0,1]$ and $L > 0$ such that for any $a \in [K]$,

$$|f_a(x) - f_a(x')| \le L \|x - x'\|_2^\beta, \quad \forall x, x' \in \mathcal{X}.$$

The second assumption depicts the separation of the reward functions of different arms. For any $x \in \mathcal{X}$, define the pointwise maximum of the reward functions at x to be

$$f^\star(x) = f^{(1)}(x) = \max_{a \in [K]} f_a(x).$$

Besides, define the second pointwise maximum to be

$$f^{(2)}(x) = \max\{f_a(x) : a \in [K], f_a(x) < f^{(1)}(x)\},$$

if $f^{(1)}(x) \neq \min_{a\in[K]} f_a(x)$, and $f^{(2)}(x) = f^{(1)}(x)$ otherwise.

Assumption 2.2 (Margin)**.** We assume that the reward functions satisfy the margin condition with parameter $\alpha > 0$, that is there exist $C_\alpha > 0$ such that

$$P_X\left(0 < f^{(1)}(X) - f^{(2)}(X) \leq \delta\right) \leq C_\alpha \delta^\alpha, \quad \forall \delta \in [0, 1].$$

Assumption 2.2 originates from the margin condition in nonparametric classification (Mammen & Tsybakov, 1999; Tsybakov, 2004; Audibert & Tsybakov, 2007). It has been introduced to nonparametric contextual bandits by (Goldenshluger & Zeevi, 2009; Rigollet & Zeevi, 2010; Perchet & Rigollet, 2013). The complexity of the decision boundary is affected by the margin parameter. As the margin parameter α grows larger, the mean reward function of the optimal action becomes more well-separated from the other arms and identifying the optimal arm is less difficult.

Remark 2.3. When $\alpha\beta > 1$, the problem reduces to a static multi-armed bandit where one arm is always optimal, regardless of the context; see Proposition 2.1 in (Rigollet & Zeevi, 2010). In this degenerate case, the context becomes irrelevant, and the decision-making task loses its inherent complexity. Since our focus is on contextual bandits, we concentrate on the case $\alpha\beta \leq 1$ in this paper.

2.2 Relaxed coverage condition

To characterize the quality of the offline data, we define

$$\mu(\cdot \mid x) = \frac{1}{N}\sum_{i=1}^{N} \mu_i(\cdot \mid x), \tag{2}$$

which is the average of the behavior policies at x over all time steps. We consider the following notion about the coverage of μ.

Definition 2.4. We define $C^\star$ to be the positive constant that satisfies

$$\inf_{x\in\mathcal{X}} \mu(\pi^\star(x) \mid x) \geq \frac{1}{C^\star}. \tag{3}$$

Namely, $1/C^\star$ reflects the minimum probability that the optimal arm is taken over the covariate space. Compared to Cai et al. (2024), which requires the minimum probability that any arm is pulled to be lower bounded, our notion here is more relaxed because it only needs the optimal action to be covered. More precisely, one would have $\inf_{a\in[K],x\in\mathcal{X}} \mu(a \mid x) \leq \inf_{x\in\mathcal{X}} \mu(\pi^\star(x) \mid x)$ since the infimum is taken over all actions.

Definition 2.4 is related to the single-policy concentrability coefficient in offline tabular RL (Rashidinejad et al., 2021). Under the nonparametric bandit setting, however, the continuity of the covariate space together with the nonparametric reward function necessitates different techniques for the algorithm design and analysis of policy learning.

Throughout the paper, we assume the number of arms K to be constant. We use $\mathcal{F}(\alpha, \beta, C^\star)$ to denote the family of K-armed bandit instances that satisfy the above conditions with parameters α, β and $C^\star$.

3 Minimax rates

The main challenge in learning an optimal policy from the batch dataset stems from the continuity of the covariate space. A common approach in nonparametric bandits literature is to decompose the state space into smaller bins and treat each bin as a multi-armed bandit problem without the covariate (Rigollet & Zeevi, 2010; Perchet & Rigollet, 2013). However, their algorithms are mainly designed for the online learning setup while in our case, the task is to learn a good policy from the offline data. The principle of pessimism has been a widely adopted method in offline reinforcement

Algorithm 1 Binning with lower confidence bound

Require: Test point x, offline dataset $\mathcal{D}_{\text{off}}$, binning parameter M, confidence level δ.
1: Generate partition $\mathcal{L} \leftarrow \{B_j : j \in [M^d]\}$.
2: Find $j \in [M^d]$ such that $x \in B_j$.
3: Return $\hat{\pi}(x) = \arg\max_{a \in \mathcal{I}} \hat{f}_{a,j} - b_j(a)$.

learning (Jin et al., 2021; Rashidinejad et al., 2021). The key is to subtract an additional term from the empirical estimate of the reward value of an action to account for the uncertainty of the offline data. Motivated by these ideas, we propose Algorithm 1—Binning with lower confidence bound—to perform policy learning from the offline dataset for the nonparametric bandits.

To facilitate the presentation, we first introduce some notations. Let $\mathcal{L} = \{B_j : j \in [M^d]\}$ be a regular partition of $\mathcal{X}$ for some positive integer M, where

$$B_j = \{x \in \mathcal{X} : (v_l - 1)/M \leq x_l < v_l/M, 1 \leq l \leq d\},$$

and $\boldsymbol{v} = (v_1, v_2, \ldots, v_d) \in [M]^d$. As a result, there are in total M^d bins in $\mathcal{L}$. For any $j \in [M^d]$, let

$$N_j(a) = \sum_{i=1}^{N} \mathbf{1}\{X_i \in B_j, A_i = a\},$$

which is the number of times the covariate goes to bin B_j and the action taken is a. Define

$$\hat{f}_{a,j} = \frac{1}{N_j(a)} \cdot \sum_{i=1}^{N} \mathbf{1}\{X_i \in B_j, A_i = a\} \cdot Y_i^a,$$

which is the empirical estimate of arm a's reward in B_j. Define the uncertainty level of arm a in B_j to be

$$b_j(a) = \sqrt{\frac{2\log(1/\delta)}{N_j(a)}},$$

for some $\delta > 0$. For any $x \in \mathcal{X}$, Algorithm 1 first assigns it to the corresponding bin B_j. Then, it returns the action $a \in \mathcal{I}$ that maximizes $\hat{f}_{a,j} - b_j(a)$, which is the lower confidence bound of the reward value within that bin.

We are ready to present the theoretical guarantee of Algorithm 1.

Theorem 3.1. *Suppose $\alpha\beta \leq 1$. Assume $N \geq (20\underline{c}^{-1}K\log(2N^5))^{(2\beta+d)/\beta}C^\star$. Algorithm 1 with inputs $M \asymp (N/C^\star)^{1/(2\beta+d)}$, $\delta = 1/N^5$ outputs a policy $\hat{\pi}$ that satisfies*

$$\sup_{\mathcal{F}(\alpha,\beta,C^\star)} \mathbb{E}\left[f_{\pi^\star(X)}(X) - f_{\hat{\pi}(X)}(X)\right] \leq \widetilde{O}\left((\frac{N}{C^\star})^{-\frac{\beta(1+\alpha)}{2\beta+d}}\right).$$

See Section 5.1 for the proof.

The coverage coefficient $C^\star$ controls the effective sample size of the offline dataset. When $C^\star$ gets larger, which means the offline dataset has worse coverage on the optimal action, the expected suboptimality decays at a slower rate.

We complement the performance upper bound with the following minimax lower bound on the suboptimality of policy learning for nonparametric bandits.

Theorem 3.2. *Suppose $\alpha\beta \leq 1$ and $C^\star \geq 2$. For any algorithm that takes in an offline dataset $\mathcal{D}_{\text{off}}$ and outputs a policy π, one has*

$$\sup_{\mathcal{F}(\alpha,\beta,C^\star)} \mathbb{E}\left[f_{\pi^\star(X)}(X) - f_{\pi(X)}(X)\right] \gtrsim \left(\frac{N}{C^\star}\right)^{-\frac{\beta(1+\alpha)}{2\beta+d}}.$$

See Appendix C for the proof.

Theorem 3.1 matches the lower bound in Theorem 3.2 up to log factors, and together they establish the minimax suboptimality gap of policy learning for nonparametric bandits under the relaxed coverage condition.

Algorithm 2 KNN with lower confidence bound

Require: Test point x, offline dataset $\mathcal{D}_{\text{off}}$, confidence level δ.
1: **for** each $a \in \mathcal{I}$ **do**
2: $k(a) \leftarrow \arg\min_{k\in[N]} U_k^a(x)$.
3: **end for**
4: Return $\tilde{\pi}(x) = \arg\max_{a\in\mathcal{I}} \hat{f}^a_{k(a)}(x) - U^a_{k(a)}(x)$.

4 Adaptivity to the coverage coefficient

While Algorithm 1 nearly achieves the minimax optimal rate, it requires knowledge of the coverage coefficient $C^\star$ to determine the optimal binning parameter M. In practice, the quality of the offline dataset is often unknown, and the learner could face difficulties in choosing the appropriate value of M without knowing $C^\star$. A natural attempt is to estimate the coverage coefficient. However, obtaining a faithful estimate of $C^\star$ is challenging because we do not know the optimal action at all. Instead of estimating $C^\star$ directly, we consider the following procedure that can optimally adapt to the quality of the batch dataset (Algorithm 2).

Our algorithm is inspired by the k-nearest neighbor UCB proposed in (Reeve et al., 2018). Their approach combines the k nearest-neighbor method with the upper confidence bound to tackle the online regret minimization problem. In our case, however, the main challenge lies in adapting to the coverage of the offline dataset. On a high level, our procedure uses k-nearest neighbor regression to estimate the nonparametric reward functions, and applies the pessimism principle to select the action based on the batch data.

We start by introducing some notations. Given any $x \in \mathcal{X}$, let $\{\tau_q(x)\}_{q=1}^N$ be an enumeration of $[N]$ such that

$$\|x - X_{\tau_q(x)}\|_2 \le \|x - X_{\tau_{q+1}(x)}\|_2,$$

for any $q \le N-1$. Denote by $\Gamma_k(x) = \{\tau_q : q \in [k]\}$ the set of indices of the k-nearest neighbors of x. Let

$$N_k^a(x) = \sum_{i\in\Gamma_k} \mathbf{1}\{A_i = a\},$$

which is the number of times arm a is taken among the k-nearest neighbors of x. Let $r_k(x) = \|x - X_{\tau_k(x)}\|_2$. Define

$$U_k^a(x) = \sqrt{\frac{2\log(1/\delta)}{N_k^a(x)}} + \log N \cdot r_k(x)^\beta,$$

which is the uncertainty value of arm a with k neighbors at x. Next, define

$$\hat{f}_k^a(x) = \frac{\sum_{i\in\Gamma_k} \mathbf{1}\{A_i = a\} Y_i^a}{N_k^a(x)},$$

which is the empirical estimate of arm a's reward with the k-nearest neighbors of x among the batch dataset. For any $x \in \mathcal{X}$, Algorithm 2 first determines a value $k(a)$ such that

$$k(a) = \arg\min_{k\in[N]} U_k^a(x), \tag{4}$$

for each $a \in \mathcal{I}$. Intuitively, $k(a)$ is the number of neighbors that can balance the bias and variance of the reward estimate at x for arm a. Then, it selects the action $a \in \mathcal{I}$ that maximizes $\hat{f}^a_{k(a)}(x) - U^a_{k(a)}(x)$, which is the lower confidence bound of the reward estimate of arm a at x. Now, we are ready to state the suboptimality guarantee of Algorithm 2.

Theorem 4.1. *Suppose $\alpha\beta \le 1$. Assume $N \ge (20\underline{c}^{-1} K \log(2N^5))^{(2\beta+d)/\beta} C^\star$. Algorithm 2 with input $\delta = 1/N^5$ outputs a policy $\tilde{\pi}$ that satisfies*

$$\sup_{\mathcal{F}(\alpha,\beta,C^\star)} \mathbb{E}\left[f_{\pi^\star(X)}(X) - f_{\tilde{\pi}(X)}(X)\right] \le \widetilde{O}\left((\frac{N}{C^\star})^{-\frac{\beta(1+\alpha)}{2\beta+d}} \right).$$

See Appendix B.1 for the proof.

Algorithm 2 attains the minimax optimal suboptimality up to log factors. In contrast to Algorithm 1, it does not need any knowledge of the coverage coefficient. As mentioned earlier, $C^\star$ dictates the effective sample size of the offline dataset. One can see from the proof of Theorem 1 that the optimal choice of the binning parameter M balances the bias and variance in some sense based on the number of effective samples. In Algorithm 2, however, the burden of adapting to the effective sample size is left to the choice of k, the number of nearest neighbors to consider for reward estimation. Crucially, the definition of $k(a)$ in equation (4) allows for balancing the bias and variance of estimation in a data-driven fashion. Such choice of $k(a)$ in turn adapts to the local effective sample size at point x for each arm $a \in \mathcal{I}$.

5 Proof of main results

In this section, we present the analysis of Algorithm 1. While the full proof of our adaptive procedure (Algorithm 2) is postponed to Appendix B.1, the framework outlined here is instrumental for the later proof.

A key difficulty stems from the challenge of partial coverage in the presence of continuous covariates. With nonparametric reward functions, the optimal arm $\pi^\star(x) \in \arg\max_{a\in\mathcal{I}} f_a(x)$ can switch arbitrarily often, even within a tiny neighborhood, due to complex intersections among the reward curves $f_a(\cdot)$. Our key insight (Lemma 5.2) is the identification of at least one arm whose reward curve closely tracks the pointwise maximum $f^\star(\cdot)$ and, crucially, receives sufficient coverage under the behavior policy.

Moreover, a naïve application of existing pessimistic MAB bounds after partitioning the context space yields an excess risk guarantee that ignores the margin condition and is therefore loose. The novelty of our analysis lies in carefully controlling the error incurred on the regions where the best and second-best reward functions exhibit a sufficient gap. To do so, we further decompose the risk on those regions based on whether a near-optimal arm is selected or not, and derive high-probability bounds that can fully leverage the gap condition.

Motivated by (Perchet & Rigollet, 2013), we begin by partitioning the covariate space into different types of regions based on the separation of the reward functions. Define

$$\mathcal{J} = \{j \in [M^d] : \exists x_j \in B_j, f^{(1)}(x_j) - f^{(2)}(x_j) > cM^{-\beta}\}, \tag{5}$$

where $c > 0$ is to be specified. For its complement, we partition $\mathcal{J}^c$ into two smaller sets

$$\mathcal{J}_1^c = \{j \in \mathcal{J}^c : \exists x_j \in B_j, f^{(1)}(x_j) = f^{(2)}(x_j)\}, \tag{6}$$

and

$$\mathcal{J}_2^c = \{j \in \mathcal{J}^c : \forall x \in B_j, 0 < f^{(1)}(x) - f^{(2)}(x) \le cM^{-\beta}\}. \tag{7}$$

For any $j \in \mathcal{J}_1^c$, the following lemma shows that the regret incurred on B_j can be controlled by the margin condition.

Lemma 5.1. *For any $j \in \mathcal{J}_1^c$ and policy $\pi : \mathcal{X} \to [K]$, one has*

$$\mathbb{E}\left[\sum_{j\in\mathcal{J}_1^c} \big(f^\star(X) - f_{\pi(X)}(X)\big)\,\mathbf{1}\{X \in B_j\}\right] \le C_\alpha \cdot c^{1+\alpha} \cdot M^{-\beta(1+\alpha)}.$$

See Section B.2.1 for the proof.

For any $j \in \mathcal{J} \cup \mathcal{J}_2^c$, let

$$\mathcal{I}_j^\star = \{a \in \mathcal{I} : \exists x \in B_j, f_a(x) = f^\star(x)\},$$

which is the set of near optimal arms in B_j. Our proof relies on the following observation that there always exists an arm in $\mathcal{I}_j^\star$ that is sufficiently covered by the offline dataset.

Lemma 5.2. *For any $j \in \mathcal{J} \cup \mathcal{J}_2^c$, there exists $a^\star \in \mathcal{I}_j^\star$ such that*

$$\mu(a^\star \mid B_j) = \frac{1}{P_X(B_j)} \int_{B_j} \mu(a^\star \mid x)\mathrm{d}P_X(x) \ge \frac{1}{KC^\star}.$$

See Section B.2.2 for the proof.

5.1 PROOF OF THEOREM 3.1

To start with, let $c_1 = 2\sqrt{\underline{c}^{-1}\log(2K\delta^{-1})K}$ and $c = c_1 + 2Ld^{\beta/2}$. For any $j \in \mathcal{J} \cup \mathcal{J}_2^c$, denote $a^\star \in \mathcal{I}_j^\star$ to be the near optimal arm with coverage in B_j given by Lemma 5.2. For any $a \in \mathcal{I}$, define

$$f_{a,j} := \mathbb{E}[f_a(X) \mid X \in B_j] = \frac{1}{P_X(B_j)} \int_{B_j} f_a(x) \mathrm{d}P_X(x).$$

Deote $f_{\star,j} = f_{a^\star,j}$, and let $\hat{\pi}_j$ to be the output of Algorithm 1 on B_j. Define

$$\mathcal{A}_j = \{N_j(a^\star) \ge \frac{1}{2K} P_X(B_j) \cdot \frac{N}{C^\star}\},$$

and

$$\mathcal{E}_j = \{f_{\star,j} - f_{\hat{\pi}_j,j} \le 2b_j(a^\star)\} \cap \mathcal{A}_j.$$

The next two lemmas state these good events happen with high probability.

Lemma 5.3. *For any $j \in \mathcal{J} \cup \mathcal{J}_2^c$, let $\hat{\pi}_j$ be the output of Algorithm 1 on B_j. With probability at least $1 - N^{-3}$,*

$$f_{\star,j} - f_{\hat{\pi}_j,j} \le 2b_j(a^\star).$$

See Section B.2.3 for the proof.

Lemma 5.4. *Assume $\mu(a^\star \mid B_j) \ge 1/(C^\star K)$. One has*

$$\mathbb{P}(\mathcal{A}_j^c) \le \frac{1}{N^5}.$$

See Section B.2.4 for the proof.

The excess risk can be decomposed as

$$\begin{aligned}
\mathbb{E}\left[f^\star(X) - f_{\hat{\pi}(X)}(X)\right] &= \sum_{j=1}^{M^d} \mathbb{E}\left[\left(f^\star(X) - f_{\hat{\pi}(X)}(X)\right) \mathbf{1}\{X \in B_j\}\right] \\
&= \underbrace{\sum_{j \in \mathcal{J}} \mathbb{E}\left[\left(f^\star(X) - f_{\hat{\pi}(X)}(X)\right) \mathbf{1}\{X \in B_j\}\right]}_{U} + \underbrace{\sum_{j \in \mathcal{J}^c} \mathbb{E}\left[\left(f^\star(X) - f_{\hat{\pi}(X)}(X)\right) \mathbf{1}\{X \in B_j\}\right]}_{V}.
\end{aligned}$$

5.1.1 CONTROL OF TERM V

We further decompose

$$V = \underbrace{\sum_{j \in \mathcal{J}_1^c} \mathbb{E}\left[\left(f^\star(X) - f_{\hat{\pi}(X)}(X)\right) \mathbf{1}\{X \in B_j\}\right]}_{V_1} + \underbrace{\sum_{j \in \mathcal{J}_2^c} \mathbb{E}\left[\left(f^\star(X) - f_{\hat{\pi}(X)}(X)\right) \mathbf{1}\{X \in B_j\}\right]}_{V_2}.$$

For term V_1, Lemma 5.1 gives

$$V_1 \le C_\alpha c^{1+\alpha} M^{-\beta(1+\alpha)}.$$

Next, we upper bound V_2. Fix any $j \in \mathcal{J}_2^c$. Let $a^\star \in \mathcal{I}_j^\star$ be the near optimal arm with coverage in B_j given by Lemma 5.2, so that $\mu(a^\star \mid B_j) \ge 1/(KC^\star)$. Applying Lemma B.3 we get

$$\mathbb{E}[(f^\star(X) - f_{\hat{\pi}(X)}(X))\mathbf{1}\{X \in B_j\}] \le 3\overline{c}cM^{-d-\beta}.$$

Besides, the margin condition implies

$$\sum_{j \in \mathcal{J}_2^c} \underline{c}M^{-d} \le P_X(0 < f^{(1)}(x) - f^{(2)}(x) \le cM^{-\beta}) \le C_\alpha c^\alpha M^{-\beta\alpha}. \tag{8}$$

Therefore, $|\mathcal{J}_2^c| \le \underline{c}^{-1} C_\alpha c^\alpha M^{d-\alpha\beta}$ and we reach

$$V_2 \le \underline{c}^{-1} C_\alpha c^\alpha M^{d-\alpha\beta} \cdot (3\overline{c}cM^{-d-\beta}) = 3\underline{c}^{-1}\overline{c} C_\alpha c^{1+\alpha} M^{-\beta(1+\alpha)}.$$

Combining the bounds of V_1 and V_2 yields

$$V = V_1 + V_2 \le (1 + 3\underline{c}^{-1}\overline{c}) C_\alpha c^{1+\alpha} M^{-\beta(1+\alpha)}.$$

5.1.2 CONTROL OF TERM U

Fix any $j \in \mathcal{J}$. Let $\mathcal{I}_j^\star = \{a \in \mathcal{I} : f_a(x_j) = f^\star(x_j)\}$ where $x_j \in B_j$ satisfies $f^{(1)}(x_j) - f^{(2)}(x_j) > cM^{-\beta}$ by definition of $\mathcal{J}$. Let $a^\star \in \mathcal{I}_j^\star$ be the near optimal arm with coverage in B_j given by Lemma 5.2, so that $\mu(a^\star \mid B_j) \geq 1/(KC^\star)$. Applying Lemma B.4 we obtain

$$\begin{aligned}&\mathbb{E}[(f^\star(X) - f_{\hat{\pi}(X)}(X))\mathbf{1}\{X \in B_j\}] \\ &\quad \leq cM^{-\beta}\mathbb{P}(X \in B_j, 0 < f^{(1)}(X) - f^{(2)}(X) \leq cM^{-\beta}) + \mathbb{E}[\mathbf{1}\{X \in B_j, f_{\star,j} - f_{\hat{\pi}_j,j} \geq c_1 M^{-\beta}\}].\end{aligned} \tag{9}$$

We further decompose the second term above into

$$\begin{aligned}&\mathbb{E}[\mathbf{1}\{X \in B_j, f_{\star,j} - f_{\hat{\pi}_j,j} \geq c_1 M^{-\beta}\}] \\ &\quad = \mathbb{E}[\mathbf{1}\{X \in B_j, f_{\star,j} - f_{\hat{\pi}_j,j} \geq c_1 M^{-\beta}\}(\mathbf{1}\{\mathcal{A}_j\} + \mathbf{1}\{\mathcal{A}_j^c\})] \\ &\quad \leq \mathbb{E}[\mathbf{1}\{X \in B_j, f_{\star,j} - f_{\hat{\pi}_j,j} \geq c_1 M^{-\beta}\}\mathbf{1}\{\mathcal{A}_j\}] + \mathbb{P}(\mathcal{A}_j^c) \\ &\quad \leq \mathbb{E}[\mathbf{1}\{X \in B_j, f_{\star,j} - f_{\hat{\pi}_j,j} \geq 2b_j(a^\star)\}\mathbf{1}\{\mathcal{A}_j\}] + \mathbb{P}(\mathcal{A}_j^c) \\ &\quad \leq \frac{2}{N^3},\end{aligned} \tag{10}$$

where the penultimate inequality uses the fact that $c_1 M^{-\beta} \geq 2b_j(a^\star)$ under $\mathcal{A}_j$, and the last inequality is due to Lemma 5.3 and Lemma 5.4. Combining relations (9) and (10), we reach

$$\begin{aligned}U &= \sum_{j \in \mathcal{J}} \mathbb{E}\left[\left(f^\star(X) - f_{\hat{\pi}(X)}(X)\right)\mathbf{1}\{X \in B_j\}\right] \\ &\leq \sum_{j \in \mathcal{J}} cM^{-\beta}\mathbb{P}(X \in B_j, 0 < f^{(1)}(X) - f^{(2)}(X) \leq cM^{-\beta}) + M^d \cdot \frac{2}{N^3} \\ &\leq cM^{-\beta}\mathbb{P}(0 < f^{(1)}(X) - f^{(2)}(X) \leq cM^{-\beta}) + M^d \cdot \frac{2}{N^3} \\ &\leq 2C_\alpha c^{1+\alpha} M^{-\beta(1+\alpha)},\end{aligned}$$

where the last inequality uses the margin condition. Therefore,

$$\begin{aligned}\mathbb{E}\left[f^\star(X) - f_{\hat{\pi}(X)}(X)\right] &= U + V \\ &\leq 2C_\alpha c^{1+\alpha}M^{-\beta(1+\alpha)} + (1 + 3\underline{c}^{-1}\overline{c})C_\alpha c^{1+\alpha}M^{-\beta(1+\alpha)} \\ &= (3 + 3\underline{c}^{-1}\overline{c})C_\alpha c^{1+\alpha}M^{-\beta(1+\alpha)} \\ &= (3 + 3\underline{c}^{-1}\overline{c})C_\alpha c^{1+\alpha}\left(\frac{N}{C^\star}\right)^{-\frac{\beta(1+\alpha)}{2\beta+d}}.\end{aligned}$$

6 DISCUSSION

In this paper, we establish policy learning guarantees for the nonparametric contextual bandits under a relaxed coverage condition which measures how well the optimal action is covered in the batch dataset. We design an adaptive procedure (Algorithm 2) that combines the k-nearest neighbors method with the pessimism principle to achieve the optimal suboptimality gap (up to log factors) without knowledge of the coverage coefficient.

Our work opens a few possible directions to pursue in the future. First, the current upper and lower bounds match up to log factors, and it would be interesting to remove the extra factors by sharpening the analysis. Besides, the smoothness parameter β might be unknown in practice as well. Nevertheless, in the nonparametric bandit literature, it is widely acknowledged that adapting to the unknown smoothness parameter is generally impossible without additional assumptions on the reward functions (Locatelli & Carpentier, 2018; Gur et al., 2022). Understanding what conditions permit smoothness adaptation in offline policy learning is another direction to explore.

References

Yasin Abbasi-Yadkori, Dávid Pál, and Csaba Szepesvári. Improved algorithms for linear stochastic bandits. *Advances in neural information processing systems*, 24, 2011.

Jean-Yves Audibert and Alexandre B Tsybakov. Fast learning rates for plug-in classifiers. *The Annals of Statistics*, 35(2):608–633, 2007.

Peter Auer. Using confidence bounds for exploitation-exploration trade-offs. *Journal of Machine Learning Research*, 3(Nov):397–422, 2002.

Hamsa Bastani and Mohsen Bayati. Online decision making with high-dimensional covariates. *Operations Research*, 68(1):276–294, 2020.

Aurélien Bibaut, Nathan Kallus, Maria Dimakopoulou, Antoine Chambaz, and Mark van Der Laan. Risk minimization from adaptively collected data: Guarantees for supervised and policy learning. *Advances in neural information processing systems*, 34:19261–19273, 2021.

Mariusz Bojarski. End to end learning for self-driving cars. *arXiv preprint arXiv:1604.07316*, 2016.

Changxiao Cai, T Tony Cai, and Hongzhe Li. Transfer learning for contextual multi-armed bandits. *The Annals of Statistics*, 52(1):207–232, 2024.

Kamalika Chaudhuri and Sanjoy Dasgupta. Rates of convergence for nearest neighbor classification. *Advances in Neural Information Processing Systems*, 27, 2014.

Jinglin Chen and Nan Jiang. Information-theoretic considerations in batch reinforcement learning. In *International Conference on Machine Learning*, pp. 1042–1051. PMLR, 2019.

Yaqi Duan, Zeyu Jia, and Mengdi Wang. Minimax-optimal off-policy evaluation with linear function approximation. In *International Conference on Machine Learning*, pp. 2701–2709. PMLR, 2020.

Germano Gabbianelli, Gergely Neu, and Matteo Papini. Importance-weighted offline learning done right. In *International Conference on Algorithmic Learning Theory*, pp. 614–634. PMLR, 2024.

Alexander Goldenshluger and Assaf Zeevi. Woodroofe's one-armed bandit problem revisited. *The Annals of Applied Probability*, 19(4):1603–1633, 2009.

Alexander Goldenshluger and Assaf Zeevi. A linear response bandit problem. *Stochastic Systems*, 3(1):230–261, 2013.

Melody Guan and Heinrich Jiang. Nonparametric stochastic contextual bandits. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 32, 2018.

Yonatan Gur, Ahmadreza Momeni, and Stefan Wager. Smoothness-adaptive contextual bandits. *Operations Research*, 70(6):3198–3216, 2022.

Yichun Hu, Nathan Kallus, and Xiaojie Mao. Smooth contextual bandits: Bridging the parametric and nondifferentiable regret regimes. *Operations Research*, 70(6):3261–3281, 2022.

Nan Jiang and Jiawei Huang. Minimax value interval for off-policy evaluation and policy optimization. *Advances in Neural Information Processing Systems*, 33:2747–2758, 2020.

Nan Jiang and Lihong Li. Doubly robust off-policy value evaluation for reinforcement learning. In *International Conference on Machine Learning*, pp. 652–661. PMLR, 2016.

Rong Jiang and Cong Ma. Batched nonparametric contextual bandits. *arXiv preprint arXiv:2402.17732*, 2024.

Ying Jin, Zhuoran Yang, and Zhaoran Wang. Is pessimism provably efficient for offline rl? In *International Conference on Machine Learning*, pp. 5084–5096. PMLR, 2021.

Ying Jin, Zhimei Ren, Zhuoran Yang, and Zhaoran Wang. Policy learning" without"overlap: Pessimism and generalized empirical bernstein's inequality. *arXiv preprint arXiv:2212.09900*, 2022.

Nathan Kallus. Balanced policy evaluation and learning. *Advances in neural information processing systems*, 31, 2018.

Edward S Kim, Roy S Herbst, Ignacio I Wistuba, J Jack Lee, George R Blumenschein Jr, Anne Tsao, David J Stewart, Marshall E Hicks, Jeremy Erasmus Jr, Sanjay Gupta, et al. The battle trial: personalizing therapy for lung cancer. *Cancer discovery*, 1(1):44–53, 2011.

Aniket Kittur, Ed H Chi, and Bongwon Suh. Crowdsourcing user studies with mechanical turk. In *Proceedings of the SIGCHI conference on human factors in computing systems*, pp. 453–456, 2008.

Samory Kpotufe. k-nn regression adapts to local intrinsic dimension. *Advances in neural information processing systems*, 24, 2011.

Sascha Lange, Thomas Gabel, and Martin Riedmiller. Batch reinforcement learning. In *Reinforcement learning: State-of-the-art*, pp. 45–73. Springer, 2012.

Jeonghwan Lee and Cong Ma. Off-policy estimation with adaptively collected data: the power of online learning. *Advances in Neural Information Processing Systems*, 37:133908–133947, 2024.

Sergey Levine, Aviral Kumar, George Tucker, and Justin Fu. Offline reinforcement learning: Tutorial, review, and perspectives on open problems. *arXiv preprint arXiv:2005.01643*, 2020.

Gen Li, Laixi Shi, Yuxin Chen, Yuejie Chi, and Yuting Wei. Settling the sample complexity of model-based offline reinforcement learning. *The Annals of Statistics*, 52(1):233–260, 2024a.

Gen Li, Weichen Wu, Yuejie Chi, Cong Ma, Alessandro Rinaldo, and Yuting Wei. High-probability sample complexities for policy evaluation with linear function approximation. *IEEE transactions on information theory*, 2024b.

Gen Li, Wenhao Zhan, Jason D Lee, Yuejie Chi, and Yuxin Chen. Reward-agnostic fine-tuning: Provable statistical benefits of hybrid reinforcement learning. *Advances in Neural Information Processing Systems*, 36, 2024c.

Gene Li, Cong Ma, and Nati Srebro. Pessimism for offline linear contextual bandits using ℓ_p confidence sets. *Advances in Neural Information Processing Systems*, 35:20974–20987, 2022.

Lihong Li, Wei Chu, John Langford, and Robert E Schapire. A contextual-bandit approach to personalized news article recommendation. In *Proceedings of the 19th international conference on World wide web*, pp. 661–670, 2010.

Andrea Locatelli and Alexandra Carpentier. Adaptivity to smoothness in x-armed bandits. In *Conference on Learning Theory*, pp. 1463–1492. PMLR, 2018.

Ben London and Ted Sandler. Bayesian counterfactual risk minimization. In *International Conference on Machine Learning*, pp. 4125–4133. PMLR, 2019.

Cong Ma, Banghua Zhu, Jiantao Jiao, and Martin J Wainwright. Minimax off-policy evaluation for multi-armed bandits. *IEEE Transactions on Information Theory*, 68(8):5314–5339, 2022.

Enno Mammen and Alexandre B Tsybakov. Smooth discrimination analysis. *The Annals of Statistics*, 27(6):1808–1829, 1999.

Rémi Munos and Csaba Szepesvári. Finite-time bounds for fitted value iteration. *Journal of Machine Learning Research*, 9(5), 2008.

Mitsuhiko Nakamoto, Simon Zhai, Anikait Singh, Max Sobol Mark, Yi Ma, Chelsea Finn, Aviral Kumar, and Sergey Levine. Cal-ql: Calibrated offline rl pre-training for efficient online fine-tuning. *Advances in Neural Information Processing Systems*, 36, 2024.

Vianney Perchet and Philippe Rigollet. The multi-armed bandit problem with covariates. *Ann. Statist.*, 41(2):693–721, 2013. ISSN 0090-5364. doi: 10.1214/13-AOS1101. URL `https://doi.org/10.1214/13-AOS1101`.

Wei Qian and Yuhong Yang. Kernel estimation and model combination in a bandit problem with covariates. *Journal of Machine Learning Research*, 17(149), 2016.

Paria Rashidinejad, Banghua Zhu, Cong Ma, Jiantao Jiao, and Stuart Russell. Bridging offline reinforcement learning and imitation learning: A tale of pessimism. *Advances in Neural Information Processing Systems*, 34:11702–11716, 2021.

Henry Reeve, Joe Mellor, and Gavin Brown. The k-nearest neighbour ucb algorithm for multi-armed bandits with covariates. In *Algorithmic Learning Theory*, pp. 725–752. PMLR, 2018.

Philippe Rigollet and Assaf Zeevi. Nonparametric bandits with covariates. *arXiv preprint arXiv:1003.1630*, 2010.

Otmane Sakhi, Imad Aouali, Pierre Alquier, and Nicolas Chopin. Logarithmic smoothing for pessimistic off-policy evaluation, selection and learning. *Advances in Neural Information Processing Systems*, 37, 2024.

Laixi Shi, Gen Li, Yuting Wei, Yuxin Chen, and Yuejie Chi. Pessimistic q-learning for offline reinforcement learning: Towards optimal sample complexity. In *International conference on machine learning*, pp. 19967–20025. PMLR, 2022.

Yuda Song, Yifei Zhou, Ayush Sekhari, J Andrew Bagnell, Akshay Krishnamurthy, and Wen Sun. Hybrid rl: Using both offline and online data can make rl efficient. *arXiv preprint arXiv:2210.06718*, 2022.

Joseph Suk and Samory Kpotufe. Self-tuning bandits over unknown covariate-shifts. In *Algorithmic Learning Theory*, pp. 1114–1156. PMLR, 2021.

Adith Swaminathan and Thorsten Joachims. Batch learning from logged bandit feedback through counterfactual risk minimization. *The Journal of Machine Learning Research*, 16(1):1731–1755, 2015.

Shengpu Tang and Jenna Wiens. Model selection for offline reinforcement learning: Practical considerations for healthcare settings. In *Machine Learning for Healthcare Conference*, pp. 2–35. PMLR, 2021.

Philip Thomas and Emma Brunskill. Data-efficient off-policy policy evaluation for reinforcement learning. In *International Conference on Machine Learning*, pp. 2139–2148, 2016.

Alexander B Tsybakov. Optimal aggregation of classifiers in statistical learning. *The Annals of Statistics*, 32(1):135–166, 2004.

Masatoshi Uehara and Wen Sun. Pessimistic model-based offline rl: Pac bounds and posterior sampling under partial coverage. *CoRR*, 2021.

Andrew Wagenmaker and Aldo Pacchiano. Leveraging offline data in online reinforcement learning. In *International Conference on Machine Learning*, pp. 35300–35338. PMLR, 2023.

Lequn Wang, Akshay Krishnamurthy, and Alex Slivkins. Oracle-efficient pessimism: Offline policy optimization in contextual bandits. In *International Conference on Artificial Intelligence and Statistics*, pp. 766–774. PMLR, 2024.

Yu-Xiang Wang, Alekh Agarwal, and Miroslav Dudık. Optimal and adaptive off-policy evaluation in contextual bandits. In *International Conference on Machine Learning*, pp. 3589–3597. PMLR, 2017.

Michael Woodroofe. A one-armed bandit problem with a concomitant variable. *Journal of the American Statistical Association*, 74(368):799–806, 1979.

Tengyang Xie and Nan Jiang. Batch value-function approximation with only realizability. In *International Conference on Machine Learning*, pp. 11404–11413. PMLR, 2021.

Tengyang Xie, Ching-An Cheng, Nan Jiang, Paul Mineiro, and Alekh Agarwal. Bellman-consistent pessimism for offline reinforcement learning. *Advances in neural information processing systems*, 34:6683–6694, 2021a.

Tengyang Xie, Nan Jiang, Huan Wang, Caiming Xiong, and Yu Bai. Policy finetuning: Bridging sample-efficient offline and online reinforcement learning. *Advances in neural information processing systems*, 34:27395–27407, 2021b.

Yuhong Yang and Dan Zhu. Randomized allocation with nonparametric estimation for a multi-armed bandit problem with covariates. *Ann. Statist.*, 30(1):100–121, 2002. doi: 10.1214/aos/1015362186. URL `https://doi.org/10.1214/aos/1015362186`.

Zhouhao Yang, Yihong Guo, Pan Xu, Anqi Liu, and Animashree Anandkumar. Distributionally robust policy gradient for offline contextual bandits. In *International Conference on Artificial Intelligence and Statistics*, pp. 6443–6462. PMLR, 2023.

Ekim Yurtsever, Jacob Lambert, Alexander Carballo, and Kazuya Takeda. A survey of autonomous driving: Common practices and emerging technologies. *IEEE access*, 8:58443–58469, 2020.

Andrea Zanette, Martin J Wainwright, and Emma Brunskill. Provable benefits of actor-critic methods for offline reinforcement learning. *Advances in neural information processing systems*, 34: 13626–13640, 2021.

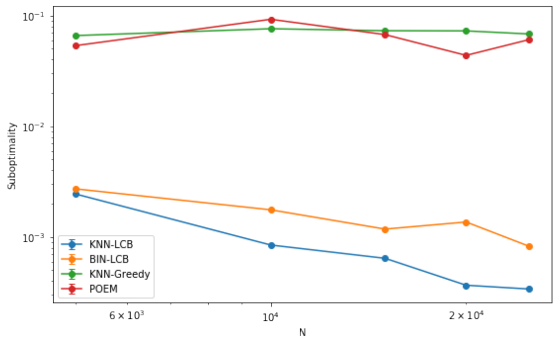
Ruohan Zhan, Zhimei Ren, Susan Athey, and Zhengyuan Zhou. Policy learning with adaptively collected data. *Management Science*, 70(8):5270–5297, 2024.

Wenhao Zhan, Baihe Huang, Audrey Huang, Nan Jiang, and Jason Lee. Offline reinforcement learning with realizability and single-policy concentrability. In *Conference on Learning Theory*, pp. 2730–2775. PMLR, 2022.

Junyu Zhang, Alec Koppel, Amrit Singh Bedi, Csaba Szepesvari, and Mengdi Wang. Variational policy gradient method for reinforcement learning with general utilities. *Advances in Neural Information Processing Systems*, 33:4572–4583, 2020.

Zhengyuan Zhou, Susan Athey, and Stefan Wager. Offline multi-action policy learning: Generalization and optimization. *Operations Research*, 71(1):148–183, 2023.

Banghua Zhu, Michael Jordan, and Jiantao Jiao. Principled reinforcement learning with human feedback from pairwise or k-wise comparisons. In *International Conference on Machine Learning*, pp. 43037–43067. PMLR, 2023.



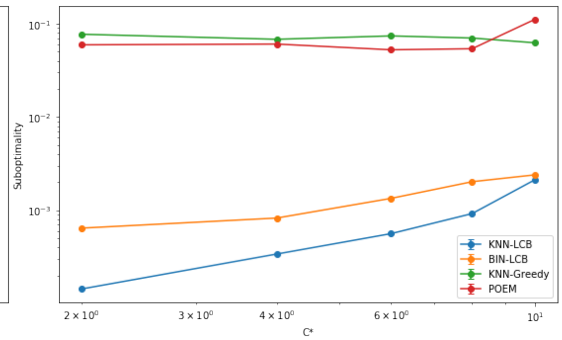


Figure 1: Suboptimality vs. N ($C^\star = 4$).

Figure 2: Suboptimality vs. $C^\star$ ($N = 25000$).

A Experiments

We evaluate the proposed pessimistic nonparametric algorithms using a controlled synthetic contextual bandit environment with smooth, nonlinear reward functions and a logging policy with tunable coverage parameter C^*. Policies are learned from logged data of size N, then evaluated using true expected rewards on fresh test contexts. We report the suboptimality

$$\mathsf{Subopt}(\pi) = \mathbb{E}[f_{\pi^*(X)}(X) - f_{\pi(X)}(X)].$$

Baselines. We compare to two standard offline bandit baselines:

- KNN-Greedy: A nonparametric estimator that chooses actions via k-nearest neighbor reward estimates, without uncertainty control.
- POEM (Swaminathan & Joachims, 2015): A self-normalized IPS method with a global variance penalty and a linear softmax policy class.

Suboptimality vs. Sample Size. Figure 1 shows suboptimality vs. N at fixed coverage $C^\star = 4$. A few observations are in order.

- KNN-LCB achieves the lowest error across all sample sizes and decreases steadily with N.
- BIN-LCB is consistently second-best and displays a similar improvement trend.
- POEM performs worse than both pessimistic methods but is generally slightly better than KNN-Greedy.
- KNN-Greedy remains nearly flat as N increases, reflecting its lack of pessimism.

Overall, the pessimistic nonparametric methods outperform both baselines, with gaps widening as the dataset grows.

Suboptimality vs. Coverage. Figure 2 shows suboptimality vs. $C^\star$ at fixed $N = 25{,}000$. Recall that as $C^\star$ increases, the coverage of the optimal action in the offline data decreases, leading to larger error.

- KNN-LCB achieves the lowest error for all coverage levels and degrades gracefully as C^* increases.
- BIN-LCB exhibits similar behavior but maintains a consistent gap above KNN-LCB.
- POEM again outperforms KNN-Greedy in general, but is still worse than the nonparametric methods.
- KNN-Greedy is nearly insensitive to C^* and remains dominated by both pessimistic methods.

These results demonstrate that the proposed algorithms adapt effectively to varying coverage, whereas POEM and KNN-GREEDY do not.

Summary. Across both experimental sweeps, KNN-LCB and BIN-LCB clearly outperform non-pessimistic and IPS-based baselines. POEM performs slightly better than KNN-GREEDY in several settings, but both are substantially worse than the pessimistic nonparametric methods, confirming the importance of local coverage-adaptive uncertainty quantification.

B PROOF OF UPPER BOUNDS

B.1 PROOF OF THEOREM 4.1

Define $M \asymp (N/C^\star)^{1/(2\beta+d)}$. Let $\{B_j\}_{j=1}^{M^d}$ be a regular partition of $\mathcal{X}$. Define $c_1 = 2(\sqrt{4\underline{c}^{-1}K\log\delta^{-1}} + \log N \cdot d^{\beta/2})$ and $c = c_1 + 2Ld^{\beta/2}$. Let $\mathcal{J}$, $\mathcal{J}_1^c$, $\mathcal{J}_2^c$ be defined as in equations (5), (6) and (7).

For any $j \in \mathcal{J} \cup \mathcal{J}_2^c$ and $x \in B_j$, let $k_j = \max\{q \in [N] : X_{\tau_q(x)} \in B_j\}$. Let $a^\star \in \mathcal{I}_j^\star$ be the near optimal arm with coverage in B_j given by Lemma 5.2. Let $\tilde{\pi}(x)$ be the output of Algorithm 2. Define

$$\mathcal{A}_j(x) = \{N_{k_j}^{a^\star}(x) \geq \frac{1}{2K} P_X(B_j) \cdot \frac{N}{C^\star}\},$$

and

$$\mathcal{E}_j(x) = \{f_{a^\star}(x) - f_{\tilde{\pi}(x)}(x) \leq 2U_{k_j}^{a^\star}(x)\} \cap \mathcal{A}_j(x). \tag{11}$$

The next two lemmas state that these good events happen with high probability.

Lemma B.1. *Suppose $j \in \mathcal{J} \cup \mathcal{J}_2^c$ and $x \in B_j$. With probability at least $1 - N^{-3}$, one has*

$$f_{a^\star}(x) - f_{\tilde{\pi}(x)}(x) \leq 2U_{k_j}^{a^\star}(x).$$

See Section B.2.5 for the proof.

Lemma B.2. *Suppose $j \in \mathcal{J} \cup \mathcal{J}_2^c$ and $x \in B_j$. Assume $\mu(a^\star \mid B_j) \geq 1/(C^\star K)$. One has*

$$\mathbb{P}(\mathcal{A}_j^c(x)) \leq \frac{1}{N^5}.$$

See Section B.2.6 for the proof.

The excess risk can be decomposed as

$$\begin{aligned}\mathbb{E}\left[f^\star(X) - f_{\tilde{\pi}(X)}(X)\right] &= \mathbb{E}\left[\sum_{j=1}^{M^d}\left(f^\star(X) - f_{\tilde{\pi}(X)}(X)\right)\mathbf{1}\{X \in B_j\}\right] \\ &= \mathbb{E}\Bigg[\underbrace{\sum_{j\in\mathcal{J}}\left(f^\star(X) - f_{\tilde{\pi}(X)}(X)\right)\mathbf{1}\{X \in B_j\}}_{U} + \underbrace{\sum_{j\in\mathcal{J}^c}\left(f^\star(X) - f_{\tilde{\pi}(X)}(X)\right)\mathbf{1}\{X \in B_j\}}_{V}\Bigg].\end{aligned}$$

B.1.1 CONTROL OF TERM V

We further decompose

$$V = \underbrace{\sum_{j\in\mathcal{J}_1^c}\mathbb{E}\left[\left(f^\star(X) - f_{\tilde{\pi}(X)}(X)\right)\mathbf{1}\{X \in B_j\}\right]}_{V_1} + \underbrace{\sum_{j\in\mathcal{J}_2^c}\mathbb{E}\left[\left(f^\star(X) - f_{\tilde{\pi}(X)}(X)\right)\mathbf{1}\{X \in B_j\}\right]}_{V_2}.$$

For V_1, Lemma 5.1 gives

$$\mathbb{E}[V_1] \leq c^{1+\alpha} C_\alpha M^{-\beta(1+\alpha)}.$$

Next, we upper bound V_2. Fix any $j \in \mathcal{J}_2^c$. Define $\mathcal{I}_j^\star = \{a \in \mathcal{I} : \exists x \in B_j, f_a(x) = f^\star(x)\}$. Let $a^\star \in \mathcal{I}_j^\star$ be the near optimal arm with coverage in B_j given by Lemma 5.2, so that $\mu(a^\star \mid B_j) \geq 1/(KC^\star)$. We have the following decomposition,

$$\begin{aligned}\mathbb{E}[(f^\star(X) - f_{\tilde{\pi}(X)}(X))\mathbf{1}\{X \in B_j\}] &= \mathbb{E}[(f^\star(X) - f_{\tilde{\pi}(X)}(X))\mathbf{1}\{X \in B_j\}(\mathbf{1}\{\mathcal{E}_j(X)\} + \mathbf{1}\{\mathcal{E}_j^c(X)\})] \\ &\leq \mathbb{E}[(f^\star(X) - f_{\tilde{\pi}(X)}(X))\mathbf{1}\{X \in B_j, \mathcal{E}_j(X)\}] + \mathbb{P}(X \in B_j, \mathcal{E}_j^c(X)) \\ &\leq \mathbb{E}[2U_{k_j}^{a^\star}(X)\mathbf{1}\{\mathcal{A}_j(X)\}]\bar{c}M^{-d} + \frac{2}{N^3} \\ &\leq c_1 M^{-\beta} \cdot \bar{c}M^{-d} + \frac{2}{N^3} \leq 2\bar{c}c_1 M^{-d-\beta},\end{aligned}$$

where the second inequality is due to the definition of $\mathcal{E}_j(X)$, and uses Lemma B.1 and Lemma B.2; the third inequality applies the definition of $\mathcal{A}_j(X)$. Reuse relation (8) we have $|\mathcal{J}_2^c| \leq \underline{c}^{-1}C_\alpha c^\alpha M^{d-\alpha\beta}$. Consequently,

$$\mathbb{E}[V_2] \leq \underline{c}^{-1}C_\alpha c^\alpha M^{d-\alpha\beta} \cdot \left(2\bar{c}c_1 M^{-d-\beta}\right) < 2\underline{c}^{-1}\bar{c}C_\alpha c^{1+\alpha}M^{-\beta(1+\alpha)}.$$

Combining the bounds of V_1 and V_2 yields

$$\mathbb{E}[V] = \mathbb{E}[V_1] + \mathbb{E}[V_2] \leq C_\alpha c^{1+\alpha}M^{-\beta(1+\alpha)} + 2\underline{c}^{-1}\bar{c}C_\alpha c^{1+\alpha}M^{-\beta(1+\alpha)} = (1 + 2\underline{c}^{-1}\bar{c})C_\alpha c^{1+\alpha}M^{-\beta(1+\alpha)}.$$

B.1.2 Control of term U

Fix any $j \in \mathcal{J}$. Let $\mathcal{I}_j^\star = \{a \in \mathcal{I} : f_a(x_j) = f^\star(x_j)\}$ where $x_j \in B_j$ satisfies $f^{(1)}(x_j) - f^{(2)}(x_j) > cM^{-\beta}$ by definition of $\mathcal{J}$. Let $a^\star \in \mathcal{I}_j^\star$ be the near optimal arm with coverage in B_j given by Lemma 5.2, so that $\mu(a^\star \mid B_j) \geq 1/(KC^\star)$. Applying Lemma B.4 we obtain

$$\begin{aligned}&\mathbb{E}[(f^\star(X) - f_{\tilde{\pi}(X)}(X))\mathbf{1}\{X \in B_j\}] \\ &\quad\leq cM^{-\beta}\mathbb{P}(X \in B_j, 0 < f^{(1)}(X) - f^{(2)}(X) \leq cM^{-\beta}) + \mathbb{E}[\mathbf{1}\{X \in B_j, f_{a^\star}(X) - f_{\tilde{\pi}(X)}(X) \geq c_1 M^{-\beta}\}].\end{aligned} \tag{12}$$

We can further decompose the second term above into

$$\begin{aligned}&\mathbb{E}[\mathbf{1}\{X \in B_j, f_{a^\star}(X) - f_{\tilde{\pi}(X)}(X) \geq c_1 M^{-\beta}\}] \\ &\quad= \mathbb{E}[\mathbf{1}\{X \in B_j, f_{a^\star}(X) - f_{\tilde{\pi}(X)}(X) \geq c_1 M^{-\beta}\}(\mathbf{1}\{\mathcal{A}_j(X)\} + \mathbf{1}\{\mathcal{A}_j^c(X)\})] \\ &\quad\leq \mathbb{E}[\mathbf{1}\{X \in B_j, f_{a^\star} - f_{\tilde{\pi}(X)} \geq c_1 M^{-\beta}\}\mathbf{1}\{\mathcal{A}_j(X)\}] + \mathbb{P}(\mathcal{A}_j^c(X)) \\ &\quad\leq \mathbb{E}[\mathbf{1}\{X \in B_j, f_{a^\star} - f_{\tilde{\pi}(X)} \geq 2U_{k_j}^{a^\star}(X)\}\mathbf{1}\{\mathcal{A}_j(X)\}] + \mathbb{P}(\mathcal{A}_j^c(X)) \\ &\quad\leq \frac{2}{N^3},\end{aligned} \tag{13}$$

where the penultimate inequality uses the fact that $c_1 M^{-\beta} \geq 2U_{k_j}^{a^\star}(x)$ under $\mathcal{A}_j(x)$; the last inequality is due to Lemma B.1 and Lemma B.2. Combining relations (12) and (13), we reach

$$\begin{aligned}\mathbb{E}[U] &= \sum_{j \in \mathcal{J}} \mathbb{E}\left[\left(f^\star(X) - f_{\pi(X)}(X)\right)\mathbf{1}\{X \in B_j\}\right] \\ &\leq \sum_{j \in \mathcal{J}} \left(cM^{-\beta}\mathbb{P}(X \in B_j, 0 < f^{(1)}(X) - f^{(2)}(X) \leq cM^{-\beta}) + \frac{2}{N^3}\right) \\ &\leq cM^{-\beta}\mathbb{P}(0 < f^{(1)}(X) - f^{(2)}(X) \leq cM^{-\beta}) + M^d \cdot \frac{2}{N^3} \\ &\leq 2C_\alpha c^{1+\alpha}M^{-\beta(1+\alpha)},\end{aligned}$$

where the last inequality is uses the margin condition. Therefore,

$$\begin{aligned}\mathbb{E}\left[f^\star(X) - f_{\hat\pi(X)}(X)\right] &= \mathbb{E}[U] + \mathbb{E}[V] \\ &\le 2C_\alpha c^{1+\alpha} M^{-\beta(1+\alpha)} + (1+2\underline{c}^{-1}\overline{c})C_\alpha c^{1+\alpha} M^{-\beta(1+\alpha)} \\ &= (3+2\underline{c}^{-1}\overline{c})C_\alpha c^{1+\alpha} M^{-\beta(1+\alpha)} \\ &= (3+3\underline{c}^{-1}\overline{c})C_\alpha c^{1+\alpha} \left(\frac{N}{C^\star}\right)^{-\frac{\beta(1+\alpha)}{2\beta+d}}.\end{aligned}$$

B.2 Proof of helper lemmas

B.2.1 Proof of Lemma 5.1

For any $B_j \in \mathcal{J}_1^c$, there exists $x_j \in B_j$ such that $f^{(1)}(x_j) = f^{(2)}(x_j) = f_a(x_j)$ for all $a \in \mathcal{I}$. Consequently, the smoothness condition gives us $f^{(1)}(x) - f_a(x) \le cM^{-\beta}$ for all $x \in B_j$. Since the set $\{x \in \mathcal{X} : f^{(1)}(x) = f^{(2)}(x)\}$ does not incur any error, we have

$$\begin{aligned}\sum_{j\in\mathcal{J}_1^c} \mathbb{E}\left[\left(f^\star(X) - f_{\pi(X)}(X)\right)\mathbf{1}\{X\in B_j\}\right] &\le \sum_{j\in\mathcal{J}_1^c} cM^{-\beta} P_X\left(X\in B_j, 0 < f^{(1)}(X) - f^{(2)}(X) \le cM^{-\beta}\right) \\ &\le cM^{-\beta} P_X\left(0 < f^{(1)}(X) - f^{(2)}(X) \le cM^{-\beta}\right) \\ &\le C_\alpha c^{1+\alpha} M^{-\beta(1+\alpha)}.\end{aligned}$$

B.2.2 Proof of Lemma 5.2

By definition, for any $k \in \mathcal{I}\setminus\mathcal{I}_j^\star$, one has $f^\star(x) - f^k(x) > 0$ for all $x \in B_j$. Since

$$\begin{aligned}\sum_{a\in\mathcal{I}_j^\star} \mu(a \mid B_j) &= \frac{1}{P_X(B_j)} \sum_{a\in\mathcal{I}_j^\star} \int_{B_j} \mu(a\mid x)\mathrm{d}P_X(x) \\ &= \frac{1}{P_X(B_j)} \int_{B_j} \sum_{a\in\mathcal{I}_j^\star} \mu(a\mid x)\mathrm{d}P_X(x) \\ &\ge \frac{1}{P_X(B_j)} \int_{B_j} \frac{1}{C^\star}\mathrm{d}P_X(x) = \frac{1}{C^\star},\end{aligned}$$

where the inequality is due to $\sum_{a\in\mathcal{I}_j^\star}\mu(a\mid x) \ge 1/C^\star$, there exists $a^\star \in \mathcal{I}_j^\star$ such that

$$\mu(a^\star \mid B_j) \ge \frac{1}{C^\star}\cdot\frac{1}{|\mathcal{I}_j^\star|} \ge \frac{1}{KC^\star}.$$

B.2.3 Proof of Lemma 5.3

Denote $\mathcal{A}_j' = \{\hat f_{a,j} - b_j(a) \le f_{a,j} \le \hat f_{a,j} + b_j(a) \text{ for all } a \in \mathcal{I}\}$. By Lemma B.5, we have $\mathbb{P}(\mathcal{A}_j') \ge 1 - N^{-3}$. Since $\mathcal{A}_j'$ implies

$$f_{\star,j} \le \hat f_{\star,j} + b_j(a^\star) = \hat f_{\star,j} - b_j(a^\star) + 2b_j(a^\star) \le \hat f_{\hat\pi_j,j} - b_j(\hat\pi_j) + 2b_j(a^\star) \le f_{\hat\pi_j,j} + 2b_j(a^\star),$$

we can conclude $\mathbb{P}(\{f_{\star,j} - f_{\hat\pi_j,j} \le 2b_j(a^\star)\}) \ge \mathbb{P}(\mathcal{A}_j') \ge 1 - N^{-3}$.

B.2.4 Proof of Lemma 5.4

For simplicity we drop the subscript on j and write B for B_j throughout the proof. Recall $N_B(a^\star) = \sum_{i=1}^N \mathbf{1}\{X_i \in B, A_i = a^\star\}$. Denote $p_i = \mathbb{P}(X_i \in B, A_i = a^\star)$. Define

$$Z_i = \mathbf{1}\{X_i\in B, A_i = a^\star\} - \mathbb{E}[\mathbf{1}\{X_i \in B, A_i = a^\star\} \mid \mathcal{F}_{i-1}].$$

One has $\mathbb{E}[\mathbf{1}\{X_i \in B, A_i = a^\star\} \mid \mathcal{F}_{i-1}] = p_i$, and it can be easily verified that $\{Z_i\}_{i=1}^N$ is a bounded martingale-difference sequence with $|Z_i| \le 1$. Besides,

$$\sum_{i=1}^N \mathbb{E}[Z_i^2 \mid \mathcal{F}_{i-1}] = \sum_{i=1}^N p_i(1-p_i) \le \sum_{i=1}^N p_i.$$

By Freedman's inequality, we have

$$\mathbb{P}\left(|\sum_{i=1}^{N} Z_i| \geq \sqrt{2\left(\sum_{i=1}^{N} p_i\right)\log(\frac{2}{\delta})}\right) \leq \delta.$$

Therefore, with probability at least $1-\delta$,

$$|N_B(a^\star) - P_X(B)\cdot N\mu(a^\star \mid B)| \leq \sqrt{3\log(\frac{2}{\delta})P_X(B)\cdot N\mu(a^\star \mid B)},$$

where we have used the relation $\mu(\cdot \mid x) = \frac{1}{N}\sum_{i=1}^{N}\mu_i(\cdot \mid x)$. Since $P_X(B)\cdot(N/C^\star) \geq 20K\log(2N^5)$ and $\delta = 1/N^5$, one has with probability at least $1-1/N^5$,

$$\begin{aligned} N_B(a^\star) &\geq P_X(B)\cdot N\mu(a^\star \mid B) - \sqrt{3\log(\frac{2}{\delta})P_X(B)\cdot N\mu(a^\star \mid B)} \\ &\geq \frac{1}{2}P_X(B)\cdot N\mu(a^\star \mid B) \geq \frac{1}{2K}P_X(B)\cdot\frac{N}{C^\star}. \end{aligned}$$

B.2.5 Proof of Lemma B.1

Denote $\mathcal{A}_j' = \{\hat{f}_{a,k} - U_k^a(x) \leq f_a(x) \leq \hat{f}_{a,k}(x) + U_k^a(x) \text{ for all } a \in \mathcal{I}, k \in [N-1]\}$. By Lemma B.6, we have $\mathbb{P}(\mathcal{A}_j') \geq 1 - N^{-3}$. Under $\mathcal{A}_j'$, we have

$$\begin{aligned} f_{a^\star}(x) &\leq \hat{f}_{a^\star,k(a^\star)}(x) + U_{k(a^\star)}^{a^\star}(x) \\ &= \hat{f}_{a^\star,k(a^\star)}(x) - U_{k(a^\star)}^{a^\star}(x) + 2U_{k(a^\star)}^{a^\star}(x) \\ &\overset{\text{(i)}}{\leq} \hat{f}_{\tilde{\pi}(x),k(\tilde{\pi}(x))}(x) - U_{k(\tilde{\pi}(x))}^{\tilde{\pi}(x)}(x) + 2U_{k(a^\star)}^{a^\star}(x) \\ &\leq f_{\tilde{\pi}(x)}(x) + 2U_{k(a^\star)}^{a^\star}(x) \overset{\text{(ii)}}{\leq} f_{\tilde{\pi}(x)}(x) + 2U_{k_j}^{a^\star}(x), \end{aligned}$$

where step (i) uses the definition of Algorithm 2, and step (ii) is due to $U_{k(a^\star)}^{a^\star}(x) \leq U_{k_j}^{a^\star}(x)$. Consequently,

$$\mathbb{P}(\{f_{a^\star}(x) - f_{\tilde{\pi}(x)}(x) \leq 2U_{k_j}^{a^\star}(x)\}) \geq \mathbb{P}(\mathcal{A}_j') \geq 1 - N^{-3}.$$

B.2.6 Proof of Lemma B.2

Recall $k_j = \max\{q \in [N] : X_{\tau_q(x)} \in B_j\}$. By definition, one has

$$N_{k_j}^{a^\star}(x) \geq \sum_{i=1}^{N}\mathbf{1}\{X_i \in B_j, A_i = a^\star\} = N_j(a^\star).$$

By Lemma 5.4,

$$\mathbb{P}(\mathcal{A}_j^c(x)) \leq \mathbb{P}(\mathcal{A}_j^c) \leq \frac{1}{N^5}.$$

B.3 Auxiliary lemmas

Lemma B.3. *For any $j \in \mathcal{J}_2^c$, one has*

$$\mathbb{E}[(f^\star(X) - f_{\hat{\pi}(X)}(X))\mathbf{1}\{X \in B_j\}] \leq 3\bar{c}cM^{-d-\beta}.$$

Proof. We have the following decomposition,

$$\begin{aligned} \mathbb{E}[(f^\star(X) - f_{\hat{\pi}(X)}(X))\mathbf{1}\{X \in B_j\}] &= \mathbb{E}[(f^\star(X) - f_{\hat{\pi}(X)}(X))\mathbf{1}\{X \in B_j\}(\mathbf{1}\{\mathcal{E}_j\} + \mathbf{1}\{\mathcal{E}_j^c\})] \\ &\leq \mathbb{E}[(f^\star(X) - f_{\hat{\pi}(X)}(X))\mathbf{1}\{X \in B_j, \mathcal{E}_j\}] + \mathbb{P}(\mathcal{E}_j^c) \\ &\leq \left(\mathbb{E}[(f_{\star,j} - f_{\hat{\pi}_j,j})\mathbf{1}\{\mathcal{E}_j\}] + cM^{-\beta}\right)\bar{c}M^{-d} + \mathbb{P}(\mathcal{E}_j^c), \end{aligned}$$

where the last inequality uses $\mathbb{E}[f^\star(X) \mid X \in B_j] \le f_{\star,j} + cM^{-\beta}$ under the smoothness condition. Applying Lemma 5.3 and Lemma 5.4 , we reach

$$\begin{aligned}\mathbb{E}[(f^\star(X) - f_{\hat\pi(X)}(X))\mathbf{1}\{X \in B_j\}] &\le \left(\mathbb{E}[(f_{\star,j} - f_{\hat\pi_j,j})\mathbf{1}\{\mathcal{E}_j\}] + cM^{-\beta}\right)\bar{c}M^{-d} + \frac{2}{N^3}\\ &\le \left(\mathbb{E}[2b_j(a^\star)\mathbf{1}\{\mathcal{A}_j\}] + cM^{-\beta}\right)\bar{c}M^{-d} + \frac{2}{N^3}\\ &\le (c_1 + c)\,M^{-\beta}\cdot\bar{c}M^{-d} + \frac{2}{N^3} \le 3\bar{c}cM^{-d-\beta},\end{aligned}$$

where the second inequality is due to the definition of $\mathcal{E}_j$, and the third inequality uses the property of $\mathcal{A}_j$. ☐

Lemma B.4. *Assume $c > 2Ld^{\beta/2}$. For any $j \in \mathcal{J}$ and any policy $\pi : \mathcal{X} \to [K]$, one has*

$$\begin{aligned}&\mathbb{E}[(f^\star(X) - f_{\pi(X)}(X))\mathbf{1}\{X \in B_j\}]\\ &\quad\le cM^{-\beta}\mathbb{P}(X \in B_j, 0 < f^{(1)}(X) - f^{(2)}(X) \le cM^{-\beta}) + \mathbb{E}[\mathbf{1}\{X \in B_j, f_{a^\star}(X) - f_{\pi(X)}(X) \ge (c - 2Ld^{\beta/2})M^{-\beta}\}].\end{aligned}$$

Furthermore, if π satisfies $\pi(x) = \pi_j \in [K]$ for all $x \in B_j$, one has

$$\begin{aligned}&\mathbb{E}[(f^\star(X) - f_{\pi(X)}(X))\mathbf{1}\{X \in B_j\}]\\ &\quad\le cM^{-\beta}\mathbb{P}(X \in B_j, 0 < f^{(1)}(X) - f^{(2)}(X) \le cM^{-\beta}) + \mathbb{E}[\mathbf{1}\{X \in B_j, f_{\star,j} - f_{\pi_j,j} \ge (c - 2Ld^{\beta/2})M^{-\beta}\}].\end{aligned}$$

Proof. Recall $\mathcal{I}_j^\star = \{a \in \mathcal{I} : f_a(x_j) = f^\star(x_j)\}$. We have the following decomposition,

$$\begin{aligned}&\mathbb{E}[(f^\star(X) - f_{\pi(X)}(X))\mathbf{1}\{X \in B_j\}]\\ &\quad= \mathbb{E}[(f^\star(X) - f_{\pi(X)}(X))\mathbf{1}\{X \in B_j\}\mathbf{1}\{\pi(X) \in \mathcal{I}_j^\star\}] + \mathbb{E}[(f^\star(X) - f_{\pi(X)}(X))\mathbf{1}\{X \in B_j\}\mathbf{1}\{\pi(X) \in \mathcal{I} \setminus \mathcal{I}_j^\star\})].\end{aligned} \tag{14}$$

For any $x \in B_j$ and $a \in \mathcal{I}_j^\star$, we have

$$f^\star(x) - f_a(x) \le cM^{-\beta}\mathbf{1}\{0 < f^{(1)}(x) - f^{(2)}(x) \le cM^{-\beta}\}.$$

So the first term in (14) can be bounded by

$$\mathbb{E}[(f^\star(X) - f_{\pi(X)}(X))\mathbf{1}\{X \in B_j\}\mathbf{1}\{\pi(X) \in \mathcal{I}_j^\star\}] \le cM^{-\beta}\mathbb{P}(X \in B_j, 0 < f^{(1)}(X) - f^{(2)}(X) \le cM^{-\beta}).$$

For any $a' \in \mathcal{I} \setminus \mathcal{I}_j^\star$ and $a \in \mathcal{I}_j^\star$, by definition $f_a(x_j) - f_{a'}(x_j) > cM^{-\beta}$. Consequently, the smoothness condition gives us

$$f_a(x) - f_{a'}(x) \ge (c - 2Ld^{\beta/2})M^{-\beta} \tag{15}$$

for all $x \in B_j$. Therefore, the second term in (14) can be bounded by

$$\begin{aligned}\mathbb{E}[(f^\star(X) - f_{\pi(X)}(X))\mathbf{1}\{X \in B_j\}\mathbf{1}\{\pi(X) \in \mathcal{I} \setminus \mathcal{I}_j^\star\})] &\le \mathbb{E}[\mathbf{1}\{X \in B_j, \pi(X) \in \mathcal{I} \setminus \mathcal{I}_j^\star\}]\\ &\le \mathbb{E}[\mathbf{1}\{X \in B_j, f_{a^\star}(X) - f_{\pi(X)}(X) \ge (c - 2Ld^{\beta/2})M^{-\beta}\}].\end{aligned}$$

Since relation (15) implies $f_{a,j} - f_{a',j} \ge (c - 2Ld^{\beta/2})M^{-\beta}$, when $\pi(x) = \pi_j \in [K]$ for all $x \in B_j$, one has

$$\begin{aligned}\mathbb{E}[(f^\star(X) - f_{\pi(X)}(X))\mathbf{1}\{X \in B_j\}\mathbf{1}\{\pi(X) \in \mathcal{I} \setminus \mathcal{I}_j^\star\})] &\le \mathbb{E}[\mathbf{1}\{X \in B_j, \pi(X) \in \mathcal{I} \setminus \mathcal{I}_j^\star\}]\\ &\le \mathbb{E}[\mathbf{1}\{X \in B_j, f_{\star,j} - f_{\pi_j,j} \ge (c - 2Ld^{\beta/2})M^{-\beta}\}].\end{aligned}$$

Combining all the above finishes the proof. ☐

Lemma B.5. *With probability at least $1 - N^{-3}$, one has*

$$\hat{f}_{a,j} - b_j(a) \le f_{a,j} \le \hat{f}_{a,j} + b_j(a) \text{ for all } a \in \mathcal{I}.$$

Proof. Fix any $a \in \mathcal{I}$. Recall

$$\hat{f}_{a,j} = \frac{1}{N_j(a)} \cdot \sum_{i=1}^{N} \mathbf{1}\{X_i \in B_j, A_i = a\} Y_i^a.$$

Denote $\epsilon_i = \mathbf{1}\{X_i \in B_j, A_i = a\}$, and $Z_i = \mathbf{1}\{X_i \in B_j\}(Y_i^a - f_{a,j})$. By Corollary 5 in (Reeve et al., 2018), one has

$$\mathbb{P}\left(|\hat{f}_{a,j} - f_{a,j}| > b_j(a)\right) = \mathbb{P}\left(|\sum_{i=1}^{N} \epsilon_i Z_i| > \sqrt{2\log(1/\delta)\sum_{i=1}^{N}\epsilon_i}\right) \le e\left(\log(1/\delta)\log N\right)\delta.$$

Applying union bound we reach

$$\mathbb{P}((\mathcal{A}_j')^c) \le Ke\left(\log(1/\delta)\log N\right)\delta \le \frac{1}{N^3}.$$

□

Lemma B.6. *For any $x \in \mathcal{X}$, with probability at least $1 - N^{-3}$,*

$$\hat{f}_{a,k} - U_k^a(x) \le f_a(x) \le \hat{f}_{a,k}(x) + U_k^a(x) \text{ for all } a \in \mathcal{I}, k \in [N].$$

Proof. Fix $a \in \mathcal{I}$ and $k \in [N]$. Denote $\mathcal{G}_{a,k} = \{\hat{f}_{a,k} - U_k^a(x) \le f_a(x) \le \hat{f}_{a,k}(x) + U_k^a(x)\}$. On $\mathcal{G}_{a,k}^c$, one has $|\hat{f}_{a,k}(x) - f_a(x)| > U_k^a(x)$. Besides,

$$\begin{aligned}
|\hat{f}_{a,k}(x) - f_a(x)| &= |\frac{1}{N_k^a(x)}\sum_{s\in\Gamma_k}\left(\mathbf{1}\{A_s = a\}Y_s - f_a(x)\right)| \\
&= |\frac{1}{N_k^a(x)}\sum_{s\in\Gamma_k}\left(\mathbf{1}\{A_s = a\}Y_s - f_a(X_s) + f_a(X_s) - f_a(x)\right)| \\
&\le |\frac{1}{N_k^a(x)}\sum_{s\in\Gamma_k}\left(\mathbf{1}\{A_s = a\}Y_s - f_a(X_s)\right)| + |\frac{1}{N_k^a(x)}\sum_{s\in\Gamma_k}\left(f_a(X_s) - f_a(x)\right)| \\
&\le |\frac{1}{N_k^a(x)}\sum_{s\in\Gamma_k}\left(\mathbf{1}\{A_s = a\}Y_s - f_a(X_s)\right)| + \log N \cdot r_k(x)^\beta,
\end{aligned}$$

where the penultimate step uses triangle inequality, and the last inequality is due to

$$|f_a(X_s) - f_a(x)| \overset{\text{(i)}}{\le} L\|x - X_s\|^\beta \overset{\text{(ii)}}{\le} L \cdot r_k(x)^\beta \overset{\text{(iii)}}{\le} \log N \cdot r_k(x)^\beta.$$

Here, step (i) is due to Assumption 2.1; step (ii) uses the definition of $r_k(x)$; step (iii) holds for N sufficiently large. This leads to

$$\sqrt{\frac{2\log(1/\delta)}{N_k^a(x)}} + \log N \cdot r_k(x)^\beta = U_k^a(x) < |\frac{1}{N_k^a(x)}\sum_{s\in\Gamma_k}\left(\mathbf{1}\{A_s = a\}Y_s - f_a(X_s)\right)| + \log N \cdot r_k(x)^\beta,$$

and we have

$$|\sum_{s\in\Gamma_k}\left(\mathbf{1}\{A_s = a\}Y_s - f_a(X_s)\right)| > \sqrt{2\log(1/\delta)N_k^a(x)}.$$

By Corollary 5 in (Reeve et al., 2018),

$$\mathbb{P}\left(|\sum_{s\in\Gamma_k}\left(\mathbf{1}\{A_s = a\}Y_s - f_a(X_s)\right)| > \sqrt{2\log(1/\delta)N_k^a(x)} \mid \{X_s\}_{s\in[N]}\right) \le e\left(\log(1/\delta)\log N\right)\delta.$$

Therefore, using the law of total expectation we reach

$$\mathbb{P}(\mathcal{G}_{a,k}^c) \le \mathbb{P}\left(|\sum_{s\in\Gamma_k}\left(\mathbf{1}\{A_s = a\}Y_s - f_a(X_s)\right)| > \sqrt{2\log(1/\delta)N_k^a(x)}\right) \le e\left(\log(1/\delta)\log N\right)\delta.$$

Applying union bound to get

$$\mathbb{P}(\cup_{a\in[K],k\in[N]}\mathcal{G}_{a,k}^c) \le e\left(\log(1/\delta)\log N\right)KN\delta \le \frac{1}{N^3}.$$

□

C PROOF OF THEOREM 3.2

Step 1: introducing the family of problem instances. Take P_X to be the uniform distribution on $\mathcal{X} = [0,1]^d$. Define $M = \lceil (N/C^\star)^{1/(2\beta+d)} \rceil$. Our construction of the reward instances is adapted from (Rigollet & Zeevi, 2010). Let $\mathcal{L} = \{B_j : j = 1, ..., M^d\}$ be a regular partition of $\mathcal{X}$ and let q_j be the center of B_j. Denote $\Omega_m := \{\pm 1\}^m$ with $m := \lceil M^{d-\alpha\beta} \rceil$. For each $\omega \in \Omega_m$, define a function $f_\omega : [0,1]^d \mapsto \mathbb{R}$:

$$f_\omega(x) = \frac{1}{2} + \sum_{j=1}^{m} \omega_j \varphi_j(x), \tag{16}$$

where $\varphi_j(x) = C_\phi M^{-\beta} \phi(2M(x - q_j)) \mathbf{1}\{x \in B_j\}$ with $\phi(x) = (1 - \|x\|_\infty)^\beta \mathbf{1}\{\|x\|_\infty \leq 1\}$, and $C_\phi = \min(2^{-\beta} L, 1/4)$.

We take $K = 2$ and $\mathcal{I} = \{1, -1\}$. Let $\mu_i(1 \mid x) = 1/C^\star$ and $\mu_i(-1 \mid x) = 1 - 1/C^\star$ for all $x \in \mathcal{X}, 1 \leq i \leq N$. By equation (2), we have $\mu(1 \mid x) = 1/C^\star$ and $\mu(-1 \mid x) = 1 - 1/C^\star$ for any $x \in \mathcal{X}$. The family of problem instances of interest is

$$\mathcal{C} := \left\{ \left(\mu, f_1(x) = f_\omega(x), f_{-1}(x) = \frac{1}{2} \right) \mid \omega \in \Omega_m \right\}. \tag{17}$$

With slight abuse of notation, we also use $\mathcal{C}$ to denote $\{f_\omega : \omega \in \Omega_m\}$. It is straightforward to verify that $\mathcal{C} \subseteq \mathcal{F}(\alpha, \beta, C^\star)$.

Step 2: reduction to the testing error. We can reduce lower bounding the suboptimality gap to the testing error due to to the following lemma.

Lemma C.1 (Lemma 3.1 in (Rigollet & Zeevi, 2010))**.** *Under the margin condition, one has*

$$\mathbb{E}\left[f^\star(X) - f_{\pi(X)}(X)\right] \geq \left(\frac{1}{D} \cdot \mathbb{E}\left[1\{\pi(X) \neq \pi^\star(X), f(X) \neq \frac{1}{2}\} \right] \right)^{\frac{\alpha+1}{\alpha}},$$

for some constant $D > 0$.

By Lemma C.1, we have

$$\begin{aligned}
\sup_{\mathcal{C}} \mathbb{E}\left[f^\star(X) - f_{\pi(X)}(X)\right] &\geq \sup_{\mathcal{C}} (\frac{1}{D})^{\frac{\alpha+1}{\alpha}} \cdot \left(\mathbb{E}\left[1\{\pi(X) \neq \pi^\star(X), f(X) \neq \frac{1}{2}\} \right] \right)^{\frac{\alpha+1}{\alpha}} \\
&= (\frac{1}{D})^{\frac{\alpha+1}{\alpha}} \cdot \left(\sup_{\mathcal{C}} \mathbb{E}\left[1\{\pi(X) \neq \pi^\star(X), f(X) \neq \frac{1}{2}\} \right] \right)^{\frac{\alpha+1}{\alpha}}.
\end{aligned}$$

Let $\mathbb{P}_\omega$ denotes the joint distribution of $\{(X_i, A_i, Y_i)\}_{i=1}^N$ under ω, and let $\mathbb{E}_\omega$ be the corresponding expectation. The supreme term within the second parenthesis can be lowered bounded by the average,

$$\begin{aligned}
\sup_{\mathcal{C}} \mathbb{E}\left[1\{\pi(X) \neq \pi^\star(X), f(X) \neq \frac{1}{2}\} \right] &\geq \frac{1}{2^m} \sum_{\omega \in \Omega_m} \mathbb{E}_\omega \left[1\{\pi(X) \neq \pi^\star(X), f_\omega(X) \neq \frac{1}{2}\} \right] \\
&= \frac{1}{2^m} \sum_{j=1}^{m} \sum_{\omega \in \Omega_m} \mathbb{E}_\omega \left[1\{\pi(X) \neq \omega_j, X \in B_j\} \right] \\
&= \frac{1}{2^m} \sum_{j=1}^{m} \sum_{\omega_{[-j]} \in \Omega_{m-1}} \underbrace{\sum_{l \in \{\pm 1\}} \mathbb{E}_{\omega^l_{[-j]}} \left[1\{\pi(X) \neq l, X \in B_j\} \right]}_{W_{j,\omega_{[-j]}}},
\end{aligned} \tag{18}$$

where $\omega^l_{[-j]}$ is the same as ω except for the j-th entry being l. Here we have used the fact that for $f_{\omega^l_{[-j]}}$, the optimal arm in the bin B_j is l. We then relate $W_{j,\omega_{[-j]}}$ to a binary testing error. By Le

Cam's method,

$$
\begin{aligned}
W_{j,\omega_{[-j]}} &= \frac{1}{M^d} \sum_{l\in\{\pm 1\}} \mathbb{P}_{\omega^l_{[-j]}}\left(\pi(X) \neq l \mid X \in B_j\right) \\
&\geq \frac{1}{4M^d} \exp\left(-\mathrm{KL}(\mathbb{P}_{\omega^{-1}_{[-j]}}, \mathbb{P}_{\omega^{1}_{[-j]}})\right) \\
&\gtrsim \frac{1}{4M^d} \exp\left(-\frac{N}{C^\star} \cdot M^{-(2\beta+d)}\right),
\end{aligned}
$$

where the last inequality uses Lemma C.2. Plugging the above back to equation (18) we obtain

$$
\begin{aligned}
\sup_{\mathcal{C}} \mathbb{E}\left[1\{\pi(X) \neq \pi^\star(X), f(X) \neq \frac{1}{2}\}\right] &\geq \frac{1}{2^m} \sum_{j=1}^{m} \sum_{\omega_{[-j]}\in\Omega_{m-1}} W_{j,\omega_{[-j]}} \\
&\gtrsim \frac{1}{2^m} \sum_{j=1}^{m} \sum_{\omega_{[-j]}\in\Omega_{m-1}} \frac{1}{4M^d} \exp\left(-\frac{N}{C^\star} \cdot M^{-(2\beta+d)}\right) \asymp M^{-\alpha\beta}.
\end{aligned}
$$

Therefore, we can conclude the proof by

$$
\begin{aligned}
\sup_{\mathcal{C}} \mathbb{E}\left[f^\star(X) - f_{\pi(X)}(X)\right] &\geq (\frac{1}{D})^{\frac{\alpha+1}{\alpha}} \cdot \left(\sup_{\mathcal{C}} \mathbb{E}\left[1\{\pi(X) \neq \pi^\star(X), f(X) \neq \frac{1}{2}\}\right]\right)^{\frac{\alpha+1}{\alpha}} \\
&\gtrsim (M^{-\alpha\beta})^{\frac{1+\alpha}{\alpha}} = M^{-\beta(1+\alpha)} \asymp \left(\frac{N}{C^\star}\right)^{-\frac{\beta(1+\alpha)}{2\beta+d}},
\end{aligned}
$$

where we have used the definition of M.

Lemma C.2. *Fix $j \in [m]$. For any policy π, one has*

$$
\mathrm{KL}(\mathbb{P}_{\omega^{-1}_{[-j]}}, \mathbb{P}_{\omega^{1}_{[-j]}}) \lesssim \frac{N}{C^\star} \cdot M^{-(2\beta+d)}.
$$

Proof. By the standard decomposition of the KL divergence and the Bernoulli reward structure,

$$
\begin{aligned}
\mathrm{KL}(\mathbb{P}_{\omega^{-1}_{[-j]}}, \mathbb{P}_{\omega^{1}_{[-j]}}) &\lesssim \sum_{i=1}^{N} \mathbb{E}_{\omega^{-1}_{[-j]}}\left[\left(f_{\omega^{-1}_{[-j]}}(X_i) - f_{\omega^{1}_{[-j]}}(X_i)\right)^2 \mathbf{1}\{A_i = 1\}\right] \\
&\lesssim \sum_{i=1}^{N} M^{-2\beta} \mathbb{E}_{\omega^{-1}_{[-j]}}\left[\mathbf{1}\{A_i = 1, X_i \in B_j\}\right] \\
&= \sum_{i=1}^{N} M^{-(2\beta+d)} \mathbb{P}_{\omega^{-1}_{[-j]}}(A_i = 1 \mid X_i \in B_j) \\
&= \frac{N}{C^\star} \cdot M^{-(2\beta+d)}.
\end{aligned}
$$

□