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# Smooth Contextual Bandits: Bridging the Parametric and Non-differentiable Regret Regimes

(Authors' names blinded for peer review)

We study a nonparametric contextual bandit problem where the expected reward functions belong to a Hölder class with smoothness parameter  $\beta$ . We show how this interpolates between two extremes that were previously studied in isolation: non-differentiable bandits ( $\beta \leq 1$ ), where rate-optimal regret is achieved by running separate non-contextual bandits in different context regions, and parametric-response bandits (satisfying  $\beta = \infty$ ), where rate-optimal regret can be achieved with minimal or no exploration due to infinite extrapolability. We develop a novel algorithm that carefully adjusts to all smoothness settings and we prove its regret is rate-optimal by establishing matching upper and lower bounds, recovering the existing results at the two extremes. In this sense, our work bridges the gap between the existing literature on parametric and non-differentiable contextual bandit problems and between bandit algorithms that exclusively use global or local information, shedding light on the crucial interplay of complexity and regret in contextual bandits.

*Key words:* Contextual bandits, local polynomial regression, minimax regret, margin condition

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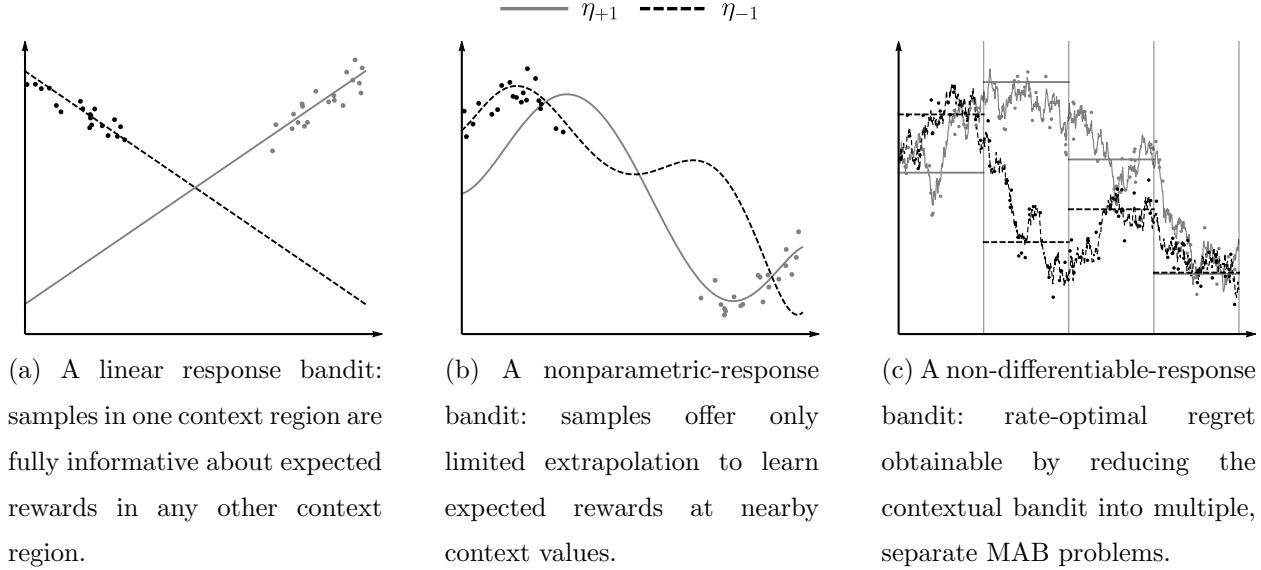
## 1. Introduction

In many domains, including healthcare and e-commerce, we frequently encounter the following decision-making problem: we sequentially and repeatedly receive context information  $X$  (*e.g.*, features of patients or users), need to choose an action  $A \in \{-1, +1\}$  (*e.g.*, whether to treat a patient with invasive therapy or whether expose a user to our ad), and receive a reward  $Y(A)$  (*e.g.*, patient's health outcome or user's click minus ad spot costs) corresponding to the chosen action. Our goal is to collect the most reward over time. When contexts  $X$  and potential rewards  $Y(-1), Y(+1)$  are drawn from a stationary, but unknown, distribution, this setting is modeled by the stochastic bandit problem (Wang et al. 2005, Bubeck and Cesa-Bianchi 2012). A special case is the multi-armed bandit (MAB) problem where there is no contextual information (Lai and Robbins 1985, Auer et al. 2002). In these problems, we quantify the quality of an algorithm for choosing actions based on available historical data in terms of its *regret* for every horizon  $T$ : the expected additional cumulative reward up to time  $T$  that we would obtain if we had full knowledge of the stationary context-reward distribution (but not the realizations). The *minimax regret* is the best (over algorithms) worst-case regret (over problem instances).

The relevant part of the context-reward distribution for maximum-expected-reward decision-making is the conditional mean reward functions,  $\eta_a(x) = \mathbb{E}[Y(a) | X = x]$ , for  $a = \pm 1$ : if we knew these functions, we would know what arm to pull. (Here we focus throughout on the case of two arms.) Since we only observe the reward of the chosen action,  $Y(A)$ , and never that of the unchosen action,  $Y(-A)$ , we face the oft-noted trade-off between exploration and exploitation: we are motivated to greedily exploit the arm we currently think is best for the context so to collect the highest reward right now, but we also need to explore the other arm to learn about its expected reward function for fear of missing better options in the future due to lack of information.

The trade-off between exploration and exploitation crucially depends on how we model the relationship between the context and the reward, *i.e.*,  $\eta_a$ . In the stochastic setting, previous literature has considered two extreme cases in isolation: a parametric reward model, usually linear (Goldenshluger and Zeevi 2013, Bastani and Bayati 2015, Bastani et al. 2017); and a nonparametric, non-differentiable reward model (Rigollet and Zeevi 2010, Perchet and Rigollet 2013, Fontaine et al. 2019). We review these below before describing our contribution. We define the problem in complete formality in Section 2.

**Linear-response bandit.** One extreme is the linear-response bandit where the expected reward function is assumed to be linear in context,  $\eta_a(x) = \theta_a^\top x$  (Goldenshluger and Zeevi 2013, Bastani and Bayati 2015). This parametric assumption imposes a global structure on the expected reward function and permits extrapolation, since *all* samples from arm  $a$  are informative about the finite-dimensional parameters  $\theta_a$  regardless of the context (see Fig. 1a). Dramatically, this global structure



**Figure 1** The fundamental nature of contextual bandit problems depends crucially on the assumed structure of expected reward functions,  $\eta_a$ .

almost entirely obviates the need for forced exploration. In particular, Bastani et al. (2017) proved that, under very mild conditions, the greedy algorithm is rate optimal for linear reward models, achieving logarithmic regret. Consequently, the result shows that the classic trade-off that characterizes contextual bandit problems is often not present in linear-response bandits. Similar behavior generally occurs when we impose other parametric models on expected rewards. At the same time, while theoretically regret is consequently very low, linear- and parametric-response bandit algorithms may actually have linear regret in practice since the parametric assumption usually fails to hold exactly.

**Non-differentiable nonparametric-response bandit.** Another line of literature considers nonparametric reward models that satisfy a Hölder continuity condition (Rigollet and Zeevi 2010, Perchet and Rigollet 2013), the strongest form of which is Lipschitz continuity. In stark contrast to the linear case, such functions need not even be differentiable. In any nonparametric-response bandit, extrapolation is limited, since only nearby samples are informative about the reward functions at each context value (Fig. 1b). Thus, we need to take a more localized learning strategy: we have to actively explore in *every* context region and learn the expected reward functions using nearby samples. In the non-differentiable extreme, Rigollet and Zeevi (2010) showed that one can achieve rate-optimal regret by partitioning the context space into small hypercubes and running completely separate MAB algorithms (*e.g.*, UCB) within each hypercube in isolation (Fig. 1c). In other words, we can almost ignore the contextual structure because we obtain so little information

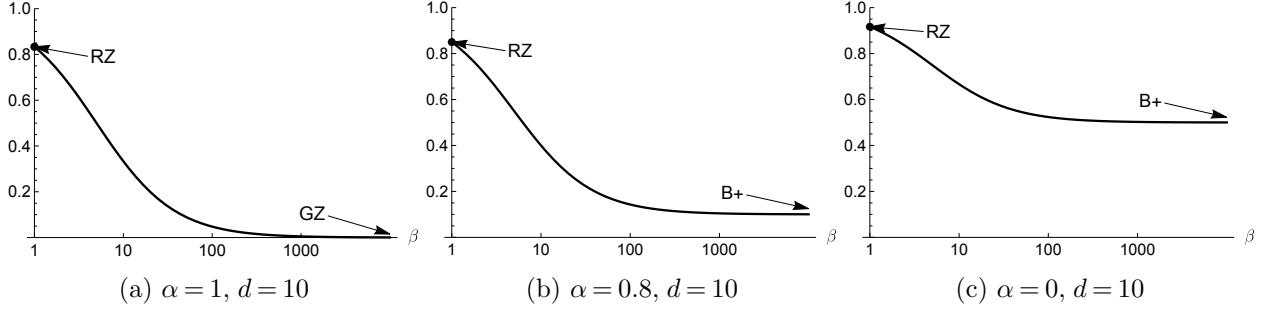
Margin Sharpness	Smoothness		
	$\# \leq 1$	$1 \leq \# < \infty$	$\# = \infty$
$0 \leq \$ < 1$			Bastani et al. (2017)
$\$ = 1$	Rigollet and Zeevi (2010)		Goldenshluger and Zeevi (2013)
$\$ > 1$	Perchet and Rigollet (2013)	<i>This paper</i>	Bastani et al. (2017)

**Table 1** The lay of the literature on stochastic contextual bandits in terms of our smoothness perspective. For the most part, there has been a significant and wide divide between non-differentiable-response and parametric-response bandits. Our work shows that (up to polylogs) the minimax regret rate  $\tilde{O}(T^{\frac{\beta+d-\alpha\beta}{2\beta+d}})$  reigns across all regimes; see also Fig. 2. (Note that additional linear restrictions are made in the  $\beta = \infty$  column.)

across contexts. However, at best, this achieves regret strictly worse than  $\sqrt{T}$  in rate whenever the dimension of contexts is more than 2 (and the bandit problem is nontrivial in that no constant decision rule is optimal; see Proposition 1).

**Our contribution: smooth contextual bandits.** In this paper, we consider a nonparametric-response bandit problem with *smooth* expected reward functions. This bridges the gap between the infinitely-smooth linear-response bandit and the unsMOOTH non-differentiable-response bandit. We characterize the smoothness of the expected reward functions in terms of the highest order of continuous derivatives, or more generally in terms of a Hölder smoothness parameter  $\#$ , which generalizes both non-differentiable Hölder continuous functions ( $\# \leq 1$ ) and infinitely-extrapolatable functions (such as linear, which we denote by  $\# = \infty$ ). Table 1 summarizes the landscape of the current literature and where our paper lies in terms of this new smoothness perspective and in terms of the sharpness  $\$$  of the margin (see Assumption 4).

We propose a novel algorithm for every level of smoothness  $1 \leq \# < \infty$  and prove that it achieves the minimax optimal regret rate up to polylogs. In particular, when  $\# > 1$ , we must leverage information across farther-apart contexts and running separate MAB algorithms will be suboptimal. And, because  $\# < \infty$ , we must ensure sufficient exploration everywhere. Thus, our algorithm interpolates between the fully-global learning of the linear-response bandit (which satisfies  $\# = \infty$ ) and the fully-local learning of the non-differentiable bandit ( $0 < \# \leq 1$ ), according to the smoothness of the expected reward functions. The smoother the expected reward functions, the more global reward information we incorporate. Moreover, our algorithm judiciously balances exploration and exploitation: it exploits only when we have certainty about which arm is optimal, and it explores economically in a shrinking margin region with fast diminishing error costs. As a result, our algorithm achieves regret bounded by  $\tilde{O}(T^{\frac{\beta+d-\alpha\beta}{2\beta+d}})$  (where  $\tilde{O}$  means up to polylogarithmic factors). We show that, for any algorithm, there exists an instance on which it must have regret lower bounded



**Figure 2** The minimax regret rate exponent,  $\lim_{T \rightarrow \infty} \log(\mathcal{R}_T)/\log(T) = \frac{\beta+d-\alpha\beta}{2\beta+d}$ , as shown by our Theorems 2 and 3. The minimax regret  $\mathcal{R}_T$  is defined in Section 2.7. Existing results shown with arrows only characterize the two extreme regimes (RZ refers to Rigollet and Zeevi 2010, GZ refers to Goldenshluger and Zeevi 2013, B+ refers to Bastani et al. 2017). In between, our results reveal the effect of complexity on regret.

by the same rate, showing that our algorithm is rate optimal and establishing the minimax regret rate for the problem. Consequently, the minimax regret,  $\mathcal{R}_T$ , which we define in Section 2.7, satisfies  $\mathcal{R}_T = \tilde{\Theta}(T^{\frac{\beta+d-\alpha\beta}{2\beta+d}})$  and hence  $\lim_{T \rightarrow \infty} \log(\mathcal{R}_T)/\log(T) = \frac{\beta+d-\alpha\beta}{2\beta+d}$ .

While this rate has the same *form* as the regret in the non-differentiable case studied by Rigollet and Zeevi (2010), our results extend to the smooth ( $\beta > 1$ ) regime where our algorithm can attain much lower regret, arbitrarily approaching polylogarithmic rates as smoothness increases. Our algorithm is fundamentally different, leveraging contextual information from farther away as smoothness increases without deteriorating estimation resolution, and our analysis is necessarily much finer. Our work connects seemingly disparate contextual bandit problems, and reveals the whole spectrum of minimax regret over varying levels of function complexity.

### 1.1. Related Literature

**Nonparametric regression.** Our algorithm leverages nonparametric regression to learn expected reward functions, namely local polynomial regression. Nonparametric regression seeks to estimate regression (aka, conditional expectation) functions without assuming that they belong to an *a priori* known parametric family. One of the most popular nonparametric regression methods is the NadarayaWatson kernel regression estimator (Nadaraya 1964, Watson 1964), which estimates the conditional expectation at a query point as the weighted average of observed outcomes, weighted by their closeness to the query using a similarity-measuring function known as a kernel. Local polynomial estimators generalize this by fitting a polynomial by kernel-weighted least squares (Stone 1977), where fitting a constant recovers the former. Stone (1980) considered function classes with different levels of differentiability and showed that local polynomial regression achieves rate-optimal point convergence. Stone (1982) further showed that a modification of this estimator can achieve rate-optimal convergence in  $p$ -norm for  $0 < p \leq \infty$ . There are a variety of

other nonparametric estimators that can achieve rate optimality in these classes, such as sieve estimators (*e.g.*, Chen 2007, Belloni et al. 2015), but we do not use these in our algorithm. For more detail and an exhaustive bibliography on nonparametric regression, see Tsybakov (2008).

Nonparametric regression also has broad applications in decision making. In classification problems, Audibert and Tsybakov (2007) established fast convergence rates for the 0-1 error of plug-in estimators based on local polynomial regression by leveraging a finite-sample concentration bound. The rate depends on a so-called margin condition number  $\alpha$  originally proposed by Mammen et al. (1999), Tsybakov et al. (2004) that quantifies how well-separated the classes are, where larger  $\alpha$  corresponds to more separation (see Assumption 4). Bertsimas and Kallus (2019) use similar locally-weighted nonparametric regression methods to solve conditional stochastic optimization problems with auxiliary observations and show that this provides model-free asymptotic optimality.

**Contextual bandits.** While the literature above usually considers an off-line problem with a given exogenous sample of data, the literature on contextual bandit problems considers adaptive data collection and sequential decision-making (see Bubeck and Cesa-Bianchi 2012 for a complete bibliography). Some contextual bandit literature allows for adversarially chosen contexts (*e.g.*, Langford and Zhang 2007, Beygelzimer et al. 2011), but this leads to high regret and may be too pessimistic in real-world applications. For example, in clinical trials for a non-infectious disease, the treatment decisions for one patient do not have direct impacts on the personal features of the next patient. One line of literature captured this stochastic structure by assuming that contexts and rewards are drawn i.i.d. (independently and identically distributed) from a stationary but unknown distribution (*e.g.*, Wang et al. 2005, Dudik et al. 2011, Agarwal et al. 2014). The aforementioned linear- and nonparametric-response bandits both fall in this setting. Rigollet and Zeevi (2010), Goldenshluger and Zeevi (2013, 2009), Perchet and Rigollet (2013) introduced the use of the margin condition in this setting to quantify how well-separated the arms are, a well-known determiner of regret in the simpler MAB problem (Lai and Robbins 1985).

Goldenshluger and Zeevi (2013) assumed a linear model between rewards and covariates for each arm and proposed a novel rate-optimal algorithm that worked by maintaining two sets of parameter estimates for each arm. Bastani et al. (2017) showed that the greedy algorithm is optimal under mild covariate diversity conditions. Bastani and Bayati (2015) considered a sparse linear model and used a LASSO estimator to accommodate high-dimensional contextual features. While Goldenshluger and Zeevi (2013), Bastani and Bayati (2015) assume a sharp margin ( $\alpha = 1$ ), Goldenshluger and Zeevi (2009) also considers more general margin conditions in the one-armed linear-response setting and Bastani et al. (2017, Appendix E) considers these in the multi-armed linear-response setting. All of the above achieve regret bounds of order  $\log T$  under a sharp margin condition ( $\alpha = 1$ ).

However, as discussed before, this relies heavily on the fact that every observation is informative about expected rewards everywhere.

Rigollet and Zeevi (2010), Perchet and Rigollet (2013) study the case where we only assume that the expected reward functions are Hölder continuous, *i.e.*, that  $|\eta_a(x) - \eta_a(x')| \leq \|x - x'\|^\beta$ . Note that  $\beta = 1$  corresponds to Lipschitz continuity and is the strongest variant of this assumption, since  $\beta > 1$  requires the function to be constant and is therefore not considered. Rigollet and Zeevi (2010) studied the two-arm case and obtained optimal minimax-regret rates for margin condition  $\alpha \leq 1$ . Perchet and Rigollet (2013) extended this to multiple arms and  $\alpha \geq 0$  (although some combinations lead to degenerate cases; see Proposition 1). The rate optimal algorithms in this case consist of segmenting the context space and running separate MAB algorithms in parallel in each segment. This cannot be improved upon in a minimax sense if we impose no additional assumptions. However, this approach will no longer be rate optimal when we impose smoothness, where we must use information from across such segments to fully leverage reward smoothness.

## 1.2. Notation

For any multiple index  $r = (r_1, \dots, r_d) \in \mathbb{Z}_+^d$  and any  $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ , define  $|r| = \sum_{i=1}^d r_i$ ,  $r! = r_1! \cdots r_d!$ ,  $x^r = x_1^{r_1} \cdots x_d^{r_d}$ , and the differential operator  $D^r := \frac{\partial^{r_1+\cdots+r_d}}{\partial x_1^{r_1} \cdots \partial x_d^{r_d}}$ . We use  $\|\cdot\|$  to represent the Euclidean norm, and  $\text{Leb}[\cdot]$  the Lebesgue measure. We let  $\mathcal{B}(x, h) = \{x' \in \mathbb{R}^d : \|x' - x\| \leq h\}$  be the ball with center  $x$  and radius  $h > 0$ , and  $v_d = \pi^{d/2}/\Gamma(d/2 + 1)$  the volume of a unit ball in  $\mathbb{R}^d$ . For any  $\beta > 0$ , let  $\mathfrak{b}(\beta) = \sup\{i \in \mathbb{Z} : i < \beta\}$  be the maximal integer that is *strictly* less than  $\beta$ , and let  $M_\beta$  be the cardinality of the set  $\{r \in \mathbb{Z}_+^d : |r| \leq \mathfrak{b}(\beta)\}$ . For an event  $A$ , the indicator function  $\mathbb{I}(A)$  is equal to 1 if  $A$  is true and 0 otherwise. For two scalars  $a, b \in \mathbb{R}$ ,  $a \wedge b = \min\{a, b\}$  and  $a \vee b = \max\{a, b\}$ . For a matrix  $\mathcal{A}$ , its minimum eigenvalue is denoted as  $\lambda_{\min}(\mathcal{A})$ . For two functions  $f_1(T) > 0$  and  $f_2(T) > 0$ , we use the standard notation for asymptotic order:  $f_1(T) = O(f_2(T))$  represents  $\limsup_{T \rightarrow \infty} \frac{f_1(T)}{f_2(T)} < \infty$ ,  $f_1(T) = \Omega(f_2(T))$  represents  $\liminf_{T \rightarrow \infty} \frac{f_1(T)}{f_2(T)} > 0$ , and  $f_1(T) = \Theta(f_2(T))$  represents simultaneously  $f_1(T) = \Omega(f_2(T))$  and  $f_1(T) = O(f_2(T))$ . We use  $\tilde{O}$ ,  $\tilde{\Omega}$ ,  $\tilde{\Theta}$  to represent the same order relationship up to polylogarithmic factors. For example,  $f_1(T) = \tilde{O}(f_2(T))$  means  $\limsup_{T \rightarrow \infty} \frac{f_1(T)}{\text{polylog}(T)f_2(T)} < \infty$  for a polylogarithmic function  $\text{polylog}(T)$ .

## 1.3. Organization

The rest of the paper is organized as follows. In Section 2, we formally introduce the smooth nonparametric bandit problem and assumptions. We describe our proposed algorithm in Section 3. In Section 4, we analyze our algorithm theoretically: we derive an upper bound on the regret of our algorithm in Section 4.1, and we prove a matching lower bound on the regret of any algorithm in Section 4.2. We conclude our paper in Section 5. While proof techniques are outlined, complete proof details are relegated to the appendix.

## 2. The Smooth Contextual Bandit Problem

In this section, we formulate the smooth contextual bandit problem that we consider in this paper. We break up this formulation into parts, explaining the significance or necessity of each part separately. In the main text, we focus on the two-armed smooth contextual bandit problem, but our algorithm and analysis can be extended to multi-armed problems (see Section A for a detailed discussion).

### 2.1. Two-Armed Stochastic Contextual Bandits

Consider the following two-armed contextual bandit problem. For  $t = 1, 2, \dots$ , nature draws  $(X_t, Y_t(1), Y_t(-1))$  i.i.d. from a common distribution  $\mathbb{P}$  of  $(X, Y(1), Y(-1))$ , where  $X \in \mathcal{X} \subseteq \mathbb{R}^d$  is the context (covariate), and  $Y(\pm 1) \in [0, 1]$  is random rewards corresponding to arm  $\pm 1$ . At each time step  $t$ , the decision maker observes the context  $X_t$ , pulls an arm  $A_t \in \{-1, 1\}$  according to the observed context and history so far, and then obtains the reward  $Y_t = Y_t(A_t)$  of the chosen arm. Specifically, an admissible policy (allocation rule),  $\pi = \{\pi_t\}$ , is a sequence of *random* functions  $\pi_t : \mathcal{X} \rightarrow \{-1, 1\}$  such that, for each  $t$ ,  $\pi_t$  is conditionally independent of  $(X_1, A_1, Y_1(1), Y_1(-1), \dots)$ , given  $(X_1, A_1, Y_1, \dots, X_{t-1}, A_{t-1}, Y_{t-1})$ , where we let  $A_t = \pi_t(X_t)$ ,  $Y_t = Y_t(A_t)$ .

For  $x \in \mathcal{X}$ , we denote the conditional expected reward functions as

$$\eta_{\pm 1}(x) = \mathbb{E}[Y(\pm 1) | X = x],$$

and the conditional average treatment effect (CATE) of pulling arm 1 versus arm  $-1$  as

$$\tau(x) = \mathbb{E}[Y(1) | X = x] - \mathbb{E}[Y(-1) | X = x] = \eta_1(x) - \eta_{-1}(x).$$

Obviously, if we had full knowledge of the regression functions  $\eta_{\pm 1}$  or the CATE function  $\tau$ , the optimal decision at each time step would be the oracle policy  $\pi^*$  that always pulls the arm with higher expected reward given  $X_t$  and regardless of history, namely,

$$\pi^*(x) = \mathbb{I}(\tau(x) \geq 0) - \mathbb{I}(\tau(x) < 0) \in \operatorname{argmax}_{a \in \{-1, 1\}} \eta_a(x). \quad (1)$$

However, since we do not know these functions, the oracle policy is infeasible in practice. We measure the performance of a policy  $\pi$  by its (*expected cumulative*) *regret* compared to the oracle policy  $\pi^*$  up to any time  $T$ , which quantifies how much the policy  $\pi$  is inferior to the oracle policy  $\pi^*$ :

$$R_T(\pi) = \mathbb{E} \left[ \sum_{t=1}^T (Y_t(\pi^*(X_t)) - Y_t(\pi_t(X_t))) \right]. \quad (2)$$

The growth of this function in  $T$  quantifies the quality of  $\pi$ .

## 2.2. Smooth Rewards

In this paper, we aim to construct a decision policy that achieves low regret *without* strong parametric assumptions on the expected reward functions. We instead focus on expected reward functions restricted to a Hölder class of functions. This is the key restriction characterizing the nature of the bandit problem we consider.

**DEFINITION 1 (HÖLDER CLASS OF FUNCTIONS).** A function  $\eta : \mathcal{X} \rightarrow [0, 1]$  belongs to the  $(\beta, L, \mathcal{X})$ -Hölder class of functions if it is  $\mathfrak{b}(\beta)$ -times continuously differentiable and for any  $x, x' \in \mathcal{X}$ ,

$$\left| \eta(x') - \sum_{|r| \leq \mathfrak{b}(\beta)} \frac{(x' - x)^r}{r!} D^r \eta(x) \right| \leq L \|x' - x\|^\beta. \quad (3)$$

Recall that  $\mathfrak{b}(\beta)$  is the largest integer *strictly* smaller than  $\beta$ . When  $\beta \leq 1$ , Eq. (3) reduces to Hölder continuity (*i.e.*,  $|\eta(x) - \eta(x')| \leq L \|x' - x\|^\beta$ ), as considered in previous non-differentiable bandit literature (Rigollet and Zeevi 2010, Perchet and Rigollet 2013). When  $\beta > 1$ ,  $\mathfrak{b}(\beta)$  is the highest order of continuous derivatives. For example, when  $\mathcal{X}$  is compact,  $k$ -times continuously differentiable functions are  $(k, L, \mathcal{X})$ -Hölder for some  $L$ . Polynomials of bounded degree  $k$  are  $(\beta, 0, \mathcal{X})$ -Hölder for all  $\beta > k$ .

In this paper we focus on  $\beta \geq 1$ , which crucially includes the smooth case ( $\beta > 1$ ).

**ASSUMPTION 1 (Smooth Conditional Expected Rewards).** For  $a = \pm 1$ ,  $\eta_a$  is  $(\beta, L, \mathcal{X})$ -Hölder for  $\beta \geq 1$  and is also  $(1, L_1, \mathcal{X})$ -Hölder.

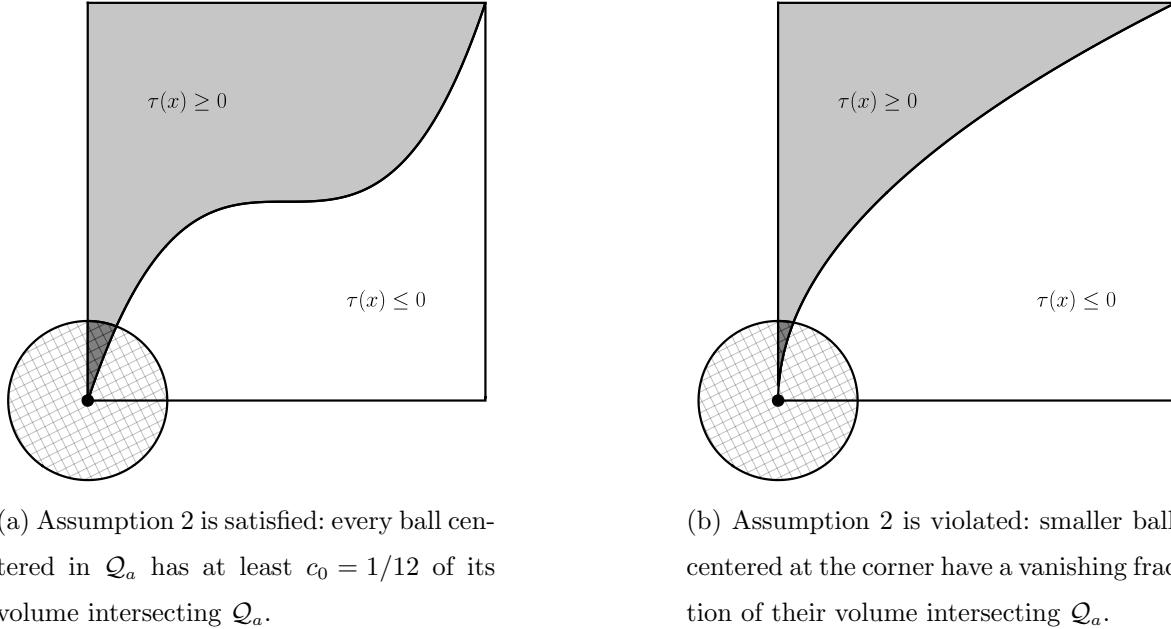
Given a function that is  $(\beta, L, \mathcal{X})$ -Hölder on a compact  $\mathcal{X}$  with  $\beta \geq 1$ , there will *always* exist a finite  $L_1 > 0$  such that the function is also  $(1, L_1, \mathcal{X})$ -Hölder (*i.e.*,  $L_1$ -Lipschitz). Thus, assuming Lipschitzness in the second part of Assumption 1 is actually *not necessary* for characterizing the regret rate of our algorithm for any single, fixed instance, if we assume a compact  $\mathcal{X}$  as we do below in Assumption 3. However, from the perspective of characterizing the *minimax* regret, where we take a supremum over instances, it is necessary, as the Lipschitz constant  $L_1$  may be arbitrarily large in the  $(\beta, L, \mathcal{X})$ -Hölder class of functions.

## 2.3. Optimal Decision Region Regularity

We next introduce a regularity condition on the context regions where each arm is optimal, namely,

$$\mathcal{Q}_a = \{x \in \mathcal{X} : a\tau(x) \geq 0\}.$$

When the expected rewards are not restricted parametrically as we imposed in the above, we *must* use local information to estimate them since extrapolation is limited. In particular, in order to estimate  $\eta_a(x)$  consistently at a given point  $x$ , we must have that the contexts of our data on outcomes from arm  $a$  eventually become dense around the point  $x$ . To formalize this notion, we introduce the  $(c_0, r_0)$ -regularity condition:



**Figure 3 Illustration of Assumption 2: each optimal decision region must be regular in that the neighborhood of every point in the region must contain at least some constant fraction of the ball.**

**DEFINITION 2 (( $c_0, r_0$ )-REGULARITY CONDITION).** A Lebesgue-measurable set  $\mathcal{S} \subseteq \mathbb{R}^d$  is called weakly  $(c_0, r)$ -regular at point  $x \in \mathcal{S}$  if

$$\text{Leb}[\mathcal{S} \cap \mathcal{B}(x, r)] \geq c_0 \text{Leb}[\mathcal{B}(x, r)].$$

If this condition holds for all  $0 \leq r \leq r_0$ , then set  $\mathcal{S}$  is called strongly  $(c_0, r_0)$ -regular at  $x$ . Furthermore, if  $\mathcal{S}$  is strongly  $(c_0, r_0)$ -regular at all  $x \in \mathcal{S}$ , then the set  $\mathcal{S}$  is called a  $(c_0, r_0)$ -regular set.

Essentially, if our data for arm  $a$  became dense in the set  $\mathcal{S}$  and if  $\mathcal{S}$  were strongly  $(c_0, r_0)$ -regular at  $x$ , then sufficient data would be available within any small neighborhood around  $x$  to estimate  $\eta_a(x)$  well. If  $\mathcal{S}$  were not regular then, even if our data became dense in  $\mathcal{S}$ , there would be diminishing amounts of data available as we looked closer and closer near  $x$ . For example, the  $\ell_q$  unit ball is regular for  $q \geq 1$  and irregular for  $q < 1$  because the points at its corners are too isolated from the rest of the set.

Naturally, we need enough data from arm  $a$  around  $x$  to estimate  $\eta_a(x)$  accurately. Luckily, we need only worry about high-accuracy estimation for *both* arms near the decision boundary, where it is hard to tell which of the arms is optimal. (Intuitively, away from the boundary, it is very easy to separate the arms with very few samples, as in the classic MAB case of Lai and Robbins 1985.) But, we cannot rely on having enough data from arm  $a$  in a whole ball around every point near the boundary, as that would require us to pull arm  $a$  too often across the boundary, in  $\mathcal{Q}_{-a}$ , where it is

not optimal. This would necessarily lead to high regret. Instead, we must be able to rely mostly on data from arm- $a$  pulls in  $\mathcal{Q}_a$ . Therefore, we must have that this set is regular. If, otherwise, there existed such a point  $x \in \mathcal{Q}_a$  that is sufficiently isolated from the rest of  $\mathcal{Q}_a$  then we cannot generate enough samples to learn  $\eta_a(x)$  accurately enough without necessarily incurring high regret.

**ASSUMPTION 2 (Optimal Decision Regions).** *For  $a = \pm 1$ ,  $\mathcal{Q}_a$  is a non-empty  $(c_0, r_0)$ -regular set.*

An illustration of this condition is given in Fig. 3. We note that this condition is a refinement of the usual condition for nonparametric estimation, which simply requires the support  $\mathcal{X}$  to be a regular set (Tsybakov 2008). This refinement is necessary for the unique bandit setting we consider where we must worry about the costs of adaptive data collection and may not simply assume a good dataset is given. Since the intersection of regular sets may not always be regular, it is insufficient to only assume the support  $\mathcal{X}$  is regular and expected rewards are smooth in order to guarantee Assumption 2, as seen in Fig. 3b.

Assumption 2 is *necessary* to guarantee the optimal minimax regret as we desire. We can show that there exists a class of problem instances satisfying Assumptions 1, 3 and 4 such that the corresponding regret lower bound is higher (See Theorem 4).

#### 2.4. Bounded Covariate Density

While Assumption 2 ensures there is sufficient volume around each point  $x$  where we need to estimate  $\eta_a(x)$ , we also need to ensure that this translates to being able to collect sufficient data around each such point. Toward this end, we make the assumption that the contexts have a density and that it is bounded away from zero and infinity.

**ASSUMPTION 3 (Strong Density).** *The marginal distribution of  $X$  has density  $\mu(x)$  with respect to Lebesgue measure and  $\mu$  is bounded away from zero and infinity on its support  $\mathcal{X}$ :*

$$0 < \mu_{\min} \leq \mu(x) \leq \mu_{\max} < \infty, \quad \forall x \in \mathcal{X}.$$

Moreover, its support  $\mathcal{X}$  is compact and  $\mathcal{X} \subseteq [0, 1]^d$ .

Note that restricting  $\mathcal{X}$  to  $[0, 1]^d$  is without loss of generality, having assumed compactness. Scaling and shifting the covariates to be in  $[0, 1]$  will only affect the constants  $L, L_1$  in Assumption 1.

Together, Assumptions 2 and 3 imply a lower bound on the probability that each arm is optimal.

**LEMMA 1.** *Under Assumptions 2 and 3, we have  $\mathbb{P}(X \in \mathcal{Q}_a) \geq p$  for  $a = \pm 1$ , where*

$$p = \mu_{\min} c_0 r_0^d v_d.$$

## 2.5. Margin Condition

We further impose a margin condition commonly used in stochastic contextual bandits (Rigollet and Zeevi 2010, Goldenshluger and Zeevi 2013) and classification (Mammen et al. 1999, Tsybakov et al. 2004), which determines how the estimation error of expected rewards translates into regret of decision-making.

**ASSUMPTION 4 (Margin Condition).** *The conditional average treatment effect function  $\tau$  satisfies the margin condition with parameters  $\alpha \geq 0$  and  $\gamma$ :*

$$\mathbb{P}(0 < |\tau(X)| \leq t) \leq \gamma t^\alpha \quad \forall t > 0.$$

The margin condition quantifies the concentration of contexts very near the decision boundary, where the optimal action transitions from one arm to the other. This measures the difficulty of determining which of the two arms is optimal. When  $\alpha$  is very small, the CATE function can be arbitrarily close to 0 with high probability, so even very small estimation error of the CATE function may lead to suboptimal decisions. In contrast, when  $\alpha$  is very large, with high probability, the CATE is either 0 so that either arm is optimal or bounded away from 0 so that the optimal arm is easy to identify.

## 2.6. On the Relationship of Margin and Smoothness

We finally remark on the relationship between the margin parameter  $\alpha$  and the smoothness parameter  $\beta$ . Assumption 1 implies that the CATE function  $\tau(x)$  is a member of the  $(\beta, 2L, \mathcal{X})$ -Hölder class. Intuitively, when  $\tau(x)$  is very smooth (*i.e.*,  $\beta$  is very large), it cannot change too abruptly at the decision boundary  $\tau(x) = 0$ , so the mass near the decision boundary must be significant (small  $\alpha$ ). This relationship is formalized in the following proposition, a straightforward extension of Proposition 3.4 of Audibert and Tsybakov (2005).

**PROPOSITION 1.** *Suppose Assumptions 3 and 4 hold and that  $\eta_a$  is  $(\beta, L, \mathcal{X})$ -Hölder ( $\beta \geq 0$ ) for  $a = \pm 1$ . If  $\mathbb{P}(X \in \mathcal{Q}_a) < 1$  for  $a = \pm 1$  then  $\alpha(1 \wedge \beta) \leq 1$ .*

In other words, Proposition 1 states that if the CATE function crosses zero in the interior of  $\mathcal{X}$  (so that each arm cannot be optimal everywhere), then the smoothness parameter and the margin condition cannot simultaneously be large, since a function that crosses zero sharply cannot be very smooth. Conversely, if  $\alpha(1 \wedge \beta) > 1$ , then the contextual bandit problem is trivial: either  $\mathbb{P}(X \in \mathcal{Q}_1) = 1$  or  $\mathbb{P}(X \in \mathcal{Q}_{-1}) = 1$ , and there exists an optimal policy that only ever pulls one arm.

Throughout this paper, we focus on the *new* setting of *smooth* contextual bandits, where  $\beta \geq 1$  (see Table 1). While our algorithm can accommodate *any* value of  $\alpha \geq 0$  and does not in fact explicitly depend on the particular value, we highlight that the *interesting* bandit problem instances in our class of problems have  $\alpha \in [0, 1]$  according to Proposition 1. Moreover, there do not actually exist any instances with very large margin conditions,  $\alpha > d$ .

**PROPOSITION 2.** *Suppose Assumptions 1 to 4 hold. Then  $\alpha \leq d$ .*

## 2.7. Minimax Regret

Having now defined the problem and our assumptions about the distribution  $\mathbb{P}$  defining the problem instance, we can introduce the notion of *minimax regret*. The minimax regret is the minimum over admissible policies  $\pi$  of the maximum of the regret of  $\pi$  over all problem instances  $\mathbb{P}$  that fit our assumptions. This describes the best-achievable behavior in the problem class we consider.

Formally, for  $\beta \geq 1$ , we let  $\mathcal{P}(\beta, L_1, L, c_0, r_0, \mu_{\min}, \mu_{\max}, \gamma, \alpha)$  be the set of all distributions  $\mathbb{P}$  on  $(X, Y(-1), Y(+1)) \in [0, 1]^d \times \mathbb{R} \times \mathbb{R}$  that satisfy Assumptions 1 to 4 with these parameters. For brevity, we write  $\mathcal{P}$ , implicitly considering the parameters as fixed. Letting  $\Pi$  denote all admissible policies, for some fixed parameters specifying a class  $\mathcal{P}$ , we then define the minimax regret as

$$\mathcal{R}_T = \inf_{\pi \in \Pi} \sup_{\mathbb{P} \in \mathcal{P}} R_T(\pi).$$

The minimax regret exactly characterizes how well we can hope to do in the given class of instances.

To understand its significance, let us fix some parameters. Now, suppose that, on the one hand, we can find a function  $f(T)$  and an admissible policy  $\hat{\pi}$  such that its regret for every instance  $\mathbb{P} \in \mathcal{P}$  is bounded by the *same* function,  $R_T(\hat{\pi}) \leq f(T)$ . Next, suppose that, on the other hand, we can show that there exists a function  $f'(T) = \tilde{\Omega}(f(T))$  where for every admissible policy  $\pi'$  there exists an instance  $\mathbb{P} \in \mathcal{P}$  such that the regret is lower bounded by this *same* function,  $R_T(\pi') \geq f'(T)$ . Then we will have shown two critical results: (a) the minimax regret satisfies the rate  $\mathcal{R}_T = \tilde{\Theta}(f(T))$  and (b) we have a specific algorithm  $\hat{\pi}$  that can actually achieve this best-possible worst-case regret in rate, which also means the regret of  $\hat{\pi}$  is known to be bounded in this rate for every single instance encountered.

In this paper, we will proceed exactly as in the above. First, in Section 3, we will develop a novel algorithm that can adapt to every smoothness level. Then, in Section 4.1 we will prove a bound on its regret in every instance. Since this bound will depend only on the parameters of  $\mathcal{P}$ , we will have in fact established an upper bound on the minimax regret as above. In Section 4.2 we will find a bad instance for every policy that yields a matching (up to polylogs) lower bound on its regret, establishing a lower bound on the minimax regret. This will exactly yield the desired conclusion: a characterization of the minimax regret and the construction of a specific algorithm that achieves it.

## 3. SmoothBandit: A Low-Regret Algorithm for Any Smoothness Level

In this section, we develop our algorithm, SMOOTHBANDIT (Algorithm 1). We first review local polynomial regression, which we use in our algorithm to estimate  $\eta_a$ .

### 3.1. The Local Polynomial Regression Estimator

A standard result of (offline) nonparametric regression is that the smoother a function is in terms of its Hölder parameter  $\beta$ , the faster it can be estimated. Appropriate convergence rates can, *e.g.*, be achieved using local polynomial regression estimators that adjusts to different smoothness levels (Stone 1982, 1980). In this section, we briefly review local polynomial regression and its statistical property in an *offline* bandit setting. Its use in our *online* algorithm is described in Section 3.2. More details about local polynomial regression can be found in Tsybakov (2008), Audibert and Tsybakov (2007).

Consider an offline setting, where we have access to an exogenously collected i.i.d. sample,  $S = \{(X_t, Y_t)\}_{t=1}^n$  drawn i.i.d. from  $(X, Y)$ , where  $X$  has support  $\mathcal{X} \subset \mathbb{R}^d$ . We can then estimate the regression function  $\eta(x) = \mathbb{E}[Y | X = x]$  at every point  $x$  using the the following local polynomial estimator.

**DEFINITION 3 (LOCAL POLYNOMIAL REGRESSION ESTIMATOR).** For any  $x \in \mathcal{X}$ , given a bandwidth  $h > 0$ , an integer  $l \geq 0$ , samples  $S = \{(X_t, Y_t)\}_{t=1}^n$ , and a degree- $l$  polynomial model  $\theta(u; x, \vartheta, l) = \sum_{|r| \leq l} \vartheta_r(S)(u - x)^r$ , define the local polynomial estimate for  $\eta(x)$  as  $\hat{\eta}^{\text{LP}}(x; S, h, l) = \theta(x; x, \hat{\vartheta}_x, l)$ , where

$$\hat{\vartheta}_x \in \arg \min_{\vartheta} \sum_{t: X_t \in \mathcal{B}(x, h)} (Y_t - \theta(X_t; x, \vartheta, l))^2. \quad (4)$$

For concreteness, we define  $\hat{\eta}^{\text{LP}}(x; S, h, l) = 0$  if the minimizer is not unique.

In words, the local polynomial regression estimator fits a polynomial by least squares to the data that is in the  $h$ -neighborhood of the query point  $x$  and evaluates this fit at  $x$  to predict  $\eta(x)$ .

Since Eq. (4) is a least squares problem, the estimation accuracy of the local polynomial estimator  $\hat{\eta}^{\text{LP}}(x; S, h, l)$  depends on the associated Gram matrix:

$$\hat{\mathcal{A}}(x; S, h, l) = \{\hat{\mathcal{A}}_{r_1, r_2}(x; S, h)\}_{|r_1|, |r_2| \leq l}, \quad \text{where } \hat{\mathcal{A}}_{r_1, r_2}(x; S, h) = \sum_{t: X_t \in \mathcal{B}(x, h)} \left(\frac{X_t - x}{h}\right)^{r_1 + r_2}. \quad (5)$$

The following proposition illustrates (using the offline setting as an example) why our Assumptions 1 to 3 are crucial in our problem. In particular, it shows that bounded density and regularity of the support of the data ensure a well-conditioned locally weighted Gram matrix. Moreover, it shows how the bandwidth and polynomial degree should adapt to the smoothness level  $\beta$ . This proposition is a direct extension of Theorem 3.2 of Audibert and Tsybakov (2007). We include this result purely for motivation, while in our *online* setting we will need to establish a more refined result that accounts for our adaptive data collection.

**PROPOSITION 3.** *Let  $S$  be an i.i.d. sample of  $(X, Y)$ , where  $\eta$  is  $(\beta, L, \mathcal{X})$ -Hölder,  $\mathcal{X}$  is compact and  $(c_0, r_0)$ -regular, and  $X$  has a density bounded away from 0 and infinity on  $\mathcal{X}$ . Then there*

exist positive constants  $\lambda_0, C_1, C_2$  such that, for any  $x \in \mathcal{X}$ , and  $\epsilon > 0$ , with probability at least  $1 - C_1 \exp\left\{-C_2 n_a^{\frac{2\beta}{2\beta+d}} \epsilon^2\right\}$ , we have

$$\lambda_{\min}(\hat{\mathcal{A}}(x; S, n^{-1/(2\beta+d)}, \mathbf{b}(\beta))) \geq \lambda_0, \quad \text{and} \quad |\hat{\eta}^{LP}(x; S, n^{-1/(2\beta+d)}, \mathbf{b}(\beta)) - \eta(x)| \leq \epsilon.$$

In our online bandit setting, the samples for each arm are collected in an adaptive way, since both exploration and exploitation can depend on data already collected. As a result, the distribution of the samples for each arm is considerably more complicated. Thus, we will need to use the local polynomial estimator in a somewhat more sophisticated way and analyze it more carefully. See Sections 3.2 and 4.1 for the details.

### 3.2. Our Algorithm

In this section we present our new algorithm for smooth contextual bandits, which uses local polynomial regression estimators that adjust to any smoothness level. The algorithm is summarized in Algorithm 1. Below we review its salient features. In what follows we assume a fixed horizon  $T$ , but can accommodate an unknown, variable  $T$  using the well-known doubling trick (see Auer et al. 1995; Cesa-Bianchi and Lugosi 2006, p. 17). Also, we assume that the smoothness parameter  $\beta$  is known, but Gur et al. (2019) adapts our algorithm to unknown  $\beta$  under extra conditions.

**3.2.1. Grid Structure** Following (Stone 1982) and similarly to previous nonparametric-response bandit literature (Rigollet and Zeevi 2010, Perchet and Rigollet 2013), we partition the context space into small hypercubes. For each time step, both our estimates of  $\eta_a(x)$  and our policy  $\pi_t(x)$  will be piecewise constant on these hypercubes. Specifically, in each hypercube, we will either pull arm +1, pull arm -1, or equiprobably pull a random arm from among the two (see Fig. 4(c)). Crucially, and **differently from Rigollet and Zeevi (2010), Perchet and Rigollet (2013), we use data from both *inside and outside* each hypercube to define the estimates and action inside each hypercube.**

We first define a grid lattice  $G'$  on  $[0, 1]^d$ : letting  $\delta = T^{-\frac{\beta}{2\beta+d}} (\log T)^{-1}$ ,

$$G' = \left\{ \left( \frac{2j_1+1}{2}\delta, \dots, \frac{2j_d+1}{2}\delta \right) : j_i \in \{0, \dots, \lceil \delta^{-1} \rceil - 1\}, i = 1, \dots, d \right\}.$$

For any  $x \in \mathcal{X} \subseteq [0, 1]^d$ , we denote by  $g(x) = \arg \min_{x' \in G'} \|x - x'\|$  the closest point to  $x$  in  $G'$ . If there are multiple closest points to  $x$ , we choose  $g(x)$  to be the one closest to  $(0, 0, \dots, 0)$ . All points that share the same closest grid point  $g(x)$  belong to a hypercube with length  $\delta$  and center  $g(x)$ . We denote this hypercube as  $\text{Cube}(x) = \{x' \in \mathcal{X} : g(x') = g(x)\}$ , and the collection of all such hypercubes overlapping with the covariate support as

$$\mathcal{C} = \{\text{Cube}(x) : x \in G\}, \quad \text{where } G = \{x \in G' : \mathbb{P}(\text{Cube}(x) \cap \mathcal{X}) > 0\}.$$

Note that the union of all cubes in  $\mathcal{C}$ ,  $\bigcup_{S \in \mathcal{C}} S$ , must cover the covariate support  $\mathcal{X} \subseteq [0, 1]^d$ .

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**Algorithm 1** SMOOTHBANDIT

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**Input:** Grid lattice  $G$ , epoch schedule  $\{\mathcal{T}_k\}_{k=1}^K$ , Hölder smoothness constant  $\beta$ , regularity constant  $c_0$ , context dimension  $d$ .

- 1: Initialize  $\mathcal{E}_{\pm 1,1} = \emptyset$ ,  $\mathcal{R}_1 = \mathcal{X}$  (explore everywhere, exploit nowhere).
- 2: **for**  $t \in \mathcal{T}_1$  **do**
- 3:   Pull  $A_t = \pm 1$  randomly, equiprobably
- 4: **end for**
- 5: Log the samples  $S_{\pm 1,1} = \{(X_t, Y_t) : t \in \mathcal{T}_1, A_t = \pm 1\}$
- 6: **for**  $k = 2, 3, \dots, K$  **do**
- 7:   Identify inestimable regions for local polynomial regression with bandwidth  $H_{a,k-1}$  ( $a = \pm 1$ ):

$$\mathcal{D}_{a,k-1} = \bigcup \left\{ \text{Cube}(x) : x \in \mathcal{R}_{k-1} \cap G, \begin{array}{l} \left( \bigcup_{j=1}^{k-1} \mathcal{E}_{a,j} \cup \mathcal{R}_{k-1} \right) \cap \mathcal{X} \text{ is not} \\ \text{weakly } \left( \frac{c_0}{2^d}, H_{a,k-1} \right)\text{-regular at } x \end{array} \right\} \quad (6)$$

- 8:   Set  $N_{\pm 1,k-1} = |S_{\pm 1,k-1}|$ ,  $H_{\pm 1,k} = N_{\pm 1,k}^{-1/(2\beta+d)}$
- 9:   Construct the CATE estimate for every  $x \in G \cap \mathcal{R}_{k-1} \cap \mathcal{D}_{1,k-1}^C \cap \mathcal{D}_{-1,k-1}^C$

$$\hat{\tau}_{k-1}(x) = \hat{\eta}^{\text{LP}}(x; S_{+1,k-1}, H_{+1,k-1}, \mathbf{b}(\beta)) - \hat{\eta}^{\text{LP}}(x; S_{-1,k-1}, H_{-1,k-1}, \mathbf{b}(\beta)) \quad (7)$$

- 10:   Update decision regions: for  $a = \pm 1$ ,

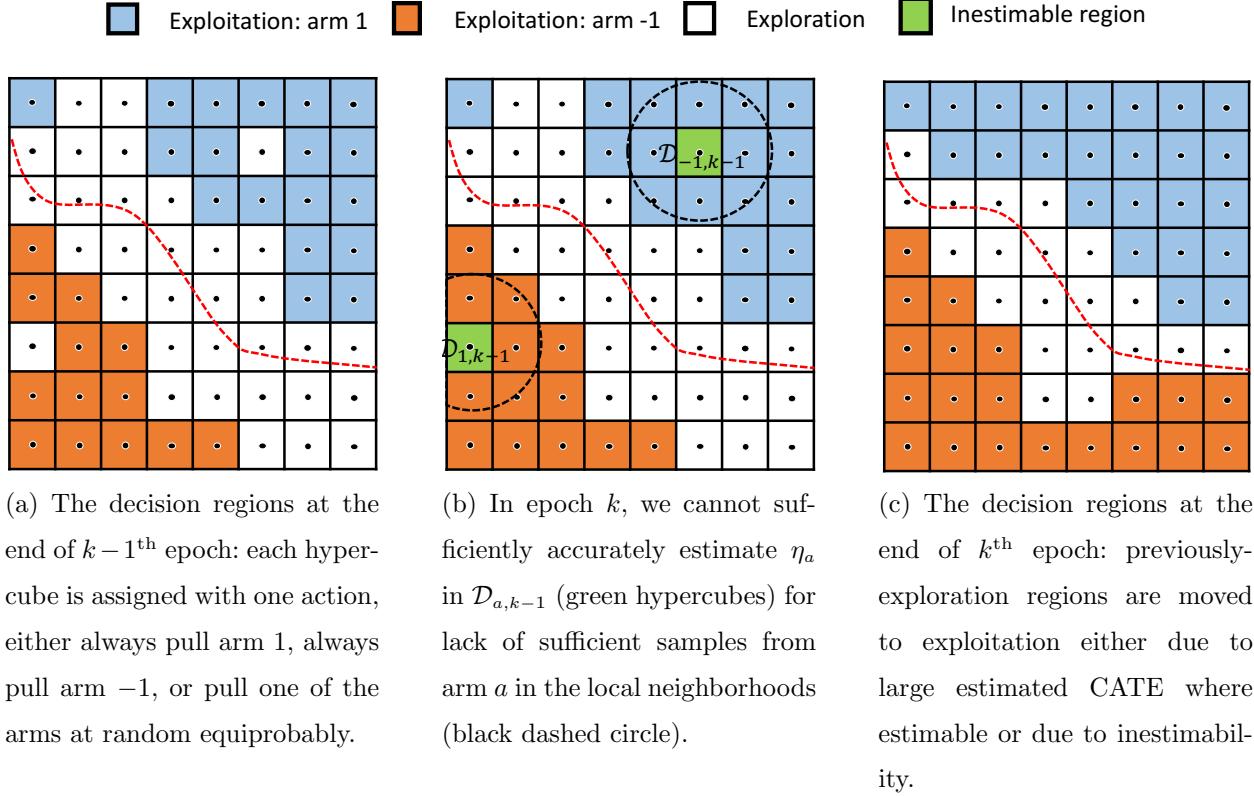
$$\mathcal{E}_{a,k} = \bigcup \left\{ \text{Cube}(x) : x \in G \cap \mathcal{R}_{k-1} \cap \mathcal{D}_{1,k-1}^C \cap \mathcal{D}_{-1,k-1}^C, a\hat{\tau}_{k-1}(x) > \epsilon_{k-1} \right\} \cup \mathcal{D}_{-a,k-1}, \quad (8)$$

$$\mathcal{R}_k = \bigcup \left\{ \text{Cube}(x) : x \in G \cap \mathcal{R}_{k-1} \cap \mathcal{D}_{1,k-1}^C \cap \mathcal{D}_{-1,k-1}^C, |\hat{\tau}_{k-1}(x)| \leq \epsilon_{k-1} \right\}. \quad (9)$$

- 11:   **for**  $t \in \mathcal{T}_k$  **do**
  - 12:     **if**  $X_t \in \bigcup_{j=1}^k \mathcal{E}_{+1,j}$  **then** pull  $A_t = +1$
  - 13:     **else if**  $X_t \in \bigcup_{j=1}^k \mathcal{E}_{-1,j}$  **then** pull  $A_t = -1$
  - 14:     **else** pull  $A_t = \pm 1$  randomly, equiprobably
  - 15:   **end for**
  - 16:   Log samples  $S_{\pm 1,k} = \{(X_t, Y_t) : t \in \mathcal{T}_k, A_t = \pm 1\}$
  - 17: **end for**
- 

**3.2.2. Epoch Structure** Our algorithm then proceeds in an epoch structure, where the estimates and actions assigned to each hypercube is fixed for the duration that epoch. For each epoch, we target a CATE-estimation error tolerance of  $\epsilon_k = 2^{-k}$ . With this target in mind, we set the length of the  $k^{\text{th}}$  epoch as follows:

$$n_k = \left\lceil \frac{4}{p} \left( \frac{\log(T\delta^{-d})}{C_0 \epsilon_k^2} \right)^{\frac{2\beta+d}{2\beta}} + \frac{2}{p^2} \log T \right\rceil, \quad (10)$$



**Figure 4** Updating the decision regions. The black dots represent hypercube centers given in  $G$ . The red dashed curve is the true decision boundary.

where  $p, C_0$  are positive constants given in Lemmas 1 and 7, respectively. We further denote the time index set associated with the  $k^{\text{th}}$  epoch as  $\mathcal{T}_k = \{t : \sum_{i=1}^{k-1} n_{i-1} + 1 \leq t \leq \min\{\sum_{i=1}^k n_i, T\}\}$ .

In our algorithm, we continually maintain a growing region, composed of hypercubes, where we are near-certain which of the arms is optimal. In these regions we always pull the seemingly optimal arm. In contrast, we randomize wherever we are not sure (denoted by the region  $\mathcal{R}_k$  for epoch  $k$ ). The first epoch,  $\mathcal{T}_1$ , is a cold-start phase where, lacking any information, we simply pull each arm uniformly at random in every hypercube ( $\mathcal{R}_1 = \mathcal{X}$ ). After that point, once we have some data, for each subsequent epoch,  $k \geq 2$ , we add the hypercubes  $\mathcal{E}_{a,k} \subseteq \mathcal{R}_{k-1}$  to the set of hypercubes where we just learned that arm  $a$  is probably optimal, never removing any hypercube that was before added. This means that, in epoch  $k$ , we are collecting data on arm  $a$  exclusively in the region  $\bigcup_{j=1}^k \mathcal{E}_{a,j} \cup \mathcal{R}_k$ . We describe in detail how we determine which hypercubes,  $\mathcal{E}_{a,k}$ , to add to the exploitation region of each arm in each epoch in Sections 3.2.4 and 3.2.5.

The total number of epochs  $K$  is the minimum integer such that  $\sum_{k=1}^K n_k \geq T$ . The following lemma shows that  $K$  grows at most logarithmically with  $T$  under the epoch schedule in Eq. (10).

LEMMA 2. When  $T \geq e^{C_0 \vee 1}$ ,

$$K \leq \left\lceil \frac{\beta}{(2\beta + d) \log 2} \log(T) \right\rceil.$$

**3.2.3. Estimating CATE** Next, we describe how we estimate the expected rewards,  $\eta_{\pm 1}(x)$ , and CATE,  $\tau(x) = \eta_1(x) - \eta_{-1}(x)$ , which we use to determine the action we take in each hypercube in each epoch. In particular, at the start of each  $k^{\text{th}}$  epoch,  $k \geq 2$ , we estimate each arm's expected reward  $\hat{\eta}_a(x)$  using the data for each arm from the last epoch, which we denote by  $S_{a,k-1}$  as in Algorithm 1. Our proposed estimate is the following piece-wise constant modification of the local polynomial regression estimate:

$$\begin{aligned} \hat{\eta}_{a,k-1}(x) &= \hat{\eta}^{\text{LP}}(g(x); S_{a,k-1}, H_{a,k-1}, \mathbf{b}(\beta)), \quad \text{where} \\ H_{a,k-1} &= N_{a,k-1}^{-1/(2\beta+d)}, \quad N_{a,k-1} = |S_{a,k-1}|. \end{aligned} \tag{11}$$

Note that by construction  $\hat{\eta}_{a,k-1}(x) = \hat{\eta}_{a,k-1}(x')$  whenever  $x$  and  $x'$  are belong to the same hypercube  $g(x) = g(x')$ . Then our CATE estimate,  $\hat{\tau}_{k-1}(x)$ , is simply the difference of these for  $a = \pm 1$ . Since we only evaluate  $\hat{\tau}_{k-1}(\cdot)$  at hypercube centers  $x \in G$  in our Algorithm 1, we simply use  $g(x)$  as the argument to the local polynomial estimates in Algorithm 2. In particular, we only need to compute two local polynomial regression estimates at a subset of the (finitely-many) grid points. Note that some grid points may not even belong to  $\mathcal{X}$  because their hypercubes may not be fully contained in  $\mathcal{X}$ ; nevertheless, we can use these centers as representative as their  $H_{\pm 1,k-1}$  neighborhood will still contain sufficient data (Lemma 3). Note also that the associated sample sizes,  $N_{\pm 1,k-1}$ , are random variables since they depend on how many samples in the  $(k-1)^{\text{th}}$  epoch fell in different decision regions and on the random decision regions themselves.

Similar to the non-differentiable bandit of Rigollet and Zeevi (2010), our estimators, Eq. (11), are **hypercube-wise constant**. That the estimate at the center of each hypercube is a good estimate for the whole hypercube is justified by the smoothness of  $\eta_{\pm 1}$  and the error is controlled by the size of the hypercubes (see Lemma EC.7 for details).

However, differently from Rigollet and Zeevi (2010), our estimate at the center of each hypercube uses data from both *inside and outside* the hypercube, instead of only inside. This is established by the next lemma.

LEMMA 3. There exists a positive constant  $c_1$  such that

$$\frac{H_{\pm 1,k}}{\sqrt{d}\delta} \geq c_1 T^{\beta-1} \log(T)^{\frac{(2\beta-1)(2\beta+d)}{2\beta}}.$$

When  $\beta \geq 1$ , there exists  $T_0 > 0$  such that for  $T > T_0$ ,  $H_{\pm 1,k} \geq \sqrt{d}\delta$  for  $1 \leq k \leq K$ .

Lemma 3 shows that the bandwidth we use, *i.e.*, the neighborhood of data used to construct the estimate, is *much larger* than the hypercube size, where the estimate is used. According to the nonparametric estimation literature (Stone 1980, 1982), the proposed hypercube size and bandwidths (up to logarithmic factors) are crucial for achieving optimal nonparametric estimation accuracy for smooth functions. This means we indeed *need* to leverage the more global information in order to leverage the smoothness of expected reward functions. This also means that separating the problems into isolated MABs within each hypercube, as would be optimal for unsMOOTH rewards, is infeasible: we must use data across hypercubes to be efficient and so decisions in different hypercubes will be interdependent. In particular, our actions in one hypercube will affect how many samples we collect to learn rewards in other hypercubes.

**3.2.4. Screening Out Inestimable Regions and Accuracy Guarantees** Although using data across multiple hypercubes enables us to improve the estimation accuracy for smooth expected reward functions, it also introduces complicated dependence between data collection in *one* hypercube and algorithm decisions in *other* hypercubes. More concretely, the number of samples available to estimate  $\eta_a$  in each hypercube, and correspondingly the accuracy of this estimate, depends on the arms we pull in *other*, neighboring hypercubes. Because in each epoch in each hypercube we either always exploit or randomly explore, this problem arises precisely when there is a hypercube that is surrounded by hypercubes where we are sure about the optimal arm (and therefore did not explore both arms) but in which we are not yet sure about the optimal arm (and therefore need to estimate both arm reward functions). (See Figs. 4b and 4c.) As a result, the local polynomial regression for estimating  $\eta_a$  in this hypercube can be ill-conditioned and fail to ensure our accuracy target  $\epsilon_k$ . Worse yet, this problem will continue to persist at all future epochs because the nearby hypercubes will continue to exploit and the accuracy target will only become sharper.

Luckily, it turns out that whenever such a problem arises, we do not actually need to estimate  $\eta_a$  in these hypercubes: the fact that the hypercube is surrounded by neighboring hypercubes where we are sure one arm is optimal means that the same arm is also optimal in this hypercube with high probability (See Lemma 5). The only thing we need to do is to detect this issue correctly. Specifically, we propose to use the rule in Eq. (6) in order to screen out the inestimable regions. This screening rule is motivated by Proposition 3 and Assumption 2, which imply that the regularity property of the support of the samples  $S_{a,k-1}$  (*i.e.*,  $(\bigcup_{j=1}^{k-1} \mathcal{E}_{a,j} \cup \mathcal{R}_{k-1}) \cap \mathcal{X}$ ) is critical for the conditioning of the local polynomial estimator. We show in Lemma EC.6 that this screening procedure is well-defined: any hypercube in  $\mathcal{C}$  can be classified into at most one of  $\mathcal{D}_{1,k}$  and  $\mathcal{D}_{-1,k}$  but not both. Moreover, although we check only weak  $(\frac{c}{2^d}, H_{a,k-1})$ -regularity with respect to *only* hypercube centers, Lemma EC.5 implies far stronger consequence for the proposed screening rule:  $(\bigcup_{j=1}^{k-1} \mathcal{E}_{a,j} \cup \mathcal{R}_{k-1}) \cap \mathcal{X}$  is not strongly  $(c_0, r_0)$ -regular at *any* point in  $\mathcal{D}_{a,k-1}$ .

After removing these inestimable regions, we can show (Theorem 1) that the our *uniform* estimation error anywhere in the remaining uncertain region from each epoch (*i.e.*,  $\mathcal{R}_k \cap D_{1,k}^C \cap D_{-1,k}^C$ ) is *exponentially* shrinking:

$$\sup_{x \in \mathcal{R}_k \cap D_{1,k}^C \cap D_{-1,k}^C} |\hat{\tau}_k(x) - \tau(x)| \leq \epsilon_k \text{ with probability } 1 - O(T^{-1}). \quad (12)$$

**3.2.5. Decision Regions** We start by randomizing everywhere,  $\mathcal{R}_1 = \mathcal{X}$ , and in each subsequent epoch, we remove the hypercubes  $\mathcal{E}_{-1,k}, \mathcal{E}_{1,k}$  from the randomization region  $\mathcal{R}_k$  and assign them to join the growing exploitation regions. The set  $\mathcal{E}_{a,k}$  is the union of two parts. The first,  $\{x \in \mathcal{R}_{k-1} \cap D_{1,k-1}^C \cap D_{-1,k-1}^C : a\hat{\tau}_{k-1}(x) > \epsilon_{k-1}\}$ , is determined by  $\hat{\tau}_{k-1}$  and consists of the points where, as long as the event in Eq. (12) holds, we are sure arm  $a$  is optimal. The second is  $\mathcal{D}_{-a,k-1}$  and, in contrast to the first, we cannot rely on the CATE estimator in order to determine that  $a$  is optimal here. Nevertheless, we can show that  $\mathcal{D}_{-a,k-1} \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : a\tau(x) > 0\}$  under Assumption 2 and as long as the event in Eq. (12) holds (Lemma 5). This means that we can conclude that the arm  $a$  is also optimal on  $\mathcal{D}_{-a,k-1}$  even though we cannot estimate CATE accurately there.

The remaining randomization region in each epoch,  $\mathcal{R}_k$ , consists of the subset of the previous randomization region where we cannot determine that either arm is optimal using either of the above criteria. In particular, the CATE estimate is below the accuracy target inside  $\mathcal{R}_k$ ,  $|\hat{\tau}_{k-1}(x)| \leq \epsilon_{k-1}$ , so, even when the event in Eq. (12) holds, we cannot be sure which arm is optimal. Thus, we may as well pull each arm uniformly at random to provide maximum exploration for estimation in future epochs. Moreover, the exploration cost is manageable since, as long as the event in Eq. (12) holds: (1) the regret incurred from pulling sub-optimal arms at the randomization region shrinks exponentially since  $|\tau(x)| \leq |\hat{\tau}_{k-1}(x)| + \epsilon_{k-1} \leq 2\epsilon_{k-1}$  for  $x \in \mathcal{R}_k$ ; and (2) the randomization region shrinks over the epochs, as Assumption 4 implies that  $\mathbb{P}(X \in \mathcal{R}_k \cap \mathcal{X}, |\tau(X)| \neq 0) \leq \mu(\{X : 0 < |\tau(X)| \leq 2\epsilon_{k-1}\}) \leq \gamma(2\epsilon_{k-1})^\alpha$ .

In each epoch, we update the CATE estimates and the decision rule only where it is needed. We estimate CATE and design new decision regions (*i.e.*,  $\mathcal{R}_k$  and  $\mathcal{E}_{\pm 1,k}$ ) only within the region where we failed to learn the optimal arm with high confidence in previous epochs (*i.e.*,  $\mathcal{R}_{k-1}$ ), and we follow previous decision rules on regions where the optimal arm is already learned with high confidence (*i.e.*,  $\bigcup_{j=1}^{k-1} \mathcal{E}_{a,j}$ ). In this way, we gradually refine the accuracy of CATE estimator in ambiguous regions, while making efficient use of the information learned in previous epochs.

**3.2.6. Finite Running Time** Finally, we remark that Algorithm 1 can be run in finite time. First, we show that all decision regions are unions of hypercubes in  $\mathcal{C}$ , as shown in Fig. 4.

LEMMA 4. *For  $1 \leq k \leq K$ ,  $\mathcal{E}_{\pm 1,k}$ ,  $\mathcal{D}_{\pm 1,k}$  and  $\mathcal{R}_k$  are all unions of hypercubes in  $\mathcal{C}$ .*

The number of hypercubes itself,  $|G|$ , is of course finite. To determine in what hypercube an arriving context falls, we need only divide each of its coordinate by  $\delta$ .

The remaining question is to compute which hypercubes belong to which decision region at the start of each epoch. To compute  $\mathcal{D}_{\pm 1,k}$ , we need to compute the volume in the intersection of  $\mathcal{X}$ , a union of cubes, and a ball and compare it to a given constant. We need to do this at most once in each epoch for every hypercube. If  $\mathcal{X}$  has a simple shape such as the unit hypercube, this can be done analytically. Alternatively, given a membership oracle for  $\mathcal{X}$ , we can compute this using rectangle quadrature integration. In particular, we can easily allow for some slowly vanishing approximation error in the quadrature integration without deteriorating the regret rate of our algorithm. Then, to compute  $\mathcal{E}_{\pm 1,k}$  and  $\mathcal{R}_k$ , we need only to compute  $\hat{\eta}_{k,a}(x)$  at most once in each epoch at each lattice point  $x \in G$ . Computing this estimate requires constructing an  $M_\beta \times M_\beta$  matrix given by averaging over the data within the bandwidth neighborhood and then pseudo-inverting this matrix.

## 4. Theoretical Guarantees: Upper and Lower Bounds on Minimax Regret

We next provide two results that together characterize the minimax regret rate (up to polylogs): an upper bound on the regret of our algorithm and a matching lower bound on the regret of any other algorithm.

### 4.1. Regret Upper Bound

In this section, we derive an upper bound on the regret of our algorithm. The performance of our algorithm, as we will show in this section, crucially depends on two events:  $\mathcal{M}_k$ , the event that sufficiently *many* samples for each arm are available for CATE estimation at the end of epoch  $k$ , and  $\mathcal{G}_k$ , the event that our estimator  $\hat{\tau}_k$  has *good* accuracy. Concretely,

$$\begin{aligned}\mathcal{M}_k &= \left\{ N_{1,k} \wedge N_{-1,k} \geq \left( \frac{\log(T\delta^{-d})}{C_0\epsilon_k^2} \right)^{\frac{2\beta+d}{2\beta}} \right\}, \\ \mathcal{G}_k &= \left\{ \sup_{x \in \mathcal{R}_k \cap D_{1,k}^C \cap D_{-1,k}^C} |\hat{\tau}_k(x) - \tau(x)| \leq \epsilon_k \right\}.\end{aligned}$$

For convenience, we also define  $\bar{\mathcal{G}}_k = \bigcap_{1 \leq j \leq k} \mathcal{G}_j$  and  $\bar{\mathcal{M}}_k = \bigcap_{1 \leq j \leq k} \mathcal{M}_j$ , where an empty intersection ( $\bar{\mathcal{G}}_0$  or  $\bar{\mathcal{M}}_0$ ) is the whole event space (always true).

**4.1.1. Characterization of the decision regions.** The following lemma shows that these two events are critical for the effectiveness of the proposed decision rules, in that whenever they hold, we have the desired behavior described in Sections 3.2.4 and 3.2.5.

**LEMMA 5.** *Fix any  $k \geq 1$ . Suppose Assumption 2 holds and that  $T \geq T_0 \vee \left(\exp\left(1 \vee \frac{C_0(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)}\right)\right)$  with  $T_0$  given in Lemma 3 and  $C_0$  given in Lemma 7. Then, under the event  $\bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}$ , we have for  $a = \pm 1$ :*

- i.  $\mathcal{R}_k \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : |\tau(x)| \leq 2\epsilon_{k-1}\}$ ,
- ii.  $(\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : a\tau(x) > 0\}$ ,
- iii.  $\mathcal{Q}_a \subseteq ((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$ , and
- iv.  $\mathcal{D}_{a,k} \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : a\tau(x) < 0\}$ .

In Lemma 5, statement i means that we cannot identify the optimal arm on the randomization region  $\mathcal{R}_k$ . Statement ii says that pulling arm  $a$  on the exploitation region  $\bigcup_{j=1}^k \mathcal{E}_{a,j}$  is optimal. Statement iii shows that the support of the sample  $S_{a,k}$  (*i.e.*,  $((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$ ) always contains the region where arm  $a$  is optimal,  $\mathcal{Q}_a$ . Statement iv says that the optimal arm on  $\mathcal{D}_{a,k}$  is  $-a$ , which justifies why we put  $\mathcal{D}_{a,k}$  into  $\mathcal{E}_{-a,k}$  in Eq. (8). Recall that on  $\mathcal{D}_{a,k}$ , the support of the sample  $S_{a,k}$  is insufficiently regular and thus we cannot hope to obtain good estimates there. Fortunately, statement iv guarantees that accurate decision making is still *possible* on  $\mathcal{D}_{a,k}$  even though accurate CATE estimation is *impossible*.

Statement iii in Lemma 5 is crucial. On the one hand, it is critical in guaranteeing that sufficient samples can be collected for both arms for future epochs (see also the discussion following Theorem 1). On the other hand, it leads to statement iv, which enables us to make correct decisions in the inestimable regions. The argument is roughly as follows. Given statement iii, if statement iv didn't hold, *i.e.*, if there were any  $x_0 \in \mathcal{D}_{a,k} \cap \mathcal{X}$  such that  $x_0 \in \mathcal{Q}_a = \{x \in \mathcal{X} : a\tau(x) \geq 0\}$ , then by the regularity of  $\mathcal{Q}_a$  imposed by Assumption 2,  $((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$  would be sufficiently regular at  $g(x_0)$ , which violates the construction of  $\mathcal{D}_{a,k}$  in Eq. (6).

**4.1.2. A preliminary regret analysis.** Based on Lemma 5, we can decompose the regret according to  $\bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}$ . Let  $\hat{\pi}$  denote our algorithm, Algorithm 1. Then:

$$\begin{aligned} R_T(\hat{\pi}) &= \sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{E}[Y_t(\pi^*(X_t)) - Y_t(A_t)] \\ &\leq \sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{E}[Y_t(\pi^*(X_t)) - Y_t(A_t) | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}] + \sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C). \end{aligned}$$

We can further decompose the regret in the  $k^{\text{th}}$  epoch given  $\bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}$  into the regret due to exploitation in  $\bigcup_{j=1}^k \mathcal{E}_{1,j} \cup \mathcal{E}_{-1,j}$  and the regret due to exploration in  $\mathcal{R}_k$ :

$$\begin{aligned} &\sum_{t \in \mathcal{T}_k} \mathbb{E}[Y_t(\pi^*(X_t)) - Y_t(A_t) | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}] \\ &\leq \sum_{t \in \mathcal{T}_k} \mathbb{E}[Y_t(\pi^*(X_t)) - Y_t(A_t) | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}, X_t \in (\bigcup_{j=1}^k \mathcal{E}_{1,j} \cup \mathcal{E}_{-1,j})] \\ &\quad + \sum_{t \in \mathcal{T}_k} \mathbb{E}[|\tau(X_t)| | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}, X_t \in \mathcal{R}_k] \mathbb{P}(X_t \in \mathcal{R}_k | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}). \end{aligned}$$

Lemma 5 statement ii implies that the proposed algorithm always pulls the optimal arm on the exploitation region. Therefore, the first term on the right-hand side, *i.e.*, the regret due to exploitation, is equal to 0. Moreover,

$$\begin{aligned} & \sum_{t \in \mathcal{T}_k} \mathbb{E}[|\tau(X_t)| \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}, X_t \in \mathcal{R}_k] \mathbb{P}(X_t \in \mathcal{R}_k \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \\ & \leq \sum_{t \in \mathcal{T}_k} 2\epsilon_{k-1} \mathbb{P}(0 < |\tau(X_t)| \leq 2\epsilon_{k-1} \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \leq \gamma 2^{1+\alpha} \epsilon_{k-1}^{1+\alpha} n_k, \end{aligned}$$

where the first inequality follows from Lemma 5 statement i, and the second inequality follows from the margin condition of Assumption 4.

Therefore, the total regret is bounded as follows:

$$\begin{aligned} R_T(\hat{\pi}) & \leq \sum_{k=1}^K \gamma 2^{1+\alpha} \epsilon_{k-1}^{1+\alpha} n_k + \sum_{k=1}^K n_k \mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C) \\ & \leq \tilde{O}(T^{\frac{\beta+d-\alpha\beta}{2\beta+d}}) + \sum_{k=1}^K n_k \mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C), \end{aligned} \quad (13)$$

where the  $\tilde{O}(\cdot)$  term depends only on the parameters of Assumptions 1 to 4 and not on the particular instance. Thus, if we can prove that  $\mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C)$  is small enough for all  $k$ , then we can (uniformly) bound the cumulative regret  $R_T(\hat{\pi})$  of our proposed algorithm.

**4.1.3. Bounding  $\mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C)$ .** The analysis in Eq. (13) shows that the cumulative regret of the proposed algorithm depends on the probability of  $\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C$ , *i.e.*, that the CATE estimator may not be accurate enough or that the total sample size for one arm is not sufficient in any epoch prior to the  $k^{\text{th}}$  epoch.

To bound this probability, we need to analyze the distribution of the samples for each arm. The sample distributions in each epoch can be distorted by decisions in previous epochs. Since a well-behaved density is crucial for nonparametric estimation, we must make sure that such distortions do not undermine our CATE estimation.

**LEMMA 6.** *For any  $1 \leq k \leq K$  and  $a = \pm 1$ ,  $S_{a,k} = \{(X_t, Y_t) : t \in \mathcal{T}_k, A_t = a\}$  are conditionally i.i.d. samples, given  $\mathcal{F}_{k-1} \cup \mathcal{A}_k$ , where  $\mathcal{F}_{k-1} = \{(X_t, A_t, Y_t) : t \in \bigcup_{k'=1}^{k-1} \mathcal{T}_{k'}\}$ ,  $\mathcal{A}_k = \{A_t : t \in \mathcal{T}_k\}$ .*

*Now suppose Assumptions 2 and 3 hold, let  $C_0$  be defined as in Lemma 7 below for any given  $\beta, L_1, c_0, r_0, \mu_{\min}$ , and suppose  $T \geq T_0 \vee \left( \exp\left(1 \vee \frac{C_0(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)}\right) \right)$ . Then, for  $a = \pm 1$ , under the event  $\bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}$ , the (common) conditional density of any of  $\{X_t : A_t = a, t \in \mathcal{T}_k\}$  with respect to Lebesgue measure, given  $\mathcal{F}_{k-1} \cup \mathcal{A}_k$ , which we denote by  $\mu_{a,k}$ , satisfies the following conditions:*

1.  $\frac{1}{2}\mu_{\min} \leq \mu_{a,k}(x) \leq \frac{2\mu_{\max}}{p}$  for any  $x \in ((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$ .
2.  $\mu_{a,k}(x) = 0$  for any  $x \in (\bigcup_{j=1}^k \mathcal{E}_{-a,j}) \cap \mathcal{X}$ .

Lemma 6 shows that in the  $k^{\text{th}}$  epoch, samples for each arm are i.i.d given the history, and it satisfies a strong density condition on the support of each sample,  $((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$ . Furthermore, this distribution support set is sufficiently regular with respect to points in  $\mathcal{R}_k \cap \mathcal{D}_{1,k}^C \cap \mathcal{D}_{-1,k}^C$ , according to the screening rule given in Eq. (6). Together, this strong density condition and support set regularity condition guarantee that we can estimate CATE using local polynomial estimators well on  $\mathcal{R}_k$  in the  $(k+1)^{\text{th}}$  epoch, after we remove the inestimable regions.

In particular, the following lemma shows that the local polynomial estimator is well-conditioned with high probability, which echoes the classic result in the offline setting (Proposition 3).

**LEMMA 7.** *Suppose the conditions of Lemma 6 hold. Let  $1 \leq k \leq K-1$ ,  $a = \pm 1$ ,  $n_{\pm 1,k}$  be given. Consider the Gram matrices of the local polynomial regression estimators in Eq. (11), i.e.,  $\hat{\mathcal{A}}(x; S_{a,k}, H_{a,k}, \mathbf{b}(\beta))$  as defined in Eq. (5). Then, given  $N_{\pm 1,k} = n_{\pm 1,k}$  and  $\overline{\mathcal{M}}_{k-1} \cap \overline{\mathcal{G}}_{k-1}$ , these satisfy the following with conditional probability at least  $1 - 2M_\beta^2 \exp\left\{-C_0(4(1+L_1\sqrt{d})^2)n_{a,k}^{2\beta/(2\beta+d)}\right\}$ :*

$$\lambda_{\min}(\hat{\mathcal{A}}(x; S_{a,k}, H_{a,k}, \mathbf{b}(\beta))) \geq \lambda_0 > 0, \quad \forall x \in \mathcal{R}_k \cap \mathcal{D}_{1,k}^C \cap \mathcal{D}_{-1,k}^C,$$

where

$$\begin{aligned} \lambda_0 &= \frac{1}{4}\mu_{\min} \inf_{\substack{W \in \mathbb{R}^d, S \subset \mathbb{R}^d : \|W\|=1 \\ S \subseteq \mathcal{B}(0,1) \text{ is compact, } \text{Leb}(S)=c_0 v_d^{d/2}}} \int_S \left( \sum_{|s| \leq \mathbf{b}(\beta)} W_s u^s \right)^2 du, \\ C_0 &= \frac{3p\lambda_0^2}{4(1+L_1\sqrt{d})^2} \min \left\{ \frac{1}{12M_\beta^4 \mu_{\max} v_d + 2p\lambda_0 M_\beta^2}, \frac{1}{108M_\beta v_d \mu_{\max} + 6\sqrt{M_\beta} p \lambda_0}, \right. \\ &\quad \left. \frac{1}{108M_\beta L^2 v_d \mu_{\max} + 6\sqrt{M_\beta} L(2v_d \mu_{\max} + p) \lambda_0} \right\}. \end{aligned}$$

In Lemma 7,  $\lambda_0$  is positive because the unit shell is compact and, for fixed  $W$ , the infimum over  $S$  is continuous in  $W$  and positive as the integrand can be zero only a measure-zero set while  $S$  has positive measure. The constant  $C_0$  dictates the epoch schedule  $\{\mathcal{T}_k\}_{k=1}^K$  of our proposed algorithm (see Section 3). Note that we can also use any positive constant no larger than  $C_0$  in our algorithm without deteriorating the regret rate.

In the following theorem, we show that  $\mathbb{P}(\overline{\mathcal{G}}_{k-1}^C \cup \overline{\mathcal{M}}_{k-1}^C)$  is indeed very small for large  $T$ , so its contribution to the cumulative regret bound in Eq. (13) is negligible.

**THEOREM 1.** *When  $T \geq T_0 \vee \left(\exp(1 \vee \frac{C_0(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)}) \vee \frac{36M_\beta L^2 v_d^2 \mu_{\max}^2 C_0(2\beta+d)}{p^2 \lambda_0^2 (2\beta+d+\beta d)}\right)$ , if we assume Assumptions 1 to 3, then for any  $1 \leq k \leq K-1$ ,*

$$\mathbb{P}(\mathcal{G}_k^C \mid \overline{\mathcal{G}}_{k-1}, \overline{\mathcal{M}}_k) \leq \frac{8+4M_\beta^2}{T}, \quad \mathbb{P}(\mathcal{M}_k^C \mid \overline{\mathcal{G}}_{k-1}, \overline{\mathcal{M}}_{k-1}) \leq \frac{2}{T}, \quad \mathbb{P}(\overline{\mathcal{G}}_k^C \cup \overline{\mathcal{M}}_k^C) \leq \frac{(10+4M_\beta^2)k}{T}.$$

Here the upper bound on  $\mathbb{P}(\mathcal{G}_k^C \mid \overline{\mathcal{G}}_{k-1}, \overline{\mathcal{M}}_k)$  is derived from the uniform convergence of local polynomial regression estimators (Stone 1982) given a well-conditioned Gram matrices (which we

ensure in Lemma 7) and sufficiently many samples for each arm (ensured by  $\mathcal{M}_k$ ) whose sample distribution satisfies strong density condition (which we ensure in Lemma 6). The upper bound on  $\mathbb{P}(\mathcal{M}_k^C \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1})$  arises from Lemma 1 and Lemma 5 statement iii, since they imply that  $\mathbb{P}(X \in (\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \geq \mathbb{P}(X \in \mathcal{Q}_a) \geq p$  for  $a = \pm 1$ . As a result, at least a constant fraction of  $n_k$  many samples will accumulate for each arm, so that  $\mathcal{M}_k$  holds with high probability as the  $n_k$  proposed in Eq. (10) is sufficiently large. The upper bound on  $\mathbb{P}(\bar{\mathcal{G}}_k^C \cup \bar{\mathcal{M}}_k^C)$  follow from the first two upper bounds by induction.

**4.1.4. Regret Upper Bound.** Given Theorem 1 and Eq. (13), we are now prepared to derive the final upper bound on our regret.

**THEOREM 2.** Suppose Assumptions 1 to 4 hold and  $T \geq T_0 \vee \left( \exp(1 \vee C_0 \vee \frac{C_0(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)} \vee \frac{36M_\beta L^2 v_d^2 \mu_{\max}^2 C_0(2\beta+d)}{p^2 \lambda_0^2 (2\beta+d+\beta d)}) \right)$ . Then

$$R_T(\pi) = \tilde{O}(T^{\frac{\beta+d-\alpha\beta}{2\beta+d}}),$$

where the  $\tilde{O}(\cdot)$  term only depends on the parameters of Assumptions 1 to 4. (An explicit form is given in the proof.)

*Proof sketch.* Theorem 1 states that for  $2 \leq k \leq K$ ,

$$n_k \mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C) \leq n_k \frac{(10 + 4M_\beta^2)(k-1)}{T} \leq (10 + 4M_\beta^2)(k-1).$$

Furthermore, Lemma 2 implies that,

$$K \leq \lceil \frac{\beta}{(2\beta+d) \log 2} \log T \rceil.$$

Thus

$$\begin{aligned} \sum_{k=1}^K n_k \mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C) &\leq (5 + 2M_\beta^2)K^2 \\ &\leq (5 + 4M_\beta^2) \frac{\beta^2 \log^2 T}{(2\beta+d)^2 \log^2 2} = \tilde{O}(1). \end{aligned}$$

The final conclusion follows from Eq. (13).

A complete and detailed proof is given in the supplement.

**COROLLARY 1.** Let any problem parameters be given. Then, for the corresponding class of contextual bandit problems  $\mathcal{P}$ , the minimax regret satisfies

$$\mathcal{R}_T = \tilde{O}(T^{\frac{\beta+d-\alpha\beta}{2\beta+d}}).$$

## 4.2. Regret Lower Bound

In this section, we prove a matching lower bound (up to polylogarithmic factors) for the regret rate in Theorem 2. This means that there does not exist any other algorithm that can achieve a lower rate of regret for all smooth bandit instances in a given smoothness class. Thus, our algorithm achieves the minimax-optimal regret rate.

**THEOREM 3 (Regret Lower Bound).** *Fix any positive parameters  $\alpha, \beta, d, L, L_1$  satisfying  $\alpha\beta \leq d$ . For any admissible policy  $\pi$  and  $T$ , there exists a contextual bandit instance satisfying Assumptions 1 to 4 with the provided parameters such that*

$$\sup_{\mathbb{P} \in \mathcal{P}} R_T(\pi) = \Omega(T^{\frac{\beta+d-\alpha\beta}{2\beta+d}}), \quad (14)$$

where the  $\Omega(\cdot)$  term only depends on the parameters of the class  $\mathcal{P}$  and not on  $\pi$ . Hence, we also have  $\mathcal{R}_T = \Omega(T^{\frac{\beta+d-\alpha\beta}{2\beta+d}})$ .

*Proof sketch.* Define the *inferior sampling rate* of a given policy  $\pi$  as the expected number of times that  $\pi$  disagrees with the oracle policy  $\pi^*$  (for a given instance  $\mathbb{P}$ ), *i.e.*,

$$I_T(\pi) = \mathbb{E} \left[ \sum_{t=1}^T \mathbb{I}(\pi^*(X_t) \neq \pi_t(X_t)) \right].$$

Lemma 3.1 in Rigollet and Zeevi (2010) relates  $R_T(\pi)$  to  $I_T(\pi)$ : under Assumption 4,

$$I_T(\pi) = O(T^{\frac{1}{1+\alpha}} R_T(\pi)^{\frac{\alpha}{1+\alpha}}). \quad (15)$$

Note the implicit dependence of  $I_T(\pi)$ ,  $R_T(\pi)$  on the instance  $\mathbb{P}$ .

We then construct a finite class,  $\mathcal{H}$ , of contextual bandit instances with smooth expected rewards and show, first, that  $\mathcal{H} \subseteq \mathcal{P}$ , *i.e.*, that our construction fits the provided parameters, and, second, that

$$\sup_{\mathbb{P} \in \mathcal{P}} I_T(\pi) \geq \sup_{\mathbb{P} \in \mathcal{H}} I_T(\pi) \geq \frac{1}{|\mathcal{H}|} \sum_{\mathbb{P} \in \mathcal{H}} I_T(\pi) = \Omega(T^{1 - \frac{\alpha\beta}{2\beta+d}}). \quad (16)$$

We arrive at the final conclusion by combining Eqs. (15) and (16).

A complete and detailed proof is given in the supplement.

Note that in Theorem 3, we allow  $\alpha, \beta, d, L, L_1$  to be given. The proof then constructs an example with appropriate values for the rest of the parameters,  $c_0, r_0, \mu_{\max}, \mu_{\min}, \gamma$ , for which the class of bandit problems  $\mathcal{P}$  satisfies the above lower bound. This shows that the rate given in Theorem 2 is tight (for the regime  $\alpha\beta \leq d$ ).

We can furthermore show that our non-standard Assumption 2 is *necessary* for achieving the minimax regret rate  $\tilde{\Theta}(T^{\frac{\beta+d-\alpha\beta}{2\beta+d}})$ . In particular, we will prove that there exists a class of problem instances satisfying Assumptions 1, 3 and 4 such that the corresponding regret lower bound is higher.

**THEOREM 4 (Regret Lower Bound, without Assumption 2).** *Under the conditions of Theorem 3, for any admissible policy  $\pi$  and  $T$ , there exists a contextual bandit instance satisfying Assumptions 1, 3 and 4 (but not necessarily Assumption 2) with the provided parameters such that*

$$\frac{R_T(\pi)}{T^{\frac{\beta+d-\alpha\beta}{2\beta+d}}} = \Omega\left(T^{\frac{\alpha(1+\alpha)\beta^2d}{2(2\beta+d)(\alpha\beta^2+2\beta d+\alpha\beta d+d^2)}}\right) \rightarrow \infty \quad \text{as } T \rightarrow \infty. \quad (17)$$

*Proof sketch.* Similar to the proof of Theorem 3, we can construct another finite class  $\mathcal{H}'$  of bandit problems that satisfy Assumptions 1, 3 and 4 but not Assumption 2 with the provided parameters, and show that for  $\Delta = \frac{1}{2}(\beta + \frac{\beta d}{\alpha\beta+d})$ ,

$$\sup_{\mathbb{P} \in \mathcal{H}'} I_T(\pi) \geq \frac{1}{|\mathcal{H}'|} \sum_{\mathbb{P} \in \mathcal{H}'} I_T(\pi) = \Omega(T^{1-\frac{\alpha\Delta}{2\Delta+d}}). \quad (18)$$

The conclusion Eq. (17) then follows from Eqs. (15) and (18).

## 5. Conclusions

In this paper, we defined and solved the smooth-response contextual bandit problem. We proposed a rate-optimal algorithm that interpolates between using global and local reward information according to the underlying smoothness structure. Our results connect disparate results for contextual bandits and bridge the gap between linear-response and non-differentiable bandits, and contribute to revealing the whole landscape of contextual bandit regret and its interplay with the inherent complexity of the underlying learning problem.

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**Supplemental Material for**  
**Smooth Contextual Bandits: Bridging the Parametric and**  
**Non-differentiable Regret Regimes**

**Algorithm 2** SMOOTHBANDIT (MULTIPLE ARMS)

**Input:** Grid lattice  $G$  and hypercubes  $\mathcal{C}$ , epoch schedule  $\{\mathcal{T}_k\}_{k=1}^K$ , Hölder smoothness constant  $\beta$ , regularity constant  $c_0$ , context dimension  $d$ .

- 1: Initialize  $\mathcal{A}_{j,1} = \mathcal{A}$  for any  $j \in \{1, \dots, |\mathcal{C}|\}$  and  $\mathcal{R}_1(\mathcal{A}) = \mathcal{X}$
- 2: **for**  $t \in \mathcal{T}_1$  **do**
- 3:   Pull  $A_t \in \mathcal{A}$  randomly, equiprobably
- 4: **end for**
- 5: Log the samples  $S_{a,1} = \{(X_t, Y_t) : t \in \mathcal{T}_1, A_t = a\}$  and set  $N_{a,1} = |S_{a,1}|$ ,  $H_{a,1} = N_{a,1}^{-1/(2\beta+d)}$  for  $a \in \mathcal{A}$
- 6: **for**  $k = 2, 3, \dots, K$  **do**
- 7:   Identify inestimable regions for local polynomial regression with bandwidth  $H_{a,k-1}$  ( $a \in \mathcal{A}$ ):

$$\mathcal{D}_{IR,k-1}(a) = \bigcup \left\{ \text{Cube}(x) : x \in \left( \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \right) \cap G, \begin{array}{l} \left( \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \right) \cap \mathcal{X} \text{ is not} \\ \text{weakly } \left( \frac{c_0}{2^d}, H_{a,k-1} \right) \text{-regular at } x \end{array} \right\}$$

- 8:   Set  $N_{a,k-1} = |S_{a,k-1}|$ ,  $H_{a,k} = N_{a,k}^{-1/(2\beta+d)}$  for  $a \in \mathcal{A}$
- 9:   Construct the local polynomial estimate for every  $a \in \mathcal{A}$  and  $x \in G \cap \left( \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \right) \cap \mathcal{D}_{IR,k-1}^C(a)$ :

$$\hat{\eta}_{a,k-1}(x) = \hat{\eta}^{\text{LP}}(x; S_{a,k-1}, H_{a,k-1}, \mathbf{b}(\beta))$$

and identify the region where arm  $a$  is estimated to be suboptimal:

$$\mathcal{D}_{Est,k}(a) = \bigcup \left\{ \text{Cube}(x) : \exists a' \in \mathcal{A}, x \in \left( \bigcup_{\mathcal{A}_0: a, a' \in \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \right) \cap G \cap \mathcal{D}_{R,k-1}^C(a) \cap \mathcal{D}_{R,k-1}^C(a'), \right. \\ \left. \hat{\eta}_{a',k-1}(x) - \hat{\eta}_{a,k-1}(x) > \epsilon_{k-1} \right\}$$

- 10:   Update active arm sets: for  $j \in \{1, \dots, |\mathcal{C}|\}$ ,

$$\mathcal{A}_{j,k} = \mathcal{A}_{j,k-1} - \{a \in \mathcal{A}_{j,k-1} : \text{Cube}_j \in \mathcal{D}_{IR,k-1}(a) \cup \mathcal{D}_{Est,k}(a)\},$$

- 11:   Update decision regions: for  $\mathcal{A}_0 \subseteq \mathcal{A}$ ,

$$\mathcal{R}_k(\mathcal{A}_0) = \bigcup_{j=1}^{|\mathcal{C}|} \{\text{Cube}_j(x) : \mathcal{A}_{j,k} = \mathcal{A}_0\}.$$

- 12:   **for**  $t \in \mathcal{T}_k$  and  $\mathcal{A}_0 \subseteq \mathcal{A}$  **do**
- 13:     **if**  $X_t \in \mathcal{R}_k(\mathcal{A}_0)$  **then** pull  $A_t \in \mathcal{A}_0$  randomly, equiprobably
- 14:     **end for**
- 15:   Log samples  $S_{a,k} = \{(X_t, Y_t) : t \in \mathcal{T}_k, A_t = a\}$  for  $a \in \mathcal{A}$
- 16: **end for**

## Appendix A: Extention to Multi-armed Setting

In this section, we consider smooth contextual bandits with multiple arms, i.e.,  $A \in \mathcal{A}$  with  $|\mathcal{A}| > 2$ . We first extend Assumptions 1 to 4 to the multi-armed setting as follows.

**ASSUMPTION EC.1.** *Suppose the following conditions hold:*

- i.  $\eta_a(\cdot) = \mathbb{E}[Y(a) | X = \cdot]$  is  $(\beta, L, \mathcal{X})$ -Hölder for  $\beta \geq 1$  and is also  $(1, L_1, \mathcal{X})$ -Hölder for any  $a \in \mathcal{A}$ .
- ii.  $\mathcal{Q}_a = \{x \in \mathcal{X} : \eta_a(x) \geq \eta_{a'}(x) \text{ for any } a' \neq a\}$  is an non-empty  $(c_0, r_0)$ -regular set for any  $a \in \mathcal{A}$ .
- iii. The strong density condition with parameters  $\mu_{\min}$  and  $\mu_{\max}$  in Assumption 3.
- iv. The following margin condition with parameters  $\alpha \geq 0$  and  $\gamma > 0$

$$\mathbb{P}(0 < |\eta_a(X) - \eta_{a'}(X)| \leq t) \leq \gamma t^\alpha$$

for any  $t > 0$ ,  $a, a' \in \mathcal{A}$ .

Note that when  $|\mathcal{A}| = 2$ , each condition above reduces its counterpart in Section 2. By following the proof of Lemma 1, we can again show that  $\min_{a \in \mathcal{A}} \mathbb{P}(X \in \mathcal{Q}_a) \geq p = \mu_{\min} c_0 r_0^d v_d > 0$ . In other words, no arm is strictly suboptimal everywhere.

**Extending the algorithm.** To extend our algorithm to multi-armed setting, we follow the same grid structure in Section 3.2.1 and the epoch structure in Section 3.2.2, and employ the hypercube-wise constant local polynomial estimator in Section 3.2.3 to estimate the conditional reward function  $\eta_a$  for each  $a \in \mathcal{A}$ . We only need to slightly change the epoch schedule by setting the length of the  $k^{\text{th}}$  according to the number of arms  $|\mathcal{A}|$ :

$$n_k = \left\lceil \frac{2|\mathcal{A}|}{p} \left( \frac{\log(T\delta^{-d})}{C_{\mathcal{A}}\epsilon_k^2} \right)^{\frac{2\beta+d}{2\beta}} + \frac{|\mathcal{A}|^2}{2p^2} \log T \right\rceil$$

where

$$C_{\mathcal{A}} = \frac{3p\lambda_0^2}{4(1+L_1\sqrt{d})^2} \min \left\{ \frac{1}{6|\mathcal{A}|M_{\beta}^4\mu_{\max}v_d + 2p\lambda_0M_{\beta}^2}, \frac{1}{54|\mathcal{A}|M_{\beta}v_d\mu_{\max} + 6\sqrt{M_{\beta}}p\lambda_0}, \frac{1}{54|\mathcal{A}|M_{\beta}L^2v_d\mu_{\max} + 6\sqrt{M_{\beta}}L(|\mathcal{A}|v_d\mu_{\max} + p)\lambda_0} \right\}.$$

We mainly need to revise the decision rules in Algorithm 1. Indeed, when only two arms are available, eliminating one arm (either due to estimated suboptimal reward or inestimability screening) unambiguously suggests that the other arm should be pulled. However, this no longer applies when there multiple arms. To tackle with this problem, we associate each region with an active arm set of all arms that we pull with positive probability in this region. Our algorithm (Algorithm 2) gradually eliminates arms from each active arm set, and explores the remaining arms with equal probability. When only a single arm remains in the active arm set of a region, we exploit this arm in this region until the end of the time horizon.

More concretely, we number the hypercubes in  $\mathcal{C}$  (see Section 3.2.1) as  $\text{Cube}_j$  for  $j = 1, \dots, |\mathcal{C}|$ . At the  $k^{\text{th}}$  epoch, we equip hypercube  $\text{Cube}_j$  with an active arm set  $\mathcal{A}_{j,k}$  where each arm within  $\mathcal{A}_{j,k}$  is pulled with equal probability at the  $k^{\text{th}}$  epoch. For example, when  $|\mathcal{A}_{j,k}| = 3$ , the decision for  $X \in \text{Cube}_j$  is  $\pi_k(X) = a$  with probability  $1/3$  for any  $a \in \mathcal{A}_{j,k}$ . When  $|\mathcal{A}_{j,k}| = 1$ , we exploit the unique arm in  $\mathcal{A}_{j,k}$  for  $X \in \text{Cube}_j$ . For

any  $\mathcal{A}_0 \subseteq \mathcal{A}$ , the following set  $\mathcal{R}_{k-1}(\mathcal{A}_0)$  denotes the region where we explore each arm in  $\mathcal{A}_0$  equiprobably in the  $(k-1)$ th epoch:

$$\mathcal{R}_{k-1}(\mathcal{A}_0) = \bigcup_{j=1}^{|\mathcal{C}|} \{\text{Cube}_j(x) : \mathcal{A}_{j,k-1} = \mathcal{A}_0\}.$$

Obviously, for each  $a \in \mathcal{A}$ ,  $\bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0)$  is the region where we can collect samples for arm  $a$  in the  $k$ th epoch, which we denote as  $S_{a,k-1}$  with sample size  $N_{a,k-1}$ . Similar to the two-arm setting (Section 3.2.4), we may not be able to estimate the conditional reward function for a certain arm because of irregularity. The following set is the irregular region for arm  $a \in \mathcal{A}$ :

$$\mathcal{D}_{IR,k-1}(a) = \bigcup \left\{ \text{Cube}(x) : x \in \left( \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \right) \cap G, \begin{array}{l} \left( \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \right) \cap \mathcal{X} \text{ is not} \\ \text{weakly } \left( \frac{c_0}{2^d}, H_{a,k-1} \right)\text{-regular at } x \end{array} \right\}.$$

We will show that although we cannot estimate  $\eta_a$  reliably on  $\mathcal{D}_{IR,k-1}$  due to irregularity, we can ensure that arm  $a$  is strictly suboptimal on  $\mathcal{D}_{IR,k-1}$ , and thus can safely remove arm  $a$  from the corresponding active arm sets (Lemma EC.1 statement iv).

The other scenario where we can safely remove one arm is when the local polynomial estimates confidently determine that this arm is suboptimal. In the following region  $\mathcal{D}_{E,k}(a)$ ,  $\eta_a$  and  $\eta_{a'}$  can both be reliably estimated based on samples from the  $k-1$ th epoch thanks to the regularity condition, and arm  $a'$  is estimated to outperform arm  $a$  in terms of the conditional reward:

$$\mathcal{D}_{E,k}(a) = \bigcup \left\{ \text{Cube}(x) : \exists a' \in \mathcal{A}, x \in \left( \bigcup_{\mathcal{A}_0: a, a' \in \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \right) \cap G \cap \mathcal{D}_{R,k-1}^C(a) \cap \mathcal{D}_{R,k-1}^C(a'), \begin{array}{l} \hat{\eta}_{a',k-1}(x) - \hat{\eta}_{a,k-1}(x) > \epsilon_{k-1} \end{array} \right\}$$

It follows that we can remove arm  $a$  from the active arm sets of all hypercubes in  $\mathcal{D}_{IR,k-1}(a)$  and  $\mathcal{D}_{E,k}(a)$ : for  $j = 1, \dots, |\mathcal{C}|$ ,

$$\mathcal{A}_{j,k} = \mathcal{A}_{j,k-1} - \{a \in \mathcal{A}_{j,k-1} : \text{Cube}_j \in \mathcal{D}_{IR,k-1}(a) \cup \mathcal{D}_{E,k}(a)\}. \quad (\text{EC.1})$$

**Regret Upper bound.** The performance of the proposed algorithm again depends on the following events:

$$\begin{aligned} \mathcal{M}_k &= \left\{ \min_{a \in \mathcal{A}} N_{a,k} \geq \left( \frac{\log(T\delta^{-d})}{C_A \epsilon_k^2} \right)^{\frac{2\beta+d}{2\beta}} \right\}, \\ \mathcal{G}_k &= \left\{ \sup_{x \in \mathcal{R}_k(\mathcal{A}_0) \cap D_{a,k}^C} |\hat{\eta}_{k,a}(x) - \eta_{k,a}(x)| \leq \epsilon_k/2 \text{ for any } a \in \mathcal{A}_0, \text{ and any } \mathcal{A}_0 \subseteq \mathcal{A} \right\}. \end{aligned}$$

where  $\mathcal{M}_k$  represents that sufficiently *many* samples for *all* arms are available, and  $\mathcal{G}_k$  represents *good* accuracy of the estimated conditional reward function for *every* arm uniformly over the region where it is estimable. We again define  $\bar{\mathcal{G}}_k = \bigcap_{1 \leq j \leq k} \mathcal{G}_k$  and  $\bar{\mathcal{M}}_k = \bigcap_{1 \leq j \leq k} \mathcal{M}_k$ , where an empty intersection ( $\bar{\mathcal{G}}_0$  or  $\bar{\mathcal{M}}_0$ ) is the whole event space (always true).

In order to upper bound the regret of our algorithm in multi-armed setting, we need to first extend Lemmas 5 to 7 and Theorem 1. The following lemma extends Lemma 5 and characterizes the decision regions of our algorithm in multi-armed setting.

LEMMA EC.1. *If the event  $\bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}$  holds, then for any  $\mathcal{A}_0 \subseteq \mathcal{A}$  and  $a \in \mathcal{A}$ ,*

- i.  $D_{Est,k}(a) \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : \eta_a(x) < \max_{a' \in \mathcal{A}} \eta_{a'}(x)\};$
- ii.  $\mathcal{R}_k(\mathcal{A}_0) \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : \arg \max_{a \in \mathcal{A}} \eta_a(x) \subseteq \mathcal{A}_0\};$
- iii.  $\mathcal{R}_k(\mathcal{A}_0) \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : \max_{a \in \mathcal{A}_0} \eta_a(x) - \min_{a \in \mathcal{A}_0} \eta_a(x) \leq 2\epsilon_{k-1}\};$
- iv.  $\mathcal{Q}_a \subseteq \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_k(\mathcal{A}_0) \cap \mathcal{X};$
- v.  $D_{IR,k}(a) \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : \eta_a(x) < \max_{a' \in \mathcal{A}} \eta_{a'}(x)\}.$

Here statement i means that arms removed according to local polynomial estimates are strictly suboptimal. Statement ii implies that optimal arms on  $\mathcal{R}_k(\mathcal{A}_0)$  are never removed by mistake, while statement iii means that arms that are being randomized (including the optimal arms) have close expected rewards relative to the tolerance level  $\epsilon_k$ , which justifies our decision to explore them randomly. Statement iv states that the support of sample  $S_{a,k}$  (i.e.,  $\bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_k(\mathcal{A}_0)$ ) always contains the region where arm  $a$  is optimal. Statement v shows that the arms removed because of irregularity are also always strictly suboptimal. Statements i and v justify the updating rule of removing arm  $a$  in hypercubes in  $D_{Est,k}(a)$  and  $D_{IR,k}(a)$  (see Eq. (EC.1)). These statements guarantee low regret of our algorithm provided  $\overline{\mathcal{M}}_k$  and  $\overline{\mathcal{G}}_k$  for  $k = 1, \dots, K$  hold.

To prove that  $\overline{\mathcal{M}}_k$  and  $\overline{\mathcal{G}}_k$  happen with high probability (Theorem EC.2, Section B.6), we further extend Lemmas 6 and 7 to multi-armed setting in Lemmas EC.8 and EC.9 (Section B.6) to ensure that local polynomial estimates are well-behaved. As a result, we can prove that the regret of our algorithm scales with the optimal rate  $\tilde{O}(T^{\frac{\beta+d-\alpha\beta}{2\beta+d}})$ , and an additional factor growing with the number of arms  $|\mathcal{A}|$ .

**THEOREM EC.1.** Suppose Assumption EC.1 holds and  $T \geq T_0$   $\vee$   
 $\left( \exp(1 \vee C_{\mathcal{A}} \vee \frac{C_{\mathcal{A}}(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)} \vee \frac{36M_{\beta}L^2v_d^2\mu_{\max}^2C_{\mathcal{A}}(2\beta+d)}{p^2\lambda_0^2(2\beta+d+\beta d)}) \right)$ . Then

$$R_T(\pi) = \tilde{O}(|\mathcal{A}|^3 T^{\frac{\beta+d-\alpha\beta}{2\beta+d}}),$$

where the  $\tilde{O}(\cdot)$  term only depends on the parameters of Assumption EC.1.

## Appendix B: Omitted Proofs

### B.1. Supporting Lemmas

**LEMMA EC.2.** Under the assumptions in Lemma 2,

$$\begin{aligned} \epsilon_K^{-1} &= 2^K \leq 2T^{\frac{\beta}{2\beta+d}}, \\ \epsilon_k &\geq \frac{1}{2}\delta. \end{aligned}$$

*Proof.* Lemma 2 implies that

$$2^K \leq 2^{\frac{\beta}{(2\beta+d)\log 2} \log(T)+1} = 2T^{\frac{\beta}{2\beta+d}}.$$

It follows that for  $1 \leq k \leq K$ ,

$$2^{-k} \geq 2^{-K} \geq \frac{1}{2}T^{-\frac{\beta}{2\beta+d}} \geq \frac{1}{2}\delta.$$

**LEMMA EC.3.** For two sets  $A \subseteq B$ , and a point  $x \in A$ , if  $A$  is  $(c_0, r_0)$ -regular at  $x$ , then  $B$  is also  $(c_0, r_0)$ -regular at  $x$ .

*Proof.* This is obvious according to the definition of  $(c_0, r_0)$ -regularity (Definition 2).

LEMMA EC.4. *Given  $\bar{\mathcal{M}}_k$ , if  $T \geq \exp(1 \vee \frac{C_0(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)})$ . for  $1 \leq k' \leq k \leq K$ .*

*Proof.* Given  $\bar{\mathcal{M}}_k$ , when  $T \geq \exp(1 \vee \frac{C_0(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)})$ ,

$$\delta^{-d}T \geq \exp\left(\frac{C_0}{4(2r_0)^{2\beta}}\right) \geq \exp(\epsilon_{k'}^2 \frac{C}{(2r_0)^{2\beta}})$$

which implies that  $H_{\pm 1, k'} = N_{\pm 1, k'}^{-\frac{1}{2\beta+d}} \leq (\frac{\log(T\delta^{-d})}{C\epsilon_{k'}^2})^{-\frac{1}{2\beta}} \leq 2r_0$ .

LEMMA EC.5. *For any  $1 \leq k \leq K$ , if  $H_{1,k} = N_{1,k}^{-\frac{1}{2\beta+d}} \in [\sqrt{d}\delta, 2r_0]$ , then  $((\bigcup_{j=1}^k \mathcal{E}_{1,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$  is not strongly  $(c_0, r_0)$ -regular at any  $x \in D_{1,k} \cap \mathcal{X}$ . Similarly, if  $H_{-1,k} = N_{-1,k}^{-\frac{1}{2\beta+d}} \in [\sqrt{d}\delta, 2r_0]$ , then  $((\bigcup_{j=1}^k \mathcal{E}_{-1,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$  is not strongly  $(c_0, r_0)$ -regular at any  $x \in D_{-1,k} \cap \mathcal{X}$ .*

*Proof.* We prove the first statement about  $D_{1,k}$  by contradiction. Suppose there exists a point  $x \in D_{1,k} \cap \mathcal{X}$  such that  $((\bigcup_{j=1}^k \mathcal{E}_{1,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$  is strongly  $(c_0, r_0)$ -regular at  $x$ . Since  $\|g(x) - x\| \leq \frac{1}{2}\sqrt{d}\delta \leq \frac{1}{2}H_{1,k}$ ,

$$\mathcal{B}(x, \frac{H_{1,k}}{2}) \subseteq \mathcal{B}(x, H_{1,k} - \frac{1}{2}\sqrt{d}\delta) \subseteq \mathcal{B}(g(x), H_{1,k}).$$

Thus,

$$\begin{aligned} \text{Leb}[\mathcal{B}(g(x), H_{1,k}) \cap (\bigcup_{j=1}^k \mathcal{E}_{1,j} \cup \mathcal{R}_k)] &\geq \text{Leb}[\mathcal{B}(x, \frac{H_{1,k}}{2}) \cap (\bigcup_{j=1}^k \mathcal{E}_{1,j} \cup \mathcal{R}_k)] \\ &\geq c_0 v_d 2^{-d} H_{1,k}^d = \frac{c_0}{2^d} \text{Leb}[\mathcal{B}(g(x), H_{1,k})], \end{aligned}$$

where  $v_d$  is the volume of a unit ball in  $\mathbb{R}^d$ . Here the second inequality uses the assumption that  $((\bigcup_{j=1}^k \mathcal{E}_{1,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$  is  $(c_0, r_0)$ -regular at  $x$  and that  $H_{a,k}/2 \leq r_0$ .

This means that if there exists any point  $x \in D_{1,k}$  such that  $((\bigcup_{j=1}^k \mathcal{E}_{1,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$  is  $(c_0, r_0)$ -regular at  $x$ , then  $((\bigcup_{j=1}^k \mathcal{E}_{1,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$  must be weakly  $(\frac{c_0}{2^d}, H_{1,k})$ -regular at  $g(x)$ , the center of the hypercube that  $x$  belongs to. By construction,  $((\bigcup_{j=1}^k \mathcal{E}_{1,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$  is not weakly  $(\frac{c_0}{2^d}, H_{1,k})$ -regular at any center of any hypercube in  $D_{1,k}$  (Eq. (6)). Thus the first statement about  $D_{1,k}$  holds. The second one about  $D_{-1,k}$  can be proved analogously.

LEMMA EC.6. *Under the conditions in Lemma 5, and suppose  $H_{\pm 1,k} \in [\sqrt{d}\delta, 2r_0]$ , any hypercube in  $\mathcal{C}$  at most belongs to one of  $\mathcal{D}_{1,k}$  and  $\mathcal{D}_{-1,k}$ .*

*Proof.* We prove this by contradiction. Suppose there exists a Cube  $\in \mathcal{C}$ , such that for  $(\bigcup_{j=1}^k \mathcal{E}_{1,j} \cup \mathcal{R}_k) \cap \mathcal{X}$  is not weakly  $(\frac{c_0}{2^d}, H_{1,k})$ -regular at the center of Cube, and  $(\bigcup_{j=1}^k \mathcal{E}_{-1,j} \cup \mathcal{R}_k) \cap \mathcal{X}$  is not weakly  $(\frac{c_0}{2^d}, H_{-1,k})$ -regular at the center of Cube either.

However, since  $\text{Cube} \cap \mathcal{X} \neq \emptyset$ , there must exist  $x \in \text{Cube} \cap \mathcal{X}$  such that either  $\tau(x) \geq 0$  or  $\tau(x) \leq 0$ . According to Lemma 5 statement iii and Lemma EC.3, either  $(\bigcup_{j=1}^{k-1} \mathcal{E}_{1,j} \cup \mathcal{R}_{k-1}) \cap \mathcal{X}$  or  $(\bigcup_{j=1}^{k-1} \mathcal{E}_{-1,j} \cup \mathcal{R}_{k-1}) \cap \mathcal{X}$  is  $(c_0, r_0)$ -regular at  $x$ . Without loss of generality, we suppose this for  $(\bigcup_{j=1}^{k-1} \mathcal{E}_{1,j} \cup \mathcal{R}_{k-1}) \cap \mathcal{X}$ . Then the proof in Lemma EC.5 implies that  $(\bigcup_{j=1}^{k-1} \mathcal{E}_{1,j} \cup \mathcal{R}_{k-1}) \cap \mathcal{X}$  must be  $(\frac{c_0}{2^d}, H_{1,k})$ -regular at the center of Cube. Thus contradiction arises.

LEMMA EC.7. For  $\forall 1 \leq k \leq K - 1$ , and integers  $n_{\pm 1,k}$  that satisfy  $n_{\pm 1,k} \geq (\frac{6\sqrt{M}Lv_d\mu_{\max}}{p\lambda_0\epsilon_k})^{\frac{2\beta+d}{\beta}}$ ,  $n_{1,k} + n_{-1,k} = n_k$ , if we assume the Assumption Assumptions 1 to 3 and that  $T \geq T_0 \vee \left(\exp(1 \vee \frac{C_0(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)})\right)$ , then the estimator  $\hat{\tau}_k$  based on samples in the  $k^{\text{th}}$  epoch satisfies that

$$\begin{aligned} & \mathbb{P}\left(\sup_{x \in \mathcal{R}_k \cap \mathcal{D}_{1,k}^C \cap \mathcal{D}_{-1,k}^C} |\hat{\tau}_k(x) - \tau(x)| \geq \epsilon_k \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{\pm 1,k} = n_{\pm 1,k}\right) \\ & \leq \delta^{-d}(8 + 4M_\beta^2) \exp(-C_0 n_{a,k}^{\frac{2\beta}{2\beta+d}} \epsilon_k^2). \end{aligned}$$

where  $C_0$  and  $\lambda_0$  are given in Lemma 7.

*Proof.* In the following proof, we condition on  $\bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{\pm 1,k} = n_{\pm 1,k}$ , and  $\mathcal{F}_{k-1}$ . According to Lemma 6, the samples  $S_{a,k} = \{(X_t, Y_t) : A_t = a, t \in \mathcal{T}_k\}$  are i.i.d whose conditional density for  $X_t$  is  $\mu_{a,k} : \frac{1}{2}\mu_{\min} \leq \mu_{a,k}(x) \leq \frac{2\mu_{\max}}{p}$  for any  $x \in ((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$ , and  $\mu_{a,k}(x) = 0$  for any  $x \in (\bigcup_{j=1}^k \mathcal{E}_{-a,j}) \cap \mathcal{X}$ . Moreover, recall that  $\eta_a(x) = \mathbb{E}[Y_t \mid X_t = x, A_t = a]$  for any  $x \in \mathcal{X}$  and  $a = \pm 1$ . Here the purpose of conditioning on  $\bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}$  is merely to guarantee the strong density condition for  $\mu_{a,k}$  by Lemma 6. In what follows,  $K(x)$  denotes the kernel function  $\mathbb{I}(\|x\| \leq 1)$ .

**Step I: Characterize the estimation error for a fixed point on the grid.** We first fix  $x_0 \in G \cap \mathcal{R}_k \cap D_{1,k}^C \cap D_{-1,k}^C$ . To estimate the CATE, we first use local polynomial regression of order  $\beta$  based on samples  $S_{a,k} = \{(X_t, Y_t) : A_t = a, t \in \mathcal{T}_k\}$  to estimate the conditional expected reward  $\eta_a(x_0)$ :

$$\begin{aligned} \hat{\eta}_{a,k}(x_0) &= e_1^T \left( \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} K\left(\frac{X_t - x_0}{h_{a,k}}\right) U\left(\frac{X_t - x_0}{h_{a,k}}\right) U^T\left(\frac{X_t - x_0}{h_{a,k}}\right) \right)^{-1} \\ &\quad \times \left( \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} K\left(\frac{X_t - x_0}{h_{a,k}}\right) U\left(\frac{X_t - x_0}{h_{a,k}}\right) Y_t \right). \end{aligned}$$

where  $U(u) = (u^r)_{|r| \leq \beta}$  is a vector-valued function from  $\mathbb{R}^d$  to  $\mathbb{R}^M$ ,  $h_{a,k} = n_{a,k}^{-\frac{1}{2\beta+d}}$  is the bandwidth,  $e_1$  is a  $M \times 1$  vector whose all elements are 0 except the first one. Recall that  $M_\beta = |\{r : |r| \leq b(\beta)\}|$ .

According to Proposition 1.12 in Tsybakov (2008), the true conditional expected reward  $\eta_a$  can be written in the following way:

$$\begin{aligned} \eta_a(x_0) &= \eta_{a,b(\beta)}(x_0; x_0) = e_1^T \left( \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} K\left(\frac{X_t - x_0}{h_{a,k}}\right) U\left(\frac{X_t - x_0}{h_{a,k}}\right) U^T\left(\frac{X_t - x_0}{h_{a,k}}\right) \right)^{-1} \\ &\quad \times \left( \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} K\left(\frac{X_t - x_0}{h_{a,k}}\right) U\left(\frac{X_t - x_0}{h_{a,k}}\right) \eta_{a,b(\beta)}(X_t; x_0) \right). \end{aligned}$$

where

$$\eta_{a,b(\beta)}(x; x_0) = \sum_{|r| \leq b(\beta)} \frac{(x - x_0)^r}{r!} D^r \eta_a(x_0).$$

After denoting

$$\hat{\mathcal{A}}_{a,k}(x_0) = \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} K\left(\frac{X_t - x_0}{h_{a,k}}\right) U\left(\frac{X_t - x_0}{h_{a,k}}\right) U^T\left(\frac{X_t - x_0}{h_{a,k}}\right),$$

the estimation error for  $\hat{\eta}_{a,k}(x_0)$  has the following upper bound:

$$|\hat{\eta}_{a,k}(x_0) - \eta_a(x_0)| \leq \left\| \left( \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} K\left(\frac{X_t - x_0}{h_{a,k}}\right) U\left(\frac{X_t - x_0}{h_{a,k}}\right) U^T\left(\frac{X_t - x_0}{h_{a,k}}\right) \right)^{-1} \right\|$$

$$\begin{aligned}
& \times \left\| \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} K\left(\frac{X_t - x_0}{h_{a,k}}\right) U\left(\frac{X_t - x_0}{h_{a,k}}\right) (Y_t - \eta_{a,\beta}(X_t; x_0)) \right\| \\
& \leq \frac{\sqrt{M_\beta}}{\lambda_{\min}(\hat{\mathcal{A}}_{a,k}(x_0))} \left| \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} (Y_t - \eta_{a,\beta}(X_t; x_0)) K\left(\frac{X_t - x_0}{h_{a,k}}\right) \right| \\
& \leq \frac{\sqrt{M_\beta}}{\lambda_{\min}(\hat{\mathcal{A}}_{a,k}(x_0))} \left| \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} (Y_t - \eta_a(X_t)) K\left(\frac{X_t - x_0}{h_{a,k}}\right) \right| \\
& + \frac{\sqrt{M_\beta}}{\lambda_{\min}(\hat{\mathcal{A}}_{a,k}(x_0))} \left| \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} (\eta_a(X_t) - \eta_{a,\beta}(X_t; x_0)) K\left(\frac{X_t - x_0}{h_{a,k}}\right) \right|,
\end{aligned}$$

where the second inequality follows from the fact that  $U\left(\frac{X_t - x_0}{h_{a,k}}\right) K\left(\frac{X_t - x_0}{h_{a,k}}\right)$  is a  $M_\beta \times 1$  vector whose elements are bounded by  $K\left(\frac{X_t - x_0}{h_{a,k}}\right)$ .

We further denote

$$\begin{aligned}
\Gamma_1 &= \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} (Y_t - \eta_a(X_t)) K\left(\frac{X_t - x_0}{h_{a,k}}\right) \\
\Gamma_2 &= \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} (\eta_a(X_t) - \eta_{a,\beta}(X_t; x_0)) K\left(\frac{X_t - x_0}{h_{a,k}}\right)
\end{aligned}$$

Then

$$|\hat{\eta}_{a,k}(x_0) - \eta_a(x_0)| \leq \frac{\sqrt{M_\beta}}{\lambda_{\min}(\hat{\mathcal{A}}_{a,k}(x_0))} (\Gamma_1 + \Gamma_2) \quad (\text{EC.2})$$

### Step II: lower bound for $\lambda_{\min}(\hat{\mathcal{A}}_{a,k}(x_0))$ .

According to Lemma 7, with high probability  $1 - 2M_\beta^2 \exp\{-C_0(4(1+L_1\sqrt{d})^2)n_{a,k}^{\frac{2\beta}{2\beta+d}}\}$ ,

$$\lambda_{\min}(\hat{\mathcal{A}}_{a,k}(x_0)) \geq \lambda_0. \quad (\text{EC.3})$$

### Step III: upper bound $\Gamma_1$ and $\Gamma_2$ .

We first bound

$$\Gamma_1 = \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} (Y_t - \eta_a(X_t)) K\left(\frac{X_t - x_0}{h_{a,k}}\right) = \frac{1}{n_{a,k}} \sum_{t \in \mathcal{T}_{a,k}} \hat{Z}_t$$

where

$$\hat{Z}_t = \frac{1}{h_{a,k}^d} (Y_t - \eta_a(X_t)) K\left(\frac{X_t - x_0}{h_{a,k}}\right).$$

It is easy to prove that

$$\begin{aligned}
|\hat{Z}_t| &\leq h_{a,k}^{-d}, \\
\mathbb{E}(\hat{Z}_t | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}) &= 0, \\
\mathbb{E}(\hat{Z}_t^2 | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}) &\leq \frac{2v_d \mu_{\max}}{p h_{a,k}^d},
\end{aligned}$$

where the last inequality uses the fact that  $|Y_t - \eta_a(X_t)| \leq 1$ . By Bernstein's inequality, for  $\forall \epsilon > 0$ ,

$$\begin{aligned}
& \mathbb{P}(|\Gamma_1| \geq \epsilon | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}) \\
&= \mathbb{P}\left(|\sum_{t \in \mathcal{T}_{a,k}} \hat{Z}_t| \geq n_{a,k} \epsilon | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}\right) \\
&\leq 2 \exp\left(-\frac{3pn_{a,k} h_{a,k}^d \epsilon^2}{12v_d \mu_{\max} + 2p\epsilon}\right).
\end{aligned} \quad (\text{EC.4})$$

We now bound

$$\Gamma_2 = \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} (\eta_a(X_t) - \eta_{a,b(\beta)}(X_t; x_0)) K\left(\frac{X_t - x_0}{h_{a,k}}\right) = \frac{1}{n_{a,k}} \sum_{t \in \mathcal{T}_{a,k}} \tilde{Z}_t,$$

where

$$\tilde{Z}_t = \frac{1}{h_{a,k}^d} (\eta_a(X_t) - \eta_{a,b(\beta)}(X_t; x_0)) K\left(\frac{X_t - x_0}{h_{a,k}}\right)$$

Note that by the definition of Hölder class (Assumption 1),

$$\left| (\eta_a(X_t) - \eta_{a,b(\beta)}(X_t; x_0)) K\left(\frac{X_t - x_0}{h_{a,k}}\right) \right| \leq L K\left(\frac{X_t - x_0}{h_{a,k}}\right) \|X_t - x_0\|^\beta \leq L h_{a,k}^\beta.$$

It follows that

$$\begin{aligned} |\mathbb{E}(\tilde{Z}_t | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1})| &\leq \frac{2}{p} L v_d \mu_{\max} h_{a,k}^\beta \\ |\tilde{Z}_t - \mathbb{E}(\tilde{Z}_t | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1})| &\leq \frac{2}{p} L v_d \mu_{\max} h_{a,k}^\beta + L h_{a,k}^{\beta-d} \\ \mathbb{E}(\tilde{Z}_t^2 | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}) &\leq \frac{2}{p} L^2 v_d \mu_{\max} h_{a,k}^{2\beta-d}. \end{aligned}$$

By Bernstein's inequality, for  $\forall \epsilon > 0$ ,

$$\begin{aligned} \mathbb{P}(|\Gamma_2| \geq \epsilon + \frac{2}{p} L v_d \mu_{\max} h_{a,k}^\beta | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}) \\ = \mathbb{P}\left(\left|\frac{1}{n_{a,k}} \sum_{t \in \mathcal{T}_{a,k}} \tilde{Z}_t\right| \geq \epsilon + \frac{2}{p} L v_d \mu_{\max} h_{a,k}^\beta | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}\right) \\ \leq \mathbb{P}\left(\frac{1}{n_{a,k}} \left|\sum_{t \in \mathcal{T}_{a,k}} \tilde{Z}_t - \mathbb{E}(\tilde{Z}_t | \bar{\mathcal{G}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1})\right| \geq \epsilon | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}\right) \\ \leq 2 \exp\left(-\frac{3pn_{a,k}h_{a,k}^d\epsilon^2}{12L^2v_d\mu_{\max}h_{a,k}^{2\beta} + 2L(2v_d\mu_{\max} + p)h_{a,k}^\beta\epsilon}\right). \end{aligned} \tag{EC.5}$$

#### Step IV: error bound for a fixed point

Plug Eqs. (EC.3) to (EC.5) with  $\epsilon = \frac{\lambda_0}{3\sqrt{M_\beta}}\epsilon_k$  into Eq. (EC.2), we can get that

$$\begin{aligned} \mathbb{P}\left(\left|\hat{\eta}_{a,k}(x_0) - \eta_a(x_0)\right| \geq \frac{\sqrt{M_\beta}}{\lambda_0} \left(\frac{2\lambda_0}{3\sqrt{M_\beta}}\epsilon_k + \frac{2}{p} L v_d \mu_{\max} h_{a,k}^\beta\right) | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}\right) \\ \leq 2M_\beta^2 \exp\left(-\frac{3pn_{a,k}h_{a,k}^d\lambda_0^2}{12M_\beta^4\mu_{\max}v_d + 2p\lambda_0M_\beta^2}\right) + 2 \exp\left(-\frac{pn_{a,k}h_{a,k}^d\lambda_0^2\epsilon_k^2}{36M_\beta v_d \mu_{\max} + 2\sqrt{M_\beta}p\epsilon_k\lambda_0}\right) \\ + 2 \exp\left(-\frac{pn_{a,k}h_{a,k}^d\lambda_0^2\epsilon_k^2}{36M_\beta L^2v_d\mu_{\max}h_{a,k}^{2\beta} + 2\sqrt{M_\beta}L(2v_d\mu_{\max} + p)h_{a,k}^\beta\epsilon_k\lambda_0}\right) \end{aligned}$$

Note that  $\frac{2}{p} L v_d \mu_{\max} h_{a,k}^\beta \leq \frac{\lambda_0}{3\sqrt{M_\beta}}\epsilon_k$  under the assumption that  $n_{\pm 1,k} \geq \left(\frac{6\sqrt{M_\beta}L v_d \mu_{\max}}{p\lambda_0\epsilon_k}\right)^{\frac{2\beta+d}{\beta}}$ . In other words,

$$\frac{\sqrt{M_\beta}}{\lambda_0} \left(\frac{2\lambda_0}{3\sqrt{M_\beta}}\epsilon_k + \frac{2}{p} L v_d \mu_{\max} h_{a,k}^\beta\right) \leq \epsilon_k.$$

After denoting

$$C = \min \left\{ \frac{3p\lambda_0^2}{12M_\beta^4\mu_{\max}v_d + 2p\lambda_0M_\beta^2}, \frac{p\lambda_0^2}{36M_\beta v_d \mu_{\max} + 2\sqrt{M_\beta}p\lambda_0}, \frac{p\lambda_0^2}{36M_\beta L^2v_d\mu_{\max}h_{a,k}^{2\beta} + 2\sqrt{M_\beta}L(2v_d\mu_{\max} + p)\lambda_0} \right\},$$

it is easy to verify that

$$\begin{aligned} 2M_\beta^2 \exp\left\{-C_0(4(1+L_1\sqrt{d})^2)n_{a,k}^{\frac{2\beta}{2\beta+d}}\right\} &\leq 2M_\beta^2 \exp(-Cn_{a,k}h_{a,k}^d\epsilon_k^2), \\ \exp\left(-\frac{3pn_{a,k}h_{a,k}^d\lambda_0^2\epsilon_k^2}{108M_\beta v_d\mu_{\max} + 6\sqrt{M_\beta p}\epsilon_k\lambda_0}\right) &\leq \exp(-Cn_{a,k}h_{a,k}^d\epsilon_k^2), \\ \exp\left(-\frac{3pn_{a,k}h_{a,k}^d\lambda_0^2\epsilon_k^2}{108M_\beta L^2v_d\mu_{\max}h_{a,k}^{2\beta} + 6\sqrt{M_\beta L}(2v_d\mu_{\max} + p)h_{a,k}^\beta\epsilon_k\lambda_0}\right) & \\ \leq \exp(-Cn_{a,k}h_{a,k}^{d-\beta}\epsilon_k^2) &\leq \exp(-Cn_{a,k}h_{a,k}^d\epsilon_k^2). \end{aligned}$$

Therefore,

$$\begin{aligned} \mathbb{P}\left(\left|\hat{\eta}_{a,k}(x_0) - \eta_a(x_0)\right| \geq \epsilon_k \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}\right) &\leq (2M_\beta^2 + 4) \exp(-Cn_{a,k}h_{a,k}^d\epsilon_k^2) \\ &= (4 + 2M_\beta^2) \exp(-Cn_{a,k}^{\frac{2\beta}{2\beta+d}}\epsilon_k^2) \end{aligned}$$

Moreover, marginalizing over the history  $\mathcal{F}_{k-1}$  gives

$$\mathbb{P}\left(\left|\hat{\eta}_{a,k}(x_0) - \eta_a(x_0)\right| \geq \epsilon_k \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}\right) \leq (4 + 2M_\beta^2) \exp(-Cn_{a,k}^{\frac{2\beta}{2\beta+d}}\epsilon_k^2)$$

#### Step V: uniform convergence

Since  $|G \cap \mathcal{R}_k \cap D_{1,k}^C \cap D_{-1,k}^C| \leq |G| = \delta^{-d}$ , we can take union bound:

$$\begin{aligned} &\mathbb{P}\left(\sup_{x \in G \cap \mathcal{R}_k \cap D_{1,k}^C \cap D_{-1,k}^C} |\hat{\eta}_{a,k}(x) - \eta_a(x)| \geq \epsilon_k \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}\right) \\ &\leq \delta^{-d} \mathbb{P}(|\hat{\eta}_{a,k}(x_0) - \eta_a(x_0)| \geq \epsilon_k \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}) \\ &\leq \delta^{-d} (4 + 2M_\beta^2) \exp(-Cn_{a,k}^{\frac{2\beta}{2\beta+d}}\epsilon_k^2). \end{aligned}$$

Moreover, since  $\eta_a$  is Lipschitz, we know that for any  $x \in \mathcal{X}$ ,

$$\begin{aligned} |\hat{\eta}_a(x) - \eta_a(x)| &= |\hat{\eta}_a(g(x)) - \eta_a(x)| \\ &\leq |\hat{\eta}_a(g(x)) - \eta_a(g(x))| + |\eta_a(g(x)) - \eta_a(x)| \\ &\leq |\hat{\eta}_a(g(x)) - \eta_a(g(x))| + L_1 \|g(x) - x\| \\ &\leq |\hat{\eta}_a(g(x)) - \eta_a(g(x))| + \frac{1}{2}L_1\sqrt{d}\delta. \end{aligned}$$

Therefore,

$$\begin{aligned} &\mathbb{P}\left(\sup_{x \in \mathcal{R}_k \cap D_{1,k}^C \cap D_{-1,k}^C} |\hat{\eta}_{a,k}(x) - \eta_a(x)| \geq (1 + L_1\sqrt{d})\epsilon_k \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}\right) \\ &\leq \mathbb{P}\left(\sup_{x \in \mathcal{R}_k \cap D_{1,k}^C \cap D_{-1,k}^C} |\hat{\eta}_{a,k}(x) - \eta_a(x)| \geq \epsilon_k + \frac{1}{2}L_1\sqrt{d}\delta \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}\right) \\ &\leq \mathbb{P}\left(\sup_{x \in G \cap \mathcal{R}_k \cap D_{1,k}^C \cap D_{-1,k}^C} |\hat{\eta}_{a,k}(x) - \eta_a(x)| \geq \epsilon_k \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}\right) \\ &\leq \delta^{-d} (4 + 2M_\beta^2) \exp(-Cn_{a,k}^{\frac{2\beta}{2\beta+d}}\epsilon_k^2). \end{aligned}$$

where the first inequality uses the fact that  $\epsilon_k = 2^{-k} \geq \frac{1}{2}\delta$  for  $1 \leq k \leq K$  (Lemma EC.2).

Taking union bound over  $a = \pm 1$  and replacing  $(1 + L_1\sqrt{d})\epsilon_k$  with  $\epsilon_k$  gives the final conclusion.

## B.2. Proofs for Section 2

*Proof of Lemma 1.* By assumption there exists some  $x^* \in \mathcal{Q}_1$ . Then

$$\begin{aligned}\mathbb{P}(X \in \mathcal{Q}_1) &\geq \mu_{\min} \text{Leb}(\mathcal{Q}_1) \\ &\geq \mu_{\min} \text{Leb}(\mathcal{Q}_1 \cap \mathcal{B}(x^*, r_0)) \\ &\geq \mu_{\min} c_0 \text{Leb}(\mathcal{B}(x^*, r_0)) \\ &= \mu_{\min} c_0 r_0^d v_d.\end{aligned}$$

Analogously, we can prove the same result for  $\mathbb{P}(\mathcal{Q}_{-1})$ .

*Proof for Proposition 2.* It is straightforward to extend the Proposition 3.4 in Audibert and Tsybakov (2005) to show that, if  $\alpha(1 \wedge \beta) = \alpha > d$ , then any bandit problem satisfying Assumptions 1, 3 and 4 necessarily satisfies either

$$\mathbb{P}(\mathcal{Q}_1) = 0 \quad \text{or} \quad \mathbb{P}(\mathcal{Q}_{-1}) = 0.$$

This violates Assumptions 2 and 3 according to Lemma 1. Thus, any bandit problem satisfying Assumptions 1 to 4 must also satisfy  $\alpha \leq d$ .

## B.3. Proofs for Section 3

*Proof for Lemma 2.* By definition,  $K$  is the smallest integer such that  $\sum_{j=1}^K n_j \geq T$ .

Note that if  $T \geq e^{C_0}$ , for an integer  $K_0$ ,

$$\sum_{j=1}^{K_0} n_j \geq \sum_{j=1}^{K_0} \frac{4}{p} \left( \frac{\log T}{C_0} \right)^{\frac{2\beta+d}{2\beta}} 2^{\frac{2\beta+d}{\beta} j} \geq \frac{4}{p} (2^{K_0 \frac{2\beta+d}{\beta}} - 1).$$

If  $K_0$  is the smallest integer such that  $\frac{4}{p} (2^{K_0 \frac{2\beta+d}{\beta}} - 1) \geq T$ , then by the definition of  $K$ , we have

$$K \leq K_0 = \lceil \frac{\beta}{(2\beta+d) \log 2} \log \left( \frac{pT}{4} + 1 \right) \rceil \leq \lceil \frac{\beta}{(2\beta+d) \log 2} \log(T) \rceil.$$

*Proof for Lemma 3.* Note that  $H_{\pm 1,k} = (\frac{1}{N_{\pm 1,k}})^{\frac{1}{2\beta+d}} \geq (\frac{1}{n_k})^{\frac{1}{2\beta+d}} \geq (\frac{1}{n_K})^{\frac{1}{2\beta+d}}$ , so we only need to prove the statement for  $(\frac{1}{n_K})^{\frac{1}{2\beta+d}}$ :

$$\begin{aligned}\frac{\frac{1}{n_K}}{(\sqrt{d}\delta)^{2\beta+d}} &= \frac{1}{d^{\frac{2\beta+d}{2}}} \frac{\delta^{-(2\beta+d)}}{\frac{4}{p} \left( \frac{\log(T\delta^{-d})}{C_0 c_K^2} \right)^{\frac{2\beta+d}{2\beta}} + \frac{2}{p^2} \log T} \\ &\geq \frac{1}{d^{\frac{2\beta+d}{2}}} \frac{T^\beta (\log T)^{2\beta+d}}{\frac{4}{p} \left[ \frac{2\beta+d+\beta d}{(2\beta+d)C_0} \right]^{\frac{2\beta+d}{2\beta}} \log(T)^{\frac{2\beta+d}{2\beta}} T + \frac{2}{p^2} \log T} \\ &= \frac{1}{d^{\frac{2\beta+d}{2}}} \frac{T^{\beta-1} (\log T)^{\frac{(2\beta-1)(2\beta+d)}{2\beta}}}{\frac{4}{p} \left[ \frac{2\beta+d+\beta d}{(2\beta+d)C_0} \right]^{\frac{2\beta+d}{2\beta}} + \frac{2}{p^2} \frac{1}{T(\log T)^{\frac{d}{2\beta}}} }.\end{aligned}$$

Thus there exists  $c_1 > 0$  such that

$$\frac{H_{1,k}}{\sqrt{d}\delta} \geq c_1 T^{\beta-1} \log(T)^{\frac{(2\beta-1)(2\beta+d)}{2\beta}}.$$

Since  $c_0 T^{\beta-1} \log(T)^{\frac{(2\beta-1)(2\beta+d)}{2\beta}} \rightarrow \infty$  when  $T \rightarrow \infty$  and  $\beta \geq 1$ , so there exists  $T_0$  such that  $\frac{H_{1,k}}{\sqrt{d}\delta} \geq 1$  for  $T \geq T_0$ .

*Proof for Lemma 4.* We prove this by induction. When  $k = 1$ , this is trivially true because  $\mathcal{E}_{\pm 1,1} = \mathcal{D}_{\pm 1,1} = \emptyset$  and  $\mathcal{R}_1$  is the union of all hypercubes in  $\mathcal{T}$ . Suppose that this statement is also true for  $1 \leq k \leq k_0$ .

For  $k = k_0 + 1$  and  $a = \pm 1$ ,

$$\begin{aligned}\mathcal{R}_k &= \{x \in \mathcal{R}_{k-1} \cap \mathcal{D}_{1,k-1}^C \cap \mathcal{D}_{-1,k-1}^C : |\hat{\tau}_{k-1}(x)| \leq \epsilon_{k-1}\}, \\ \mathcal{E}_{a,k} &= \{x \in \mathcal{R}_{k-1} \cap \mathcal{D}_{1,k-1}^C \cap \mathcal{D}_{-1,k-1}^C : a\hat{\tau}_{k-1}(x) > \epsilon_{k-1}\} \cup \mathcal{D}_{-a,k-1}.\end{aligned}$$

Obviously  $\mathcal{R}_k$  can be written as unions of hypercubes in  $\mathcal{C}$  because  $\mathcal{R}_{k-1} \cap \mathcal{D}_{1,k-1}^C \cap \mathcal{D}_{-1,k-1}^C$  can be written as unions of hypercubes according to the induction assumption, and  $\hat{\tau}_{k-1}$  is constant within each hypercube in  $\mathcal{C}$  (Eq. (11)). Similarly,  $\mathcal{E}_{a,k}$  can be written as unions of hypercubes in  $\mathcal{C}$ .

Moreover, by the definition of  $\mathcal{D}_{a,k}$ , it can be also written as unions of hypercubes in  $\mathcal{C}$  (Eq. (6)).

#### B.4. Proofs for Section 4.1

*Proof for Lemma 5.* We will prove all statements for  $a = 1$ , and those for  $a = -1$  can be proved analogously. We prove the statements by induction. For  $k = 1$ ,  $\bigcup_{j=1}^k \mathcal{E}_{1,j} = \emptyset \subseteq \{x \in \mathcal{X} : \tau(x) > 0\}$ ,  $\bigcup_{j=1}^k \mathcal{E}_{-1,j} = \emptyset \subseteq \{x \in \mathcal{X} : \tau(x) < 0\}$ ,  $\mathcal{R}_k \cap \mathcal{X} = \mathcal{X}$ ,  $\{x \in \mathcal{X} : a\tau(x) \leq 2\epsilon_{k-1}\} = \mathcal{X}$ , and  $\mathcal{D}_{\pm 1,k} = \emptyset$  since  $\bigcup_{j=1}^k \mathcal{E}_{\pm 1,j} \cup \mathcal{R}_k = \mathcal{X}$  is strongly  $(c_0, r_0)$  regular at any  $x \in \mathcal{X}$  according to assumption 2. So statements 1-4 hold for  $k = 1$ .

Assume that statements 1-4 hold for  $k \leq k_0$ . We only need to prove that the statements also holds for  $k_0 + 1$ .

**Statement 1.** Statement 1 follows from the following fact: under the event  $\bar{\mathcal{G}}_{k_0}$ ,

$$\begin{aligned}\mathcal{R}_{k_0+1} \cap \mathcal{X} &= \{x \in \mathcal{R}_{k_0} \cap \mathcal{D}_{1,k_0}^C \cap \mathcal{D}_{-1,k_0}^C \cap \mathcal{X} : |\hat{\tau}_{k_0}(x)| \leq \epsilon_{k_0}\} \\ &\subseteq \{x \in \mathcal{R}_{k_0} \cap \mathcal{X} : |\tau(x)| \leq 2\epsilon_{k_0}\}.\end{aligned}$$

**Statement 2.** According to the decision updating rule Eq. (8),

$$\begin{aligned}\left(\bigcup_{j=1}^{k_0+1} \mathcal{E}_{1,j}\right) \cap \mathcal{X} &= \left(\left(\bigcup_{j=1}^{k_0} \mathcal{E}_{1,j}\right) \cap \mathcal{X}\right) \cup \{x \in \mathcal{R}_{k_0} \cap \mathcal{D}_{1,k_0}^C \cap \mathcal{D}_{-1,k_0}^C \cap \mathcal{X} : \\ &\quad \hat{\tau}_{k_0}(x) > \epsilon_{k_0}\} \cup (\mathcal{D}_{-1,k_0} \cap \mathcal{X}).\end{aligned}$$

According to induction assumption,  $\left(\bigcup_{j=1}^{k_0} \mathcal{E}_{1,j}\right) \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : \tau(x) > 0\}$  and  $\mathcal{D}_{-1,k_0} \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : \tau(x) > 0\}$ .  $\bar{\mathcal{G}}_{k_0}$  implies that  $\{x \in \mathcal{R}_{k_0} \cap \mathcal{D}_{1,k_0}^C \cap \mathcal{D}_{-1,k_0}^C \cap \mathcal{X} : \hat{\tau}_{k_0}(x) > \epsilon_{k_0}\} \subseteq \{x \in \mathcal{X} : \tau(x) > 0\}$ .

**Statement 3.** For  $k \geq 2$ , according to statement 2,

$$\left(\left(\bigcup_{j=1}^k \mathcal{E}_{1,j}\right) \cup \mathcal{R}_k\right)^C \cap \mathcal{X} = \bigcup_{j=1}^k \mathcal{E}_{-1,j} \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : \tau(x) < 0\},$$

which implies  $\{x \in \mathcal{X} : \tau(x) \geq 0\} \subseteq \left(\left(\bigcup_{j=1}^k \mathcal{E}_{1,j}\right) \cup \mathcal{R}_k\right) \cap \mathcal{X}$ .

**Statement 4.** We prove  $\mathcal{D}_{-1,k_0+1} \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : \tau(x) > 0\}$  by showing that for any  $x \in \mathcal{X}$  such that  $\tau(x) \leq 0$ ,  $x \notin \mathcal{D}_{-1,k_0+1}$ . Recall that  $\mathcal{D}_{-1,k_0+1} \subseteq \mathcal{R}_{k_0+1} \subseteq \bigcup_{j=1}^{k_0+1} \mathcal{E}_{-1,j} \cup \mathcal{R}_{k_0+1}$ . According to statement 2 and statement 3,

$$\left(\left(\bigcup_{j=1}^{k_0+1} \mathcal{E}_{-1,j}\right) \cup \mathcal{R}_{k_0+1}\right)^C \cap \mathcal{X} = \left(\bigcup_{j=1}^{k_0+1} \mathcal{E}_{1,j}\right) \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : \tau(x) > 0\},$$

which implies that

$$\{x \in \mathcal{X} : \tau(x) \leq 0\} \subseteq \left( \left( \bigcup_{j=1}^{k_0+1} \mathcal{E}_{-1,j} \right) \cup \mathcal{R}_{k_0+1} \right) \cap \mathcal{X}.$$

If there exists any point  $x \in \mathcal{X}$  such that  $\tau(x) \leq 0$ , then by Assumption 2 and Lemma EC.3,  $\left( \left( \bigcup_{j=1}^{k_0+1} \mathcal{E}_{-1,j} \right) \cup \mathcal{R}_{k_0+1} \right) \cap \mathcal{X}$  is strongly  $(c_0, r_0)$ -regular at  $x$ . Since  $T \geq T_0 \vee \left( \exp\left(1 \vee \frac{C_0(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)}\right)\right)$ , Lemma 3 and Lemma EC.4 implies that  $H_{\pm 1, k'} = N_{\pm 1, k'}^{-\frac{1}{2\beta+d}} \in [\sqrt{d}\delta, 2r_0]$  for  $1 \leq k' \leq k_0$ . Thus we can use Lemma EC.5, which implies that  $x \notin D_{-1, k_0+1}$ . Therefore,  $D_{-1, k_0+1} \cap \mathcal{X} \subseteq \{x \in \mathcal{X} : \tau(x) > 0\}$ .

*Proof for Lemma 6.* When  $k = 1$ , the conclusions hold trivially since  $\mathcal{E}_{\pm 1} = \emptyset, R_1 = \mathcal{X}$ , i.e., we pull each arm with prob. 1/2 for all samples in the first stage. This implies that  $\mu_{\pm 1, 1} = \mu(x)$  for  $x \in \mathcal{X}$ . Then the conclusion follows from Assumption 3. Denote  $\mathcal{T}_{a,k} = \{t \in \mathcal{T}_k : A_t = a\}$ .

When  $k \geq 2$ ,  $\{(X_t, Y_t), t \in \mathcal{T}_{a,k}\}$  are obviously i.i.d conditionally on  $\mathcal{F}_{k-1}, \bar{\mathcal{G}}_{k-1}$  and  $\bar{\mathcal{M}}_{k-1}$ , since  $A_t$  only depends on  $X_t$  and  $\mathcal{F}_{k-1}$ . This implies that  $\{X_t : t \in \mathcal{T}_{a,k}\}$  are i.i.d conditionally on  $\mathcal{F}_{k-1}, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}$ . Furthermore,  $X_t \perp\!\!\!\perp N_{\pm 1, k} | A_t$ , thus  $\{X_t : t \in \mathcal{T}_{a,k}\}$  are i.i.d given  $\mathcal{F}_{k-1}, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{\pm 1, k} = n_{\pm 1, k}$ . This also implies that for any  $x \in \mathcal{X}$ ,

$$\begin{aligned} \mu_{a,k}(x) &= \mu_{X_t | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{\pm 1, k} = n_{\pm 1, k}, \mathcal{F}_{k-1}}(x) \\ &= \mu_{X_t | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}}(x) \end{aligned}$$

For any  $x \in \mathcal{X}$ , obviously  $\mu_{X_t | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}}(x) = \mu_{X_t}(x)$  for  $t \in \mathcal{T}_k$ . Thus

$$\begin{aligned} &\mu_{X_t | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}}(x) \\ &= \frac{\mathbb{P}(A_t = a | X_t = x, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1})}{\mathbb{P}(A_t = a | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1})} \mu_{X_t | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}}(x) \\ &= \frac{\mathbb{P}(A_t = a | X_t = x, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1})}{\mathbb{P}(A_t = a | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1})} \mu_{X_t}(x). \end{aligned} \tag{EC.6}$$

For  $\forall x \in (\bigcup_{j=1}^k \mathcal{E}_{-a,j}) \cap \mathcal{X}$ , our algorithm ensures that

$$\mathbb{P}(A_t = a | X_t = x, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}) = 0.$$

Therefore, for  $\forall x \in (\bigcup_{j=1}^k \mathcal{E}_{-a,j}) \cap \mathcal{X}$ ,  $\mu_{a,k}(x) = 0$ , which proves statement 2.

For any  $x \in ((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$ , our algorithm ensures that

$$\mathbb{P}(A_t = a | X_t = x, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}) \in \left\{ \frac{1}{2}, 1 \right\}.$$

Plus, since  $T \geq T_0 \vee \left( \exp\left(1 \vee \frac{C_0(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)}\right)\right)$ , Lemma 5 implies that  $\{x : a\tau(x) \geq 0\} \subseteq ((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$ . By Assumption 2,

$$\begin{aligned} &\mathbb{P}(A_t = a | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}) \\ &= \mathbb{P}(A_t = a | X_t \in ((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}) \\ &\quad \times \mathbb{P}(X_t \in ((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X} | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}) \\ &\geq \frac{1}{2} \mathbb{P}(a\tau(x) \geq 0) \geq \frac{p}{2}, \end{aligned}$$

where the last inequality follows from Lemma 1.

Then it follows from Assumption 3 and Eq. (EC.11) that for  $\forall x \in ((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$ ,

$$\frac{1}{2}\mu_{\min} \leq \mu_{a,k}(x) \leq \frac{2\mu_{\max}}{p},$$

which proves statement 1.

*Proof for Lemma 7.* In the following proof, we condition on  $\bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{\pm 1,k} = n_{\pm 1,k}$ , and  $\mathcal{F}_{k-1}$ . According to Lemma 6, the samples  $S_{a,k} = \{(X_t, Y_t) : A_t = a, t \in \mathcal{T}_k\} = \{(X_t, Y_t) : t \in \mathcal{T}_{k,a}\}$  are i.i.d whose conditional density for  $X_t$  is  $\mu_{a,k} : \frac{1}{2}\mu_{\min} \leq \mu_{a,k}(x) \leq \frac{2\mu_{\max}}{p}$  for any  $x \in ((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}$ , and  $\mu_{a,k}(x) = 0$  for any  $x \in (\bigcup_{j=1}^k \mathcal{E}_{-a,j}) \cap \mathcal{X}$ . Moreover, recall that  $\eta_a(x) = \mathbb{E}[Y_t | X_t = x, A_t = a]$  for any  $x \in \mathcal{X}$  and  $a = \pm 1$ . Here the purpose of conditioning on  $\bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}$  is merely to guarantee the strong density condition for  $\mu_{a,k}$ . We fix  $x_0 \in G \cap \mathcal{R}_k \cap D_{1,k}^C \cap D_{-1,k}^C$ .

Recall that

$$\hat{\mathcal{A}}_{a,k}(x_0; S_{a,k}) = \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} K\left(\frac{X_t - x_0}{h_{a,k}}\right) U\left(\frac{X_t - x_0}{h_{a,k}}\right) U^T\left(\frac{X_t - x_0}{h_{a,k}}\right).$$

where  $U(u) = (u^r)_{|r| \leq \beta}$  is a vector-valued function from  $\mathbb{R}^d$  to  $\mathbb{R}^M$ ,  $h_{a,k} = n_{a,k}^{-\frac{1}{2\beta+d}}$  is the bandwidth,  $e_1$  is a  $M \times 1$  vector whose all elements are 0 except the first one.

Note that the  $(r_1, r_2)$ -th entry of  $\hat{\mathcal{A}}_{a,k}(x_0)$  is

$$(\hat{\mathcal{A}}_{a,k}(x_0))_{r_1, r_2} = \frac{1}{n_{a,k} h_{a,k}^d} \sum_{t \in \mathcal{T}_{a,k}} \left(\frac{X_t - x_0}{h_{a,k}}\right)^{r_1+r_2} K\left(\frac{X_t - x_0}{h_{a,k}}\right)$$

whose conditional expectation is

$$\begin{aligned} & \mathbb{E}[(\hat{\mathcal{A}}_{a,k}(x_0))_{r_1, r_2} | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}] \\ &= \frac{1}{h_{a,k}^d} \int_{\|\frac{x-x_0}{h_{a,k}}\| \leq 1, x \in (\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k} \left(\frac{x - x_0}{h_{a,k}}\right)^{r_1+r_2} \mu_{a,k}(x) dx \\ &= \int_{\|u\| \leq 1, x_0 + u h_{a,k} \in (\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k} u^{s_1+s_2} \mu_{a,k}(x_0 + h_{a,k} u) du \\ &:= (\mathcal{A}_{a,k}(x_0))_{r_1, r_2} \end{aligned}$$

It follows that

$$\begin{aligned} \lambda_{\min}(\hat{\mathcal{A}}_{a,k}(x_0)) &\geq \min_{\|W\|=1} W^T \mathcal{A}_{a,k}(x_0) W + \min_{\|W\|=1} W^T (\hat{\mathcal{A}}_{a,k}(x_0) - \mathcal{A}_{a,k}(x_0)) W \\ &\geq \min_{\|W\|=1} W^T \mathcal{A}_{a,k}(x_0) W - \sum_{|r_1|, |r_2| \leq \mathfrak{b}(\beta)} |(\hat{\mathcal{A}}_{a,k}(x_0))_{r_1, r_2} - (\mathcal{A}_{a,k}(x_0))_{r_1, r_2}|. \end{aligned} \quad (\text{EC.7})$$

We first derive lower bound for  $\min_{\|W\|=1} W^T \mathcal{A}_{a,k}(x_0) W$ :

$$\begin{aligned} W^T \mathcal{A}_{a,k}(x_0) W &= \int_{B_{a,k}(x_0)} \left( \sum_{|r| \leq \mathfrak{b}(\beta)} W_r u^r \right)^2 \mu_{a,k}(x_0 + h_{a,k} u) du \\ &\geq \frac{1}{2} \mu_{\min} \int_{B_{a,k}(x_0)} \left( \sum_{|r| \leq \mathfrak{b}(\beta)} W_r u^r \right)^2 du, \end{aligned}$$

where  $B_{a,k}(x_0) = \{u \in \mathbb{R}^d : \|u\| \leq 1, x_0 + u h_{a,k} \in ((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X}\}$ .

Note that

$$\begin{aligned}\text{Leb}[B_{a,k}(x_0)] &= h_{a,k}^{-d} \text{Leb}[\mathcal{B}(x_0, h_{a,k}) \cap (((\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k) \cap \mathcal{X})] \\ &\geq h_{a,k}^{-d} \frac{c_0}{2^d} \text{Leb}[\mathcal{B}(x_0, h_{a,k})] = h_{a,k}^{-d} \frac{c_0}{2^d} v_d h_{a,k}^d = \frac{c_0}{2^d} v_d\end{aligned}$$

where the first equality holds because of change of variable, and the inequality holds since  $x_0 \notin D_{\pm 1,k}$  and our construction of  $D_{\pm 1,k}$  guarantees that  $(\bigcup_{j=1}^k \mathcal{E}_{a,j}) \cup \mathcal{R}_k$  is weakly  $(\frac{c_0}{2^d}, h_{a,k})$ -regular at  $x_0 \in G_K$ .

Thus

$$\begin{aligned}\lambda_{\min}(\mathcal{A}_{a,k}(x_0)) &= \min_{\|W\|=1} W^T \mathcal{A}_{a,k}(x_0) W \\ &\geq \frac{1}{2} \mu_{\min} \min_{\|W\|=1, S \subseteq \mathcal{B}(0,1), \text{Leb}(S)=\frac{c_0}{2^d} v_d} \int_S \left( \sum_{|s| \leq b(\beta)} W_s u^s \right)^2 du = 2\lambda_0.\end{aligned}\quad (\text{EC.8})$$

Now we derive upper bound for  $\sum_{|r_1|, |r_2| \leq b(\beta)} |(\hat{\mathcal{A}}_{a,k}(x_0))_{r_1, r_2} - (\mathcal{A}_{a,k}(x_0))_{r_1, r_2}|$ .

For  $t \in S_{a,k}$  and  $|r_1|, |r_2| \leq \beta$ , denote  $Z_t(r_1, r_2) = \frac{1}{h_{a,k}^d} (\frac{x_t - x_0}{h_{a,k}})^{r_1 + r_2} K(\frac{x_t - x_0}{h_{a,k}})$ . Obviously,  $|Z_t(r_1, r_2)| \leq \frac{1}{h_{a,k}^d}$ , and

$$\begin{aligned}&\mathbb{E}(Z_t^2(r_1, r_2) | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}) \\ &= \frac{1}{h_{a,k}^{2d}} \int_{\mathcal{X}} (\frac{x - x_0}{h_{a,k}})^{2(r_1 + r_2)} K^2(\frac{x - x_0}{h_{a,k}}) \mu_{a,k}(x) dx \\ &\leq \frac{2\mu_{\max}}{ph_{a,k}^d} \int_{B_{a,k}(x_0)} u^{2(r_1 + r_2)} du \leq \frac{2\mu_{\max}}{ph_{a,k}^d} \text{Leb}[B_{a,k}(x_0)] \leq \frac{2\mu_{\max} v_d}{ph_{a,k}^d},\end{aligned}$$

where the first inequality follows from the fact that  $\mu_{a,k}(x) \leq \frac{2\mu_{\max}}{p}$ .

By Bernstein inequality,

$$\begin{aligned}\mathbb{P}(|(\hat{\mathcal{A}}_{a,k}(x_0))_{r_1, r_2} - (\mathcal{A}_{a,k}(x_0))_{r_1, r_2}| \geq \frac{\lambda_0}{M_{\beta}^2} | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1} ) \\ &= \mathbb{P}\left(\left| \sum_{i \in \mathcal{T}_{a,k}} Z_t(r_1, r_2) - n_{a,k} \mathbb{E}\left(\sum_{i \in \mathcal{T}_{a,k}} Z_t(r_1, r_2) | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}\right)\right| \geq n_{a,k} \frac{\lambda_0}{M_{\beta}^2} | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}\right) \\ &\leq 2 \exp\left(-\frac{3pn_{a,k}h_{a,k}^d\lambda_0^2}{12M_{\beta}^4\mu_{\max}v_d + 2p\lambda_0 M_{\beta}^2}\right).\end{aligned}$$

By taking union bound over all possible  $r_1, r_2$ ,

$$\begin{aligned}\mathbb{P}\left(\sum_{|r_1|, |r_2| \leq b(\beta)} |(\hat{\mathcal{A}}_{a,k}(x_0))_{r_1, r_2} - (\mathcal{A}_{a,k}(x_0))_{r_1, r_2}| \geq \lambda_0 | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}\right) \\ &\leq 2M_{\beta}^2 \exp\left(-\frac{3pn_{a,k}h_{a,k}^d\lambda_0^2}{12M_{\beta}^4\mu_{\max}v_d + 2p\lambda_0 M_{\beta}^2}\right) \\ &\leq 2M_{\beta}^2 \exp\left\{-C_0(4(1+L_1\sqrt{d})^2)n_{a,k}h_{a,k}^d\right\} \\ &\leq 2M_{\beta}^2 \exp\left\{-C_0(4(1+L_1\sqrt{d})^2)n_{a,k}^{\frac{2\beta}{2\beta+d}}\right\}\end{aligned}\quad (\text{EC.9})$$

According to Eqs. (EC.7) to (EC.9), with high probability  $1 - 2M_{\beta}^2 \exp\left\{-C_0(4(1+L_1\sqrt{d})^2)n_{a,k}^{\frac{2\beta}{2\beta+d}}\right\}$ ,

$$\lambda_{\min}(\hat{\mathcal{A}}_{a,k}(x_0)) \geq \lambda_0.$$

*Proof for Theorem 1.* **I. Proof for**  $\mathbb{P}(\mathcal{G}_k^C \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_k) \leq \frac{8+4M_\beta^2}{T}$ . When  $T \geq \exp(1 \vee \frac{36M_\beta L^2 v_d^2 \mu_{\max}^2 C_0(2\beta+d)}{p^2 \lambda_0^2 (2\beta+d+\beta d)})$ ,

$$\delta^{-d} T \geq \exp\left(\frac{36M_\beta L^2 v_d^2 \mu_{\max}^2 C_0}{p^2 \lambda_0^2}\right),$$

which implies that  $N_{\pm 1,k} \geq \left(\frac{\log(T\delta^{-d})}{C_0 \epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} \geq \left(\frac{6\sqrt{M_\beta} L v_d \mu_{\max}}{p \lambda_0 \epsilon_k}\right)^{\frac{2\beta+d}{\beta}}$  when  $\mathcal{M}_k$  holds.

So all conditions in Lemma EC.7 are satisfied. Thus the conclusion follows from the fact that

$$\delta^{-d} (8 + 4M_\beta^2) \exp(-C_0 \min\{N_{-1,k}, N_{1,k}\}^{\frac{2\beta}{2\beta+d}} \epsilon_k^2) \leq \frac{8 + 4M_\beta^2}{T}.$$

since  $\mathcal{M}_k$  states that

$$\min\{N_{1,k}, N_{-1,k}\} \geq \left(\frac{\log(T\delta^{-d})}{C_0 \epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}}.$$

**II. Proof for**  $\mathbb{P}(\mathcal{M}_k^C \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) \leq \frac{2}{T}$ . Lemma 5 implies that given  $\bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}$ ,  $\{x : \tau(x) \geq 0\} \subseteq \bigcup_{j=1}^k \mathcal{E}_{1,j} \cup \mathcal{R}_k$ . Thus

$$\begin{aligned} \mathbb{E}(N_{1,k} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) &= \mathbb{E}\left(\sum_{t \in \mathcal{T}_k} \mathbb{I}\{X_t \in \bigcup_{j=1}^k \mathcal{E}_{1,j}\} + \sum_{t \in \mathcal{T}_k} \mathbb{I}\{X_t \in \mathcal{R}_k, A_t = 1\} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}\right) \\ &= n_k \mathbb{P}(X_t \in \bigcup_{j=1}^k \mathcal{E}_{1,j} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) + \frac{1}{2} n_k \mathbb{P}(X_t \in \mathcal{R}_k \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) \\ &\geq \frac{1}{2} n_k \mathbb{P}(X_t \in \bigcup_{j=1}^k \mathcal{E}_{1,j} \cup \mathcal{R}_k \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) \\ &\geq \frac{1}{2} n_k \mathbb{P}(\tau(X_t) \geq 0 \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) \geq \frac{p}{2} n_k, \end{aligned}$$

where the last inequality uses Assumption 2.

By Hoeffding's inequality,

$$\begin{aligned} &\mathbb{P}\left(N_{1,k} < \left(\frac{\log(T\delta^{-d})}{C_0 \epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}\right) \\ &\leq \mathbb{P}\left(\mathbb{E}(N_{1,k} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) - N_{1,k} > \frac{p}{2} n_k - \left(\frac{\log(T\delta^{-d})}{C_0 \epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}\right) \\ &\leq \exp\left(-\frac{2}{n_k} \left[\frac{p}{2} n_k - \left(\frac{\log(T\delta^{-d})}{C_0 \epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}}\right]^2\right). \end{aligned}$$

When  $n_k \geq \frac{4}{p} \left(\frac{\log(T\delta^{-d})}{C_0 \epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} + \frac{2}{p^2} \log T$

$$\frac{2}{n_k} \left[\frac{p}{2} n_k - \left(\frac{\log(T\delta^{-d})}{C_0 \epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}}\right]^2 \geq \frac{p^2}{2} n_k - 2p \left(\frac{\log(T\delta^{-d})}{C_0 \epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} \geq \log T.$$

Thus

$$\mathbb{P}\left(N_{1,k} < \left(\frac{\log(T\delta^{-d})}{C_0 \epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}\right) \leq \frac{1}{T}.$$

Similarly, we can prove the result for  $N_{-1,k}$ . Then the conclusion follows by taking union bound for  $N_{-1,k}$  and  $N_{1,k}$ .

**III. Proof for**  $\mathbb{P}(\bar{\mathcal{G}}_k^C \cup \bar{\mathcal{M}}_k^C) \leq \frac{(10+4M^2)k}{T}$ . Recall that  $\bar{\mathcal{G}}_k = \bigcap_{j=1}^k \mathcal{G}_j$  and  $\bar{\mathcal{M}}_k = \bigcap_{j=1}^k \mathcal{M}_j$ . It is easy to verify that

$$\bar{\mathcal{G}}_k^C \cup \bar{\mathcal{M}}_k^C \subseteq \left(\bigcup_{j=0}^{k-1} \mathcal{G}_{j+1}^C \cap \bar{\mathcal{M}}_{j+1} \cap \bar{\mathcal{G}}_j\right) \cup \left(\bigcup_{j=0}^{k-1} \mathcal{M}_{j+1}^C \cap \bar{\mathcal{G}}_j \cap \bar{\mathcal{M}}_j\right).$$

It follows that

$$\begin{aligned}
\mathbb{P}(\bar{\mathcal{G}}_k^C \cup \bar{\mathcal{M}}_k^C) &\leq \sum_{j=0}^{k-1} \mathbb{P}(\mathcal{G}_{j+1}^C \cap \bar{\mathcal{M}}_{j+1} \cap \bar{\mathcal{G}}_j) + \sum_{j=0}^{k-1} \mathbb{P}(\mathcal{M}_{j+1}^C \cap \bar{\mathcal{G}}_j \cap \bar{\mathcal{M}}_j) \\
&\leq \sum_{j=0}^{k-1} \mathbb{P}(\mathcal{G}_{j+1}^C | \bar{\mathcal{G}}_j, \bar{\mathcal{M}}_{j+1}) + \sum_{j=0}^{k-1} \mathbb{P}(\mathcal{M}_{j+1}^C | \bar{\mathcal{G}}_j, \bar{\mathcal{M}}_j) \\
&\leq \sum_{j=0}^{k-1} \frac{8+4M_\beta^2}{T} + \frac{2}{T} = \frac{(10+4M_\beta^2)k}{T}.
\end{aligned}$$

*Proof for Theorem 2.* According to the definition of the expected cumulative regret,

$$\begin{aligned}
R_T(\hat{\pi}) &= \mathbb{E}\left(\sum_{t=1}^T Y_t(\pi^*(X_t)) - Y_t(A_t)\right) \\
&= \sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t)) \\
&\leq \sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t) | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \\
&\quad + \sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t) | \bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C) \mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C) \\
&\leq \sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t) | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \\
&\quad + \sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C)
\end{aligned}$$

where the last inequality follows from the fact that  $Y_t(\pm 1) \in [0, 1]$ .

Theorem 1 states that for  $2 \leq k \leq K$ ,

$$\sum_{t \in \mathcal{T}_k} \mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C) \leq n_k \frac{(10+4M_\beta^2)(k-1)}{T} \leq (10+4M_\beta^2)(k-1).$$

Furthermore,

$$\begin{aligned}
&\sum_{t \in \mathcal{T}_k} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t) | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \\
&= \sum_{t \in \mathcal{T}_k} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t) | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}, X_t \in \mathcal{R}_k) \mathbb{P}(X_t \in \mathcal{R}_k) \\
&\quad + \sum_{t \in \mathcal{T}_k} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t) | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}, X_t \in \bigcup_{j=1}^k \mathcal{E}_{1,j} \cup \mathcal{E}_{-1,j}) \\
&\quad \times \mathbb{P}(X_t \in \bigcup_{j=1}^k \mathcal{E}_{1,j} \cup \mathcal{E}_{-1,j}).
\end{aligned}$$

Lemma 5 implies that given  $\bar{\mathcal{G}}_{k-1}$ ,  $\bigcup_{j=1}^k \mathcal{E}_{1,j} \subseteq \{x : \tau(x) > 0\}$  and  $\bigcup_{j=1}^k \mathcal{E}_{-1,j} \subseteq \{x : \tau(x) < 0\}$ . This means that the decisions made on these regions exactly coincide with the decisions made by the oracle policy. Therefore,

$$\sum_{t \in \mathcal{T}_k} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t) | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}, X_t \in \bigcup_{j=1}^k \mathcal{E}_{1,j} \cup \mathcal{E}_{-1,j}) = 0.$$

Moreover, Lemma 5 states that given  $\bar{\mathcal{G}}_{k-1}$ ,  $\mathcal{R}_k \subseteq \{x : |\tau(x)| \leq 2\epsilon_{k-1}\}$ .

$$\begin{aligned} & \sum_{t \in \mathcal{T}_k} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t) | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}, X_t \in \mathcal{R}_k) \mathbb{P}(X_t \in \mathcal{R}_k | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \\ &= \sum_{t \in \mathcal{T}_k} \mathbb{E}(|\tau(X_t)| | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}, X_t \in \mathcal{R}_k) \mathbb{P}(X_t \in \mathcal{R}_k | \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \\ &= \sum_{t \in \mathcal{T}_k} 2\epsilon_{k-1} \mathbb{P}(|\tau(X_t)| \leq 2\epsilon_{k-1}) \\ &\leq \gamma 2^{1+\alpha} \epsilon_{k-1}^{1+\alpha} n_k, \end{aligned}$$

where the last inequality uses the margin condition in Assumption 4.

Moreover, according to Lemma 2,

$$K \leq \lceil \frac{\beta}{(2\beta+d)\log 2} \log T \rceil.$$

Thus,

$$\begin{aligned} R_T(\hat{\pi}) &\leq \sum_{k=1}^K \gamma 2^{1+\alpha} \epsilon_{k-1}^{1+\alpha} n_k + (10 + 4M^2)(k-1) \\ &\leq \frac{\gamma}{p} 4^{2+\alpha} C_0^{-\frac{2\beta+d}{2\beta}} \frac{2^{2(\beta+d-\alpha\beta)/\beta}}{2^{(\beta+d-\alpha\beta)/\beta}-1} T^{\frac{\beta+d-\alpha\beta}{2\beta+d}} \\ &\quad \times \left( \frac{2\beta+d+\beta d}{2\beta+d} \log T \right)^{\frac{2\beta+d}{2\beta}} + \frac{4}{p^2(2^{1+\alpha}-1)} \gamma 4^{1+\alpha} \log T \\ &\quad + (5 + 4M^2) \frac{\beta^2 \log^2 T}{(2\beta+d)^2 \log^2 2} \\ &= \tilde{O}(T^{\frac{\beta+d-\alpha\beta}{2\beta+d}}). \end{aligned}$$

## B.5. Proofs for Section 4.2

*Proof of Theorem 3.* Our proof of Theorem 3 combines ideas from the proofs of Theorem 3.5 in Audibert and Tsybakov (2007) and Theorem 4.1 in Rigollet and Zeevi (2010).

**First, we construct a class  $\mathcal{H} = \{\mathbb{P}_\sigma : \sigma \in \Sigma_m = \{-1, 1\}^m\}$  of probability distributions of  $(X, Y_1, Y_{-1})$ .**

Fix constants  $\delta_0 \in (0, \frac{1}{2})$ ,  $\kappa^2 = \frac{1}{4} - \delta_0^2$ ,  $q = \lceil (\frac{T}{4e\kappa^2})^{\frac{1}{2\beta+d}} \rceil$ ,  $m = \lceil q^{d-\alpha\beta} \rceil$  and  $\omega = q^{-d}$ . Assume  $T$  is sufficiently large so that  $m \leq q^d$ ,  $\omega \leq \frac{1}{m}$  and  $T > 4\kappa^2 q^{2\beta+d}$ .

Define

$$G_q = \left\{ \left( \frac{2j_1+1}{2q}, \dots, \frac{2j_d+1}{2q} \right) : j_i \in \{0, \dots, q-1\}, i = 1, \dots, d \right\},$$

and we number the points in  $G_q$  as  $x_1, \dots, x_{q^d}$ . For any  $x \in [0, 1]^d$ , we denote by  $g_q(x) = \arg \min_{x' \in G'} \|x - x'\|$  the closest point to  $x$  in  $G'$ . If there are multiple closest points to  $x$ , we choose  $g_q(x)$  to be the one closest to  $(0, 0, \dots, 0)$ . All points that share the same closest grid point  $g_q(x)$  belong to a hypercube with length  $\frac{1}{q}$  and center  $g_q(x)$ . We denote this hypercube as  $\text{Cube}_q(x) = \{x' \in \mathcal{X} : g_q(x') = g_q(x)\}$ . Define  $\mathcal{X}_i = \text{Cube}_q(x_i)$  for  $i = 1, \dots, m$  and  $\mathcal{X}_0 = [0, 1]^d - \bigcup_{i=1}^m \mathcal{X}_i$ .

The marginal distribution of  $X$  (denoted by  $\mathbb{P}_X$ ) does not depend on  $\sigma$ . Its density in  $\mathbb{R}^d$  is

$$\mu_X(x) = \begin{cases} \frac{\omega}{\text{Leb}[\mathcal{B}(0, \frac{1}{4q})]}, & \text{if } x \in \bigcup_{i=1}^m \mathcal{B}(x_i, \frac{1}{4q}), \\ \frac{1-m\omega}{\text{Leb}[\mathcal{A}_0]}, & \text{if } x \in \mathcal{X}_0, \\ 0, & \text{otherwise.} \end{cases}$$

The conditional distribution of  $Y(-1)$  given  $X$  does not depend on  $\sigma$  either. It is simply Bernoulli distribution with conditional expectation is  $\eta_{-1}^\sigma \equiv \frac{1}{2}$ .

We now define the conditional distribution of  $Y(1)$  given  $X$  for  $\mathbb{P}_\sigma \in \mathcal{H}$ .

Consider an infinitely differentiable function  $u_1$  defined as

$$u_1(x) = \begin{cases} \exp\left\{-\frac{1}{(\frac{1}{2}-x)(x-\frac{1}{4})}\right\}, & \text{if } x \in (\frac{1}{4}, \frac{1}{2}), \\ 0, & \text{otherwise,} \end{cases}$$

and take  $u : \mathbb{R}_+ \rightarrow \mathbb{R}_+$  to be

$$u(x) = \left( \int_{\frac{1}{4}}^{\frac{1}{2}} u_1(t) dt \right)^{-1} \int_x^\infty u_1(t) dt.$$

It is easy to verify that  $u$  is a non-increasing infinitely differentiable function satisfying  $u = 1$  on  $[0, \frac{1}{4}]$  and  $u = 0$  on  $[\frac{1}{2}, \infty)$ . Moreover, for any integer  $l \geq 1$ , the  $l$ -th derivative of  $u(x)$  at  $x \in (\frac{1}{4}, \frac{1}{2})$  is in the form of  $\frac{\text{poly}(x)}{((\frac{1}{2}-x)(x-\frac{1}{4}))^{2(l-1)}} \exp\left(-\frac{1}{(\frac{1}{2}-x)(x-\frac{1}{4})}\right)$ , which is bounded in the domain. Therefore, we can find small enough constant  $C_\phi \in (0, \delta_0]$  such that  $\phi : \mathbb{R}^d \rightarrow R_+$  defined as

$$\phi(x) \triangleq C_\phi u(\|x\|) \quad (\text{EC.10})$$

satisfies the condition that for any  $x, x' \in \mathbb{R}^d$  and  $|r| = \mathfrak{b}(\beta)$ ,  $|D^r \phi(x') - D^r \phi_x(x')| \leq \frac{L}{C_\beta} \|x' - x\|^{\beta - \mathfrak{b}(\beta)}$  and  $|\phi(x') - \phi(x)| \leq L_1 \|x' - x\|$ , where  $C_\beta = \sum_{|r|=\mathfrak{b}(\beta)} \frac{1}{r!}$ .

Define  $\eta_1^\sigma : [0, 1]^d \rightarrow \mathbb{R}$  as

$$\eta_1^\sigma(x) = \frac{1}{2} + \sum_{j=1}^m \sigma_j \varphi_j(x),$$

where  $\varphi_j(x) = q^{-\beta} \phi(q[x - x_j]) \mathbb{I}(x \in \mathcal{X}_j)$ . Since  $C_\phi \leq \delta_0$ ,  $\eta_1^\sigma \in [\frac{1}{2} - \delta_0, \frac{1}{2} + \delta_0] \subset [0, 1]$ . Therefore, we can define  $\mathbb{E}_\sigma(Y(1)|X) = \eta_1^\sigma(X)$ , and the conditional distribution of  $Y(1)$  given  $X$  is Bernoulli distribution with mean  $\eta_1^\sigma(X)$ . This completes the construction.

**Second, we check that  $\mathcal{H} \subseteq \mathcal{P}$ .**

Fix any  $\sigma \in \Sigma_m$  and consider distribution  $\mathbb{P}_\sigma$ .

1. Smooth Conditional Expected Rewards (Assumption 1)

The verification for  $\eta_{-1}^\sigma$  is trivial.

For any  $l \in \mathbb{N}_+^d$  such that  $|l| \leq \mathfrak{b}(\beta)$  and  $j \in \{1, \dots, m\}$ ,

$$D^l \varphi_j(x) = q^{|l|-\beta} D^l \phi(q[x - g_q(x)]) \mathbb{I}\{x \in \mathcal{X}_j\}.$$

Recall that our choice of  $C_\phi$  ensures that for any  $|r| = \mathfrak{b}(\beta)$ ,  $|D^r \phi(x') - D^r \phi_x(x')| \leq \frac{L}{C_\beta} \|x' - x\|^{\beta - \mathfrak{b}(\beta)}$ .

When  $x$  and  $x'$  are in the same cube, we have

$$\begin{aligned} \|D^r \eta_1^\sigma(x') - D^r \eta_1^\sigma(x)\| &\leq \|D^r \varphi_j(x') - D^r \varphi_j(x)\| \\ &\leq q^{\mathfrak{b}(\beta)-\beta} \|D^r \phi(q(x' - g_q(x'))) - D^r \phi(q(x - g_q(x)))\| \\ &\leq \frac{L}{C_\beta} q^{\mathfrak{b}(\beta)-\beta} \|q(x' - g_q(x')) - q(x - g_q(x))\|^{\beta - \mathfrak{b}(\beta)} \\ &\leq \frac{L}{C_\beta} \|(x' - g_q(x')) - (x - g_q(x))\|^{\beta - \mathfrak{b}(\beta)} \\ &= \frac{L}{C_\beta} \|x' - x\|^{\beta - \mathfrak{b}(\beta)}. \end{aligned}$$

When  $x$  and  $x'$  are in different cubes, we can always find  $x''$  in the same cube as  $x$  such that  $D^r \eta_1^\sigma(x'') = D^r \eta_1^\sigma(x')$  and

$$\|D^r \eta_1^\sigma(x') - D^r \eta_1^\sigma(x)\| = \|D^r \eta_1^\sigma(x'') - D^r \eta_1^\sigma(x)\| \leq \frac{L}{C_\beta} \|x'' - x\|^{\beta - b(\beta)} \leq \frac{L}{C_\beta} \|x' - x\|^{\beta - b(\beta)}.$$

Therefore, for any  $x, x' \in [0, 1]^d$ , there exists  $\lambda \in [0, 1]$  such that

$$\begin{aligned} \|\eta_1^\sigma(x') - \sum_{|r| \leq b(\beta)} \frac{(x' - x)^r}{r!} D^r \eta_1^\sigma(x)\| &\leq \left\| \sum_{|r|=b(\beta)} \frac{(x' - x)^r}{r!} D^r \eta_1^\sigma(x' + \lambda(x - x')) - \sum_{|r|=b(\beta)} \frac{(x' - x)^r}{r!} D^r \eta_1^\sigma(x) \right\| \\ &\leq C_\beta \|x' - x\|^{b(\beta)} \frac{L}{C_\beta} \|x' - x\|^{\beta - b(\beta)} \\ &= L \|x' - x\|^\beta, \end{aligned}$$

and  $|\eta_1^\sigma(x') - \eta_1^\sigma(x)| \leq L_1 \|x' - x\|$ .

## 2. Optimal Decision Regions (Assumption 2)

Note that by construction  $\mathcal{X}_0 \subseteq \mathcal{Q}_a = \{x : a\tau(x) \geq 0\} \cap \mathcal{X}$ . Moreover, by the construction of  $m$  and  $w$ ,  $\text{Leb}[\mathcal{X}_0] = (1 + o(1))\text{Leb}([0, 1]^d) = (1 + o(1))\text{Leb}(\mathcal{X})$ , or equivalently  $\text{Leb}[\cup_{i=1}^m \mathcal{X}_i] \ll \text{Leb}[\mathcal{X}_0]$ . This means that for sufficiently large  $T$ , the whole covariate support is almost entirely occupied by  $\mathcal{X}_0$ .

Let's fix a point  $x \in \mathcal{Q}_a$  and a sufficiently large  $T$ . We consider two cases:

- When  $r \gg \frac{1}{q}$ , then by the fact that the whole covariate support is almost entirely occupied by  $\mathcal{X}_0$ ,  $\text{Leb}[\mathcal{B}(x, r) \cap \mathcal{Q}_a] \geq \text{Leb}[\mathcal{B}(x, r) \cap \mathcal{X}_0] = (1 + o(1))\text{Leb}[\mathcal{B}(x, r)]$ , so regularity is satisfied.
- When  $r = O(\frac{1}{q})$ , if  $x \in \mathcal{X}_0$ , the regularity condition is satisfied because each hypercube satisfies the regularity condition. On the other hand, if  $x \in \mathcal{Q}_a \setminus \mathcal{X}_0 = \cup_{i=1}^m \mathcal{X}_i \cap \mathcal{Q}_a$  (and without loss of generality let  $x \in \mathcal{B}(x_1, \frac{1}{4q})$ ), then  $\text{Leb}[\mathcal{B}(x, r) \cap \mathcal{Q}_a] \geq \text{Leb}[\mathcal{B}(x, r) \cap \mathcal{B}(x_1, \frac{1}{4q})]$ . Then the regularity condition is satisfied by the fact that the ball  $\mathcal{B}(x_1, \frac{1}{4q})$  is regular.

## 3. Strong Density (Assumption 3)

The support of  $X$  is  $\mathcal{X} = \cup_{i=1}^m \mathcal{B}(x_i, \frac{1}{4q}) \cup \mathcal{X}_0$ , which is compact. By definition,

$$\mu_X(x) = \begin{cases} \frac{4^d}{v_d}, & \text{if } x \in \cup_{i=1}^m \mathcal{B}(x_i, \frac{1}{4q}), \\ \frac{1-m\omega}{1-mq^{-d}} = 1, & \text{if } x \in \mathcal{X}_0. \end{cases}$$

The strong density condition is satisfied with  $\mu_{\max} = \frac{4^d}{v_d}$  and  $\mu_{\min} = 1$ .

## 4. Margin Condition (Assumption 4)

Let  $x_0 = (\frac{1}{2q}, \dots, \frac{1}{2q})$ . We have

$$\begin{aligned} \mathbb{P}_\sigma(0 < |\tau(X)| \leq t) &= \mathbb{P}_\sigma(0 < |\eta_1^\sigma(X) - \frac{1}{2}| \leq t) \\ &= m \mathbb{P}_\sigma(0 < \phi[q(X - x_0)] \leq tq^\beta) \\ &= m \int_{\mathcal{B}(x_0, \frac{1}{4q})} \mathbb{I}\{0 < \phi[q(x - x_0)] \leq tq^\beta\} \frac{\omega}{\text{Leb}[\mathcal{B}(0, \frac{1}{4q})]} dx \\ &= \frac{m\omega}{\text{Leb}[\mathcal{B}(0, \frac{1}{4})]} \int_{\mathcal{B}(0, \frac{1}{4})} \mathbb{I}\{\phi(x) \leq tq^\beta\} dx \\ &= m\omega \mathbb{I}\{t \geq C_\phi q^{-\beta}\}. \end{aligned}$$

Note that  $m\omega = O(q^{-\alpha\beta})$ , and Assumption 4 with is satisfied with  $\gamma = 2C_\phi^{-\alpha}$ .

**Finally, we prove a lower bound for  $\mathbb{E}I_t(\pi)$  based on problem instances in  $\mathcal{H}$ .**

For any policy  $\pi$  and any  $t = 1, \dots, T$ , denote by  $\mathbb{P}_{\pi,\sigma}^t$  the joint distribution of

$$(X_1, Y_1(\pi_1(X_1))), \dots, (X_t, Y_t(\pi_t(X_t)))$$

where  $(X_t, Y_t(1), Y_t(-1))$  are generated i.i.d from  $\mathbb{P}_\sigma$ , and  $\mathbb{E}_{\pi,\sigma}^t$  the corresponding expectation.

Observe that

$$\begin{aligned} \sup_{\sigma \in \Sigma_m} \mathbb{E}_\sigma I_t(\pi) &= \sup_{\sigma \in \Sigma_m} \sum_{t=1}^T \mathbb{E}_{\pi,\sigma}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq \text{sign}(\eta_1^\sigma(X_t))] \\ &= \sup_{\sigma \in \Sigma_m} \sum_{j=1}^m \sum_{t=1}^T \mathbb{E}_{\pi,\sigma}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq \sigma_j, X_t \in \mathcal{X}_j] \\ &\geq \frac{1}{2^m} \sum_{j=1}^m \sum_{t=1}^T \sum_{\sigma \in \Sigma_m} \mathbb{E}_{\pi,\sigma}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq \sigma_j, X_t \in \mathcal{X}_j] \\ &= \frac{1}{2^m} \sum_{j=1}^m \sum_{t=1}^T \sum_{\sigma_{[-j]} \in \Sigma_{m-1}} \sum_{i \in \{-1, 1\}} \mathbb{E}_{\pi,\sigma_{[-j]}^i}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq i, X_t \in \mathcal{X}_j], \end{aligned}$$

where  $\sigma_{[-j]} = (\sigma_1, \dots, \sigma_{j-1}, \sigma_{j+1}, \dots, \sigma_m)$  and  $\sigma_{[-j]}^i = (\sigma_1, \dots, \sigma_{j-1}, i, \sigma_{j+1}, \dots, \sigma_m)$ .

For  $j = 1, \dots, m$ , define  $\mathbb{P}_X^j(\cdot) = \mathbb{P}_X(\cdot | X \in \mathcal{X}_j)$ . By Theorem 2.2(iii) in Tsybakov (2008),

$$\begin{aligned} \sum_{i \in \{-1, 1\}} \mathbb{E}_{\pi,\sigma_{[-j]}^i}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq i, X_t \in \mathcal{X}_j] &= \frac{1}{q^d} \sum_{i \in \{-1, 1\}} \mathbb{E}_{\pi,\sigma_{[-j]}^i}^{t-1} \mathbb{P}_X^j[\pi_t(X_t) \neq i] \\ &\geq \frac{1}{4q^d} \exp[-\mathcal{K}(\mathbb{P}_{\pi,\sigma_{[-j]}^{-1}}^{t-1} \times \mathbb{P}_X^j, \mathbb{P}_{\pi,\sigma_{[-j]}^1}^{t-1} \times \mathbb{P}_X^j)] \\ &= \frac{1}{4q^d} \exp[-\mathcal{K}(\mathbb{P}_{\pi,\sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi,\sigma_{[-j]}^1}^{t-1})], \end{aligned}$$

where  $\mathcal{K}(\cdot, \cdot)$  denotes the KL-divergence of two probability distributions (Kullback and Leibler (1951)).

For  $t = 2, \dots, T$ , denote by  $\mathcal{F}_t^+$  the  $\sigma$ -algebra generated by  $X_t$  and  $(X_s, Y_s(\pi_s(X_s))), s = 1, \dots, t-1$ . Denote by  $\mathbb{P}_{\pi,\sigma}^{|\mathcal{F}_t^+}$  the conditional distribution given  $\mathcal{F}_t^+$ . By the chain rule for KL divergence, for  $t = 1, \dots, T$ ,

$$\begin{aligned} \mathcal{K}(\mathbb{P}_{\pi,\sigma_{[-j]}^{-1}}^t, \mathbb{P}_{\pi,\sigma_{[-j]}^1}^t) &= \mathcal{K}(\mathbb{P}_{\pi,\sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi,\sigma_{[-j]}^1}^{t-1}) + \mathbb{E}_{\pi,\sigma_{[-j]}^{-1}}^{t-1} \mathbb{E}_X[\mathcal{K}(\mathbb{P}_{\pi,\sigma_{[-j]}^{-1}}^{(X_t, Y_t(\pi_t(X_t)))|\mathcal{F}_t^+}, \mathbb{P}_{\pi,\sigma_{[-j]}^1}^{(X_t, Y_t(\pi_t(X_t)))|\mathcal{F}_t^+})] \\ &= \mathcal{K}(\mathbb{P}_{\pi,\sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi,\sigma_{[-j]}^1}^{t-1}) + \mathbb{E}_{\pi,\sigma_{[-j]}^{-1}}^{t-1} \mathbb{E}_X[\mathcal{K}(\mathbb{P}_{\pi,\sigma_{[-j]}^{-1}}^{Y_t(\pi_t(X_t))|\mathcal{F}_t^+}, \mathbb{P}_{\pi,\sigma_{[-j]}^1}^{Y_t(\pi_t(X_t))|\mathcal{F}_t^+})]. \end{aligned}$$

Lemma 4.1 in Rigollet and Zeevi (2010) shows that for any  $\eta', \eta'' \in (\frac{1}{2} - \delta_0, \frac{1}{2} + \delta_0)$ , the KL-divergence of two Bernoulli distributions with mean  $\eta'$  and  $\eta''$  respectively satisfies

$$\mathcal{K}(\text{Bernoulli}(\eta'), \text{Bernoulli}(\eta'')) \leq \frac{1}{\kappa^2} (\eta' - \eta'')^2.$$

This implies,

$$\begin{aligned} \mathcal{K}(\mathbb{P}_{\pi,\sigma_{[-j]}^{-1}}^t, \mathbb{P}_{\pi,\sigma_{[-j]}^1}^t) &\leq \mathcal{K}(\mathbb{P}_{\pi,\sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi,\sigma_{[-j]}^1}^{t-1}) + \mathbb{E}_{\pi,\sigma_{[-j]}^{-1}}^{t-1} \mathbb{E}_X[\frac{1}{\kappa^2} (\eta_1^{\sigma_{[-j]}^1}(X_t) - \eta_1^{\sigma_{[-j]}^{-1}}(X_t))^2 \mathbb{I}\{\pi_t(X_t) = 1\}] \\ &\leq \mathcal{K}(\mathbb{P}_{\pi,\sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi,\sigma_{[-j]}^1}^{t-1}) + \mathbb{E}_{\pi,\sigma_{[-j]}^{-1}}^{t-1} \mathbb{E}_X[\frac{4C_\phi^2}{\kappa^2 q^{2\beta}} \mathbb{I}\{\pi_t(X_t) = 1, X_t \in \mathcal{X}_j\}] \\ &\leq \mathcal{K}(\mathbb{P}_{\pi,\sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi,\sigma_{[-j]}^1}^{t-1}) + \mathbb{E}_{\pi,\sigma_{[-j]}^{-1}}^{t-1} \mathbb{E}_X[\frac{1}{\kappa^2 q^{2\beta}} \mathbb{I}\{\pi_t(X_t) = 1, X_t \in \mathcal{X}_j\}], \end{aligned}$$

where the last inequality follows from  $C_\phi \leq \delta_0 < \frac{1}{2}$ . Define

$$\mathcal{N}_{j,\pi} = \mathbb{E}_{\pi, \sigma_{[-j]}^{-1}}^{T-1} \mathbb{E}_X \left[ \sum_{t=1}^T \mathbb{I}\{\pi_t(X_t) = 1, X_t \in \mathcal{X}_j\} \right].$$

By induction, for  $t = 1, \dots, T$ ,

$$\mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi, \sigma_{[-j]}^1}) \leq \frac{1}{\kappa^2 q^{2\beta}} \mathcal{N}_{j,\pi}.$$

This implies

$$\sum_{\sigma_{[-j]} \in \Sigma_{m-1}} \sum_{i \in \{-1, 1\}} \mathbb{E}_{\pi, \sigma_{[-j]}^i}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq i, X_t \in \mathcal{X}_j] \geq \frac{2^{m-1}}{4q^d} \exp(-\frac{1}{\kappa^2 q^{2\beta}} \mathcal{N}_{j,\pi}).$$

Moreover, it is trivially true that

$$\sum_{t=1}^T \sum_{\sigma \in \Sigma_m} \mathbb{E}_{\pi, \sigma}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq \sigma_j, X_t \in \mathcal{X}_j] \geq 2^{m-1} \mathcal{N}_{j,\pi}.$$

Therefore,

$$\begin{aligned} \sup_{\sigma \in \Sigma_m} \mathbb{E}_\sigma I_t(\pi) &\geq \frac{2^{m-1}}{2^m} \sum_{j=1}^m \max\left\{ \frac{T}{4q^d} \exp\left(-\frac{1}{\kappa^2 q^{2\beta}} \mathcal{N}_{j,\pi}\right), \mathcal{N}_{j,\pi} \right\} \\ &\geq \frac{1}{4} \sum_{j=1}^m \left\{ \frac{T}{4q^d} \exp\left(-\frac{1}{\kappa^2 q^{2\beta}} \mathcal{N}_{j,\pi}\right) + \mathcal{N}_{j,\pi} \right\} \\ &\geq \frac{m}{4} \inf_{z \geq 0} \left\{ \frac{T}{4q^d} \exp\left(-\frac{z}{\kappa^2 q^{2\beta}}\right) + z \right\}. \end{aligned}$$

Since  $T > 4\kappa^2 q^{2\beta+d}$ , we have

$$z^* = \operatorname{argmin}_{z \geq 0} \left\{ \frac{T}{4q^d} \exp\left(-\frac{z}{\kappa^2 q^{2\beta}}\right) + z \right\} = \kappa^2 q^{2\beta} \log\left(\frac{T}{4\kappa^2 q^{2\beta+d}}\right) = c^* T^{\frac{2\beta}{2\beta+d}},$$

where  $c^*$  is a positive constant. It follows that

$$\sup_{\sigma \in \Sigma_m} \mathbb{E}_\sigma I_t(\pi) \geq c T^{1 - \frac{\alpha\beta}{2\beta+d}}.$$

*Proof of Theorem 4* **First, we construct a class  $\mathcal{H}' = \{\mathbb{P}_\sigma : \sigma \in \Sigma_{\bar{m}} = \{-1, 1\}^{\bar{m}}\}$  of probability distributions of  $(X, Y_1, Y_{-1})$ .**

Fix constants  $\Delta = \frac{1}{2}(\beta + \frac{\beta d}{\alpha\beta+d})$ ,  $\delta_0 \in (0, \frac{1}{2})$ ,  $\kappa^2 = \frac{1}{4} - \delta_0^2$ ,  $\bar{p} = (\frac{v_d T}{2^d e \kappa^2})^{\frac{1}{2\Delta+d}}$ ,  $\bar{q} = \lceil \bar{p}^{\Delta/\beta} \rceil$ ,  $\bar{m} = \lceil \bar{p}^{d-\alpha\Delta} \rceil$  and  $\bar{\omega} = \frac{1}{1-\bar{m}(\bar{q}^{-d} - v_d(2\bar{p})^{-d})}$ . Assume  $T$  is sufficiently large so that  $\bar{m} \leq \bar{q}^d/2$  and  $2\bar{q} \leq \bar{p}$ .

Define

$$G_{\bar{q}} = \left\{ \left( \frac{2j_1+1}{2\bar{q}}, \dots, \frac{2j_d+1}{2\bar{q}} \right) : j_i \in \{0, \dots, \bar{q}-1\}, i = 1, \dots, d \right\},$$

and we number the points in  $G_{\bar{q}}$  as  $x_1, \dots, x_{\bar{q}^d}$ . For any  $x \in [0, 1]^d$ , we denote by  $g_{\bar{q}}(x) = \arg \min_{x' \in G_{\bar{q}}} \|x - x'\|$  the closest point to  $x$  in  $G_{\bar{q}}$ . If there are multiple closest points to  $x$ , we choose  $g_{\bar{q}}(x)$  to be the one closest to  $(0, 0, \dots, 0)$ . All points that share the same closest grid point  $g_{\bar{q}}(x)$  belong to a hypercube with length  $\frac{1}{\bar{q}}$  and center  $g_{\bar{q}}(x)$ . We denote this hypercube as  $\text{Cube}_{\bar{q}}(x) = \{x' \in \mathcal{X} : g_{\bar{q}}(x') = g_{\bar{q}}(x)\}$ . Define  $\mathcal{X}_i = \text{Cube}_{\bar{q}}(x_i)$  for  $i = 1, \dots, \bar{m}$  and  $\mathcal{X}_0 = [0, 1]^d - \bigcup_{i=1}^{\bar{m}} \mathcal{X}_i$ .

The marginal distribution of  $X$  (denoted by  $\mathbb{P}_X$ ) does not depend on  $\sigma$ . Its density in  $\mathbb{R}^d$  is

$$\mu_X(x) = \begin{cases} \bar{\omega}, & \text{if } x \in \bigcup_{i=1}^{\bar{m}} \mathcal{B}(x_i, \frac{1}{2\bar{p}}) \cup \mathcal{X}_0, \\ 0, & \text{otherwise.} \end{cases}$$

Note here the radius of the  $\bar{m}$  balls is  $\frac{1}{2\bar{p}}$  and it is (much) smaller than the cube size  $\frac{1}{\bar{q}}$ .

The conditional distribution of  $Y(-1)$  given  $X$  does not depend on  $\sigma$  either. It is simply Bernoulli distribution with conditional expectation is  $\eta_{-1}^\sigma \equiv \frac{1}{2}$ .

We now define the conditional distribution of  $Y(1)$  given  $X$  for  $\mathbb{P}_\sigma \in \mathcal{H}$ . Let  $\phi(x)$  be defined as in Eq. (EC.10). Define  $\eta_1^\sigma : [0, 1]^d \rightarrow \mathbb{R}$  as

$$\eta_1^\sigma(x) = \frac{1}{2} + \sum_{j=1}^{\bar{m}} \sigma_j \varphi_j(x),$$

where  $\varphi_j(x) = \bar{q}^{-\beta} \phi(\bar{q}[x - n_{\bar{q}}(x)]) \mathbb{I}(x \in \mathcal{X}_j)$ . Since  $C_\phi \leq \delta_0$ ,  $\eta_1^\sigma \in [\frac{1}{2} - \delta_0, \frac{1}{2} + \delta_0] \subset [0, 1]$ . Therefore, we can define  $\mathbb{E}_\sigma(Y(1)|X) = \eta_1^\sigma(X)$ , and the conditional distribution of  $Y(1)$  given  $X$  is Bernoulli distribution with mean  $\eta_1^\sigma(X)$ . This completes the construction.

**Second, we check that functions in  $\mathcal{H}'$  satisfy Assumption 1, Assumption 3 and Assumption 4.**

Fix any  $\sigma \in \Sigma_{\bar{m}}$  and consider distribution  $\mathbb{P}_\sigma$ .

### 1. Smooth Conditional Expected Rewards (Assumption 1)

This can be verified in the same way as discussed in the proof of Theorem 3 (we only need to change  $q$  to  $\bar{q}$ ), so we omit the details here.

### 2. Strong Density (Assumption 3)

The support of  $X$  is  $\mathcal{X} = \bigcup_{i=1}^{\bar{m}} \mathcal{B}(x_i, \frac{1}{2\bar{p}}) \cup \mathcal{X}_0$ , which is compact. By definition, since  $\bar{m} \leq \bar{q}^d / 2$ ,  $\mu_X(x) = \bar{\omega} \in (1, 2)$  on its support, so the strong density condition is satisfied with  $\mu_{\max} = 2$  and  $\mu_{\min} = 1$ .

### 3. Margin Condition (Assumption 4)

Let  $x_0 = (\frac{1}{2\bar{q}}, \dots, \frac{1}{2\bar{q}})$ . We have

$$\begin{aligned} \mathbb{P}_\sigma(0 < |\tau(X)| \leq t) &= \mathbb{P}_\sigma(0 < |\eta_1^\sigma(X) - \frac{1}{2}| \leq t) \\ &= \bar{m} \mathbb{P}_\sigma(0 < \phi[\bar{q}(X - x_0)] \leq t\bar{q}^\beta) \\ &= \bar{m}\bar{\omega} \int_{\mathcal{B}(x_0, \frac{1}{2\bar{p}})} \mathbb{I}\{0 < \phi[\bar{q}(x - x_0)] \leq t\bar{q}^\beta\} dx \\ &= \frac{\bar{m}\bar{\omega}v_d}{(2\bar{p})^d} \mathbb{I}\{t \geq C_\phi \bar{q}^{-\beta}\}. \end{aligned}$$

Since  $\frac{\bar{m}\bar{\omega}}{\bar{p}^d} = O(\bar{p}^{-\alpha\Delta}) = O(\bar{q}^{-\alpha\beta})$ , Assumption 4 with is satisfied.

Note here  $\frac{1}{2\bar{p}} = o(\frac{1}{\bar{q}})$ , i.e., the radius of the  $\bar{m}$  balls is (much) smaller than the hypercube size, in contrast to instances in the proof of Theorem 3 where the ball size is proportional to the hypercube size. As a result, for any  $x \in \bigcup_{i=1}^{\bar{m}} \mathcal{B}(x_i, \frac{1}{2\bar{p}}) \cap \mathcal{Q}_a$  and  $r = \Theta(\frac{1}{\bar{q}})$ ,  $\text{Leb}[\mathcal{B}(x, r) \cap \mathcal{Q}_a] = O\left(\text{Leb}[\mathcal{B}(x, r) \cap B(g_{\bar{q}}(x), \frac{1}{2\bar{p}})]\right) = O\left(\text{Leb}[B(g_{\bar{q}}(x), \frac{1}{2\bar{p}})]\right) = o(\text{Leb}[\mathcal{B}(x, r)])$ , i.e., Assumption 2 is violated.

**Finally, we prove a lower bound for  $\mathbb{E}I_t(\pi)$  based on problem instances in  $\mathcal{H}$ .**

For any policy  $\pi$  and any  $t = 1, \dots, T$ , denote by  $\mathbb{P}_{\pi,\sigma}^t$  the joint distribution of

$$(X_1, Y_1(\pi_1(X_1))), \dots, (X_t, Y_t(\pi_t(X_t)))$$

where  $(X_t, Y_t(1), Y_t(-1))$  are generated i.i.d from  $\mathbb{P}_\sigma$ , and  $\mathbb{E}_{\pi,\sigma}^t$  the corresponding expectation.

Observe that

$$\begin{aligned}
\sup_{\sigma \in \Sigma_{\bar{m}}} \mathbb{E}_\sigma I_t(\pi) &= \sup_{\sigma \in \Sigma_{\bar{m}}} \sum_{t=1}^T \mathbb{E}_{\pi, \sigma}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq \text{sign}(\eta_1^\sigma(X_t))] \\
&= \sup_{\sigma \in \Sigma_{\bar{m}}} \sum_{j=1}^{\bar{m}} \sum_{t=1}^T \mathbb{E}_{\pi, \sigma}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq \sigma_j, X_t \in \mathcal{X}_j] \\
&\geq \frac{1}{2^{\bar{m}}} \sum_{j=1}^{\bar{m}} \sum_{t=1}^T \sum_{\sigma \in \Sigma_{\bar{m}}} \mathbb{E}_{\pi, \sigma}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq \sigma_j, X_t \in \mathcal{X}_j] \\
&= \frac{1}{2^{\bar{m}}} \sum_{j=1}^{\bar{m}} \sum_{t=1}^T \sum_{\sigma_{[-j]} \in \Sigma_{\bar{m}-1}} \sum_{i \in \{-1, 1\}} \mathbb{E}_{\pi, \sigma_{[-j]}^i}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq i, X_t \in \mathcal{X}_j],
\end{aligned}$$

where  $\sigma_{[-j]} = (\sigma_1, \dots, \sigma_{j-1}, \sigma_{j+1}, \dots, \sigma_m)$  and  $\sigma_{[-j]}^i = (\sigma_1, \dots, \sigma_{j-1}, i, \sigma_{j+1}, \dots, \sigma_m)$ .

For  $j = 1, \dots, \bar{m}$ , define  $\mathbb{P}_X^j(\cdot) = \mathbb{P}_X(\cdot | X \in \mathcal{X}_j)$ . By Theorem 2.2(iii) in Tsybakov (2008),

$$\begin{aligned}
\sum_{i \in \{-1, 1\}} \mathbb{E}_{\pi, \sigma_{[-j]}^i}^{t-1} \mathbb{P}_X[\pi_t(X_t) \neq i, X_t \in \mathcal{X}_j] &= \frac{v_d \bar{\omega}}{(2\bar{p})^d} \sum_{i \in \{-1, 1\}} \mathbb{E}_{\pi, \sigma_{[-j]}^i}^{t-1} \mathbb{P}_X^j[\pi_t(X_t) \neq i] \\
&\geq \frac{v_d}{4(2\bar{p})^d} \exp[-\mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^{t-1} \times \mathbb{P}_X^j, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^{t-1} \times \mathbb{P}_X^j)] \\
&= \frac{v_d}{4(2\bar{p})^d} \exp[-\mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^{t-1})],
\end{aligned}$$

where  $\mathcal{K}(\cdot, \cdot)$  denotes the KL-divergence of two probability distributions (Kullback and Leibler (1951)).

For  $t = 2, \dots, T$ , denote by  $\mathcal{F}_t^+$  the  $\sigma$ -algebra generated by  $X_t$  and  $(X_s, Y_s(\pi_s(X_s))), s = 1, \dots, t-1$ . Denote by  $\mathbb{P}_{\pi, \sigma}^{|\mathcal{F}_t^+}$  the conditional distribution given  $\mathcal{F}_t^+$ . By the chain rule for KL divergence, for  $t = 1, \dots, T$ ,

$$\begin{aligned}
\mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^t, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^t) &= \mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^{t-1}) + \mathbb{E}_{\pi, \sigma_{[-j]}^{-1}}^{t-1} \mathbb{E}_X [\mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^{(X_t, Y_t(\pi_t(X_t)))|\mathcal{F}_t^+}, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^{(X_t, Y_t(\pi_t(X_t)))|\mathcal{F}_t^+})] \\
&= \mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^{t-1}) + \mathbb{E}_{\pi, \sigma_{[-j]}^{-1}}^{t-1} \mathbb{E}_X [\mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^{Y_t(\pi_t(X_t))|\mathcal{F}_t^+}, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^{Y_t(\pi_t(X_t))|\mathcal{F}_t^+})].
\end{aligned}$$

Lemma 4.1 in Rigollet and Zeevi (2010) shows that for any  $\eta', \eta'' \in (\frac{1}{2} - \delta_0, \frac{1}{2} + \delta_0)$ , the KL-divergence of two Bernoulli distributions with mean  $\eta'$  and  $\eta''$  respectively satisfies

$$\mathcal{K}(\text{Bernoulli}(\eta'), \text{Bernoulli}(\eta'')) \leq \frac{1}{\kappa^2} (\eta' - \eta'')^2.$$

This implies

$$\begin{aligned}
\mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^t, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^t) &\leq \mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^{t-1}) + \mathbb{E}_{\pi, \sigma_{[-j]}^{-1}}^{t-1} \mathbb{E}_X \left[ \frac{1}{\kappa^2} (\eta_1^{\sigma_{[-j]}^{-1}}(X_t) - \eta_1^{\sigma_{[-j]}^{-1}}(X_t))^2 \mathbb{I}\{\pi_t(X_t) = 1\} \right] \\
&\leq \mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^{t-1}) + \mathbb{E}_{\pi, \sigma_{[-j]}^{-1}}^{t-1} \mathbb{E}_X \left[ \frac{4C_\phi^2}{\kappa^2 \bar{q}^{2\beta}} \mathbb{I}\{\pi_t(X_t) = 1, X_t \in \mathcal{X}_j\} \right] \\
&\leq \mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^{t-1}) + \mathbb{E}_{\pi, \sigma_{[-j]}^{-1}}^{t-1} \mathbb{E}_X \left[ \frac{1}{\kappa^2 \bar{p}^{2\Delta}} \mathbb{I}\{\pi_t(X_t) = 1, X_t \in \mathcal{X}_j\} \right],
\end{aligned}$$

where the last inequality follows from  $C_\phi \leq \delta_0 < \frac{1}{2}$  and  $\bar{q}^{-2\beta} \leq \bar{p}^{-2\Delta}$ . Define

$$\mathcal{N}_{j, \pi} = \mathbb{E}_{\pi, \sigma_{[-j]}^{-1}}^{T-1} \mathbb{E}_X \left[ \sum_{t=1}^T \mathbb{I}\{\pi_t(X_t) = 1, X_t \in \mathcal{X}_j\} \right].$$

By induction, for  $t = 1, \dots, T$ ,

$$\mathcal{K}(\mathbb{P}_{\pi, \sigma_{[-j]}^{-1}}^{t-1}, \mathbb{P}_{\pi, \sigma_{[-j]}^1}^{t-1}) \leq \frac{1}{\kappa^2 \bar{p}^{2\Delta}} \mathcal{N}_{j, \pi}.$$

This implies

$$\sum_{\sigma_{[-j]} \in \Sigma_{\bar{m}-1}} \sum_{i \in \{-1, 1\}} \mathbb{E}_{\pi, \sigma_{[-j]}^{t-1}}^{\pi} \mathbb{P}_X[\pi_t(X_t) \neq i, X_t \in \mathcal{X}_j] \geq \frac{2^{\bar{m}-1} v_d}{4(2\bar{p})^d} \exp(-\frac{1}{\kappa^2 \bar{p}^{2\Delta}} \mathcal{N}_{j, \pi}).$$

Moreover, it is trivially true that

$$\sum_{t=1}^T \sum_{\sigma \in \Sigma_{\bar{m}}} \mathbb{E}_{\pi, \sigma}^{\pi-1} \mathbb{P}_X[\pi_t(X_t) \neq \sigma_j, X_t \in \mathcal{X}_j] \geq 2^{\bar{m}-1} \mathcal{N}_{j, \pi}.$$

Therefore,

$$\begin{aligned} \sup_{\sigma \in \Sigma_{\bar{m}}} \mathbb{E}_{\sigma} I_t(\pi) &\geq \frac{2^{\bar{m}-1}}{2^{\bar{m}}} \sum_{j=1}^{\bar{m}} \max\left\{\frac{v_d T}{4(2\bar{p})^d} \exp(-\frac{1}{\kappa^2 \bar{p}^{2\Delta}} \mathcal{N}_{j, \pi}), \mathcal{N}_{j, \pi}\right\} \\ &\geq \frac{1}{4} \sum_{j=1}^{\bar{m}} \left\{ \frac{v_d T}{4(2\bar{p})^d} \exp(-\frac{1}{\kappa^2 \bar{p}^{2\Delta}} \mathcal{N}_{j, \pi}) + \mathcal{N}_{j, \pi} \right\} \\ &\geq \frac{\bar{m}}{4} \inf_{z \geq 0} \left\{ \frac{v_d T}{4(2\bar{p})^d} \exp(-\frac{z}{\kappa^2 \bar{p}^{2\Delta}}) + z \right\}. \end{aligned}$$

Since  $T > \frac{2^d \kappa^2 \bar{p}^{2\Delta+d}}{v_d}$ , we have

$$z^* = \operatorname{argmin}_{z \geq 0} \left\{ \frac{v_d T}{4(2\bar{p})^d} \exp(-\frac{z}{\kappa^2 \bar{p}^{2\Delta}}) + z \right\} = \frac{1}{2} \kappa^2 \bar{p}^{2\Delta} \log\left(\frac{v_d T}{2^d \kappa^2 \bar{p}^{2\Delta+d}}\right) = c^* T^{\frac{2\Delta}{2\Delta+d}},$$

where  $c^*$  is a positive constant. It follows that

$$\sup_{\sigma \in \Sigma_{\bar{m}}} \mathbb{E}_{\sigma} I_t(\pi) \geq c^* T^{1 - \frac{\alpha\Delta}{2\Delta+d}}.$$

## B.6. Proofs for Appendix A

*Proof for Lemma EC.1* We prove this lemma by induction. Suppose the statements above hold up to  $k = k_0$ th epoch.

Statement i:  $D_{Est, k_0+1}(a)$  is the region within  $\mathcal{R}_{k_0}(a)$  where arm  $a$  is estimable, and it was outperformed by another estimable arm according to the estimated expected reward  $\hat{\eta}_{a, k_0}$ . Thus under  $\mathcal{G}_{k_0}$ , it is indeed outperformed by another arm, i.e.,  $D_{Est, k_0+1}(a) \subseteq \{x \in \mathcal{X} : \eta_a(x) < \max_{a' \in \mathcal{A}} \eta_{a'}(x)\}$ .

Statement ii: it holds for  $k = k_0 + 1$  because compared to  $\mathcal{R}_{k_0}$  we have only removed strictly suboptimal arms according to statement i for  $k = k_0 + 1$  and statement v for  $k = k_0$ .

Statement iii: (1) only one arm remains in  $k_0 + 1$  so the statement is trivially true; (2) at least two arms remain, and given that inestimable arms have been removed, these remaining arms have to be estimable with close estimated expected rewards, then  $\mathcal{G}_{k_0}$  implies that their true expected rewards should be close.

Statement iv:  $\left( \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_{k_0+1}(\mathcal{A}_0) \cap \mathcal{X} \right)^C$  are regions where arm  $a$  has already been removed, which means

$$\left( \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_{k_0+1}(\mathcal{A}_0) \cap \mathcal{X} \right)^C \subseteq (D_{IR, k_0}(a) \cup D_{Est, k_0+1}(a)) \cap \mathcal{X} \subseteq \left\{ x \in \mathcal{X} : \eta_a(x) < \max_{a' \in \mathcal{A}} \eta_{a'}(x) \right\} \subseteq \mathcal{Q}_a^C,$$

according to statement 1 for  $k = k_0 + 1$  and statement 5 for  $k = k_0$ . Statement 4 for time  $k = k_0 + 1$  then follows.

Statement v:  $D_{IR, k_0+1}(a) \subseteq \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_{k_0+1}(\mathcal{A}_0) \cap \mathcal{X}$  and by statement 4 for  $k = k_0 + 1$ , we know  $\mathcal{Q}_a \subseteq \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_{k_0+1}(\mathcal{A}_0) \cap \mathcal{X}$ , which implies that for any point  $x$  in  $\mathcal{Q}_a$ ,  $\bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_{k_0+1}(\mathcal{A}_0) \cap \mathcal{X}$  should be regular at  $x$  by the regularity of  $\mathcal{Q}_a$ . This means that  $x$  does not belong to  $D_{IR, k_0+1}(a)$ . Thus  $D_{IR, k_0+1}(a) \subseteq \mathcal{Q}_a^C = \{x \in \mathcal{X} : \eta_a(x) < \max_{a' \in \mathcal{A}} \eta_{a'}(x)\}$ .

LEMMA EC.8. For any  $1 \leq k \leq K$  and  $a \in \mathcal{A}$ ,  $S_{a,k} = \{(X_t, Y_t) : t \in \mathcal{T}_k, A_t = a\}$  are conditionally i.i.d. samples, given  $\mathcal{F}_{k-1} \cup \mathcal{A}_k$ , where  $\mathcal{F}_{k-1} = \{(X_t, A_t, Y_t) : t \in \bigcup_{k'=1}^{k-1} \mathcal{T}_{k'}\}$ ,  $\mathcal{A}_k = \{A_t : t \in \mathcal{T}_k\}$ .

Now suppose Assumption EC.1 holds, let  $C_{\mathcal{A}}$  be defined as in Lemma EC.9 for any given  $\beta$ ,  $L_1, c_0, r_0, \mu_{\min}$ , and suppose  $T \geq T_0 \vee \left(\exp(1 \vee \frac{C_{\mathcal{A}}(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)})\right)$ . Then, for  $a \in \mathcal{A}$ , under the event  $\bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}$ , the (common) conditional density of any of  $\{X_t : A_t = a, t \in \mathcal{T}_k\}$  with respect to Lebesgue measure, given  $\mathcal{F}_{k-1} \cup \mathcal{A}_k$ , which we denote by  $\mu_{a,k}$ , satisfies the following conditions:

1.  $\frac{1}{|\mathcal{A}|} \mu_{\min} \leq \mu_{a,k}(x) \leq \frac{|\mathcal{A}| \mu_{\max}}{p}$  for any  $x \in \bigcup_{\mathcal{A}_0 : a \in \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \cap \mathcal{X}$ ;
2.  $\mu_{a,k}(x) = 0$  for any  $x \in \bigcup_{\mathcal{A}_0 : a \notin \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \cap \mathcal{X}$ .

*Proof for Lemma EC.8.* When  $k = 1$ , the conclusions hold trivially since  $\mathcal{R}_k(\mathcal{A}) = \mathcal{X}$ , i.e., we pull each arm with equal probability for all samples in the first stage. This implies that  $\mu_{a,1} = \mu(x)$  for  $x \in \mathcal{X}$ . Then the conclusion follows from Assumption EC.1 condition iii. Denote  $\mathcal{T}_{a,k} = \{t \in \mathcal{T}_k : A_t = a\}$ ,  $N_{\mathcal{A},k} = \{N_{a,k}\}_{a \in \mathcal{A}}$  and  $n_{\mathcal{A},k} = \{n_{a,k}\}_{a \in \mathcal{A}}$ .

When  $k \geq 2$ ,  $\{(X_t, Y_t), t \in \mathcal{T}_{a,k}\}$  are obviously i.i.d conditionally on  $\mathcal{F}_{k-1}$ ,  $\bar{\mathcal{G}}_{k-1}$  and  $\bar{\mathcal{M}}_{k-1}$ , since  $A_t$  only depends on  $X_t$  and  $\mathcal{F}_{k-1}$ . This implies that  $\{X_t : t \in \mathcal{T}_{a,k}\}$  are i.i.d conditionally on  $\mathcal{F}_{k-1}$ ,  $\bar{\mathcal{G}}_{k-1}$ ,  $\bar{\mathcal{M}}_{k-1}$ . Furthermore,  $X_t \perp\!\!\!\perp N_{a,k} | A_t$ , thus  $\{X_t : t \in \mathcal{T}_{a,k}\}$  are i.i.d given  $\mathcal{F}_{k-1}$ ,  $\bar{\mathcal{G}}_{k-1}$ ,  $\bar{\mathcal{M}}_{k-1}$ ,  $N_{a,k} = n_{a,k}$ . This also implies that for any  $x \in \mathcal{X}$ ,

$$\begin{aligned} \mu_{a,k}(x) &= \mu_{X_t | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{\mathcal{A},k} = n_{\mathcal{A},k}, \mathcal{F}_{k-1}}(x) \\ &= \mu_{X_t | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}}(x) \end{aligned}$$

For any  $x \in \mathcal{X}$ , obviously  $\mu_{X_t | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}}(x) = \mu_{X_t}(x)$  for  $t \in \mathcal{T}_k$ . Thus

$$\begin{aligned} &\mu_{X_t | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}}(x) \\ &= \frac{\mathbb{P}(A_t = a | X_t = x, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1})}{\mathbb{P}(A_t = a | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1})} \mu_{X_t | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}}(x) \\ &= \frac{\mathbb{P}(A_t = a | X_t = x, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1})}{\mathbb{P}(A_t = a | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1})} \mu_{X_t}(x). \end{aligned} \tag{EC.11}$$

For any  $x \in \bigcup_{\mathcal{A}_0 : a \notin \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \cap \mathcal{X}$ , our algorithm ensures that

$$\mathbb{P}(A_t = a | X_t = x, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}) = 0.$$

Therefore, for  $x \in \bigcup_{\mathcal{A}_0 : a \notin \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \cap \mathcal{X}$ ,  $\mu_{a,k}(x) = 0$ , which proves statement 2.

For any  $x \in \bigcup_{\mathcal{A}_0 : a \in \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \cap \mathcal{X}$ , our algorithm ensures that

$$\mathbb{P}(A_t = a | X_t = x, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}) \geq \frac{1}{|\mathcal{A}|}.$$

Plus, since  $T \geq T_0 \vee \left(\exp(1 \vee \frac{C_{\mathcal{A}}(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)})\right)$ , Lemma EC.1 implies that  $\mathcal{Q}_a \subseteq \bigcup_{\mathcal{A}_0 : a \in \mathcal{A}_0} \mathcal{R}_k(\mathcal{A}_0) \cap \mathcal{X}$ . By following Lemma 1, we can analogously prove that  $\mathbb{P}(X_t \in \mathcal{Q}_a) \geq p$ . It follows from Assumption 2 that

$$\begin{aligned} &\mathbb{P}(A_t = a | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}) \\ &= \mathbb{P}(A_t = a | X_t \in \bigcup_{\mathcal{A}_0 : a \in \mathcal{A}_0} \mathcal{R}_k(\mathcal{A}_0) \cap \mathcal{X}, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}) \\ &\quad \times \mathbb{P}(X_t \in \bigcup_{\mathcal{A}_0 : a \in \mathcal{A}_0} \mathcal{R}_k(\mathcal{A}_0) \cap \mathcal{X} | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, \mathcal{F}_{k-1}) \\ &\geq \frac{1}{|\mathcal{A}|} \mathbb{P}(X_t \in \mathcal{Q}_a) \geq \frac{p}{|\mathcal{A}|}, \end{aligned}$$

where the last inequality follows from Lemma 1.

Then it follows from Assumption 3 and Eq. (EC.11) that for any  $x \in \bigcup_{\mathcal{A}_0 : a \in \mathcal{A}_0} \mathcal{R}_k(\mathcal{A}_0) \cap \mathcal{X}$ ,

$$\frac{1}{|\mathcal{A}|} \mu_{\min} \leq \mu_{a,k}(x) \leq \frac{|\mathcal{A}| \mu_{\max}}{p},$$

which proves statement 1.

**LEMMA EC.9.** Suppose the conditions of Lemma EC.8 hold. Let  $1 \leq k \leq K - 1$ ,  $n_{\pm a,k}$  for  $a \in \mathcal{A}$  be given. Consider the Gram matrices of the local polynomial regression estimators in Eq. (11), i.e.,  $\hat{\mathcal{A}}(x; S_{a,k}, H_{a,k}, \mathbf{b}(\beta))$  as defined in Eq. (5). Then, given  $N_{a,k} = n_{a,k}$  and  $\bar{\mathcal{M}}_{k-1} \cap \bar{\mathcal{G}}_{k-1}$ , these satisfy the following with conditional probability at least  $1 - 2M_\beta^2 \exp\{-C_{\mathcal{A}}(4(1 + L_1 \sqrt{d})^2)n_{a,k}^{2\beta/(2\beta+d)}\}$ :

$$\lambda_{\min}(\hat{\mathcal{A}}(x; S_{a,k}, H_{a,k}, \mathbf{b}(\beta))) \geq \lambda_0 > 0, \quad \forall x \in \mathcal{R}_k \cap \mathcal{D}_{1,k}^C \cap \mathcal{D}_{-1,k}^C,$$

where

$$\begin{aligned} \lambda_0 &= \frac{1}{4} \mu_{\min} \inf_{\substack{W \in \mathbb{R}^d, S \subset \mathbb{R}^d : \|W\|=1 \\ S \subseteq \mathcal{B}(0,1) \text{ is compact, } \text{Leb}(S)=c_0 v_d / 2^d}} \int_S \left( \sum_{|s| \leq \mathbf{b}(\beta)} W_s u^s \right)^2 du, \\ C_{\mathcal{A}} &= \frac{3p\lambda_0^2}{4(1 + L_1 \sqrt{d})^2} \min \left\{ \frac{1}{6|\mathcal{A}| M_\beta^4 \mu_{\max} v_d + 2p\lambda_0 M_\beta^2}, \frac{1}{54|\mathcal{A}| M_\beta v_d \mu_{\max} + 6\sqrt{M_\beta} p \lambda_0}, \right. \\ &\quad \left. \frac{1}{54|\mathcal{A}| M_\beta L^2 v_d \mu_{\max} + 6\sqrt{M_\beta} L(|\mathcal{A}| v_d \mu_{\max} + p) \lambda_0} \right\}. \end{aligned}$$

*Proof for Lemma EC.9.* We can condition on  $\bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}$ , and  $\mathcal{F}_{k-1}$ , and then follow the proof of Lemma 7. The only difference is that now samples  $S_{a,k} = \{(X_t, Y_t) : A_t = a, t \in \mathcal{T}_k\} = \{(X_t, Y_t) : t \in \mathcal{T}_{k,a}\}$  are i.i.d whose conditional density for  $X_t$  has different strong density parameters:  $\frac{1}{|\mathcal{A}|} \mu_{\min} \leq \mu_{a,k}(x) \leq \frac{|\mathcal{A}| \mu_{\max}}{p}$  for any  $x \in \bigcup_{\mathcal{A}_0 : a \in \mathcal{A}_0} \mathcal{R}_{k-1}(\mathcal{A}_0) \cap \mathcal{X}$ . This only influences the estimation error bound of  $|(\hat{\mathcal{A}}_{a,k}(x_0))_{r_1, r_2} - (\mathcal{A}_{a,k}(x_0))_{r_1, r_2}|$ . Note that For  $t \in S_{a,k}$  and  $|r_1|, |r_2| \leq \beta$ , and  $Z_t(r_1, r_2) = \frac{1}{h_{a,k}^d} \left( \frac{x_t - x_0}{h_{a,k}} \right)^{r_1+r_2} K\left(\frac{x_t - x_0}{h_{a,k}}\right)$ , we obviously have  $|Z_t(r_1, r_2)| \leq \frac{1}{h_{a,k}^d}$ , and

$$\begin{aligned} &\mathbb{E}(Z_t^2(r_1, r_2) | A_t = a, \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1}) \\ &= \frac{1}{h_{a,k}^{2d}} \int_{\mathcal{X}} \left( \frac{x - x_0}{h_{a,k}} \right)^{2(r_1+r_2)} K^2\left(\frac{x - x_0}{h_{a,k}}\right) \mu_{a,k}(x) dx \\ &\leq \frac{|\mathcal{A}| \mu_{\max}}{p h_{a,k}^d} \int_{B_{a,k}(x_0)} u^{2(r_1+r_2)} du \leq \frac{|\mathcal{A}| \mu_{\max}}{p h_{a,k}^d} \text{Leb}[B_{a,k}(x_0)] \leq \frac{|\mathcal{A}| \mu_{\max} v_d}{p h_{a,k}^d}, \end{aligned}$$

where the first inequality follows from the fact that  $\mu_{a,k}(x) \leq \frac{|\mathcal{A}| \mu_{\max}}{p}$  according to Lemma EC.8. Similarly, we can use Bernstein inequality to show that

$$\mathbb{P}(|(\hat{\mathcal{A}}_{a,k}(x_0))_{r_1, r_2} - (\mathcal{A}_{a,k}(x_0))_{r_1, r_2}| \geq \frac{\lambda_0}{M_\beta^2} | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1} ) \leq 2 \exp\left(-\frac{3pn_{a,k}h_{a,k}^d\lambda_0^2}{6|\mathcal{A}| M_\beta^4 \mu_{\max} v_d + 2p\lambda_0 M_\beta^2}\right).$$

Then we can apply union bound to show that taking union bound over all possible  $r_1, r_2$ ,

$$\begin{aligned} &\mathbb{P}\left(\sum_{|r_1|, |r_2| \leq \mathbf{b}(\beta)} |(\hat{\mathcal{A}}_{a,k}(x_0))_{r_1, r_2} - (\mathcal{A}_{a,k}(x_0))_{r_1, r_2}| \geq \lambda_0 | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}, \mathcal{F}_{k-1} \right) \\ &\leq 2M_\beta^2 \exp\left(-\frac{3pn_{a,k}h_{a,k}^d\lambda_0^2}{6|\mathcal{A}| M_\beta^4 \mu_{\max} v_d + 2p\lambda_0 M_\beta^2}\right) \leq 2M_\beta^2 \exp\left\{-C_{\mathcal{A}}(4(1 + L_1 \sqrt{d})^2)n_{a,k}^{\frac{2\beta}{2\beta+d}}\right\}. \end{aligned}$$

If follows from the inequality above and Eqs. (EC.7) and (EC.8) that with high probability  $1 - 2M_\beta^2 \exp\{-C_{\mathcal{A}}(4(1 + L_1 \sqrt{d})^2)n_{a,k}^{\frac{2\beta}{2\beta+d}}\}$ ,

$$\lambda_{\min}(\hat{\mathcal{A}}_{a,k}(x_0)) \geq \lambda_0.$$

**THEOREM EC.2.** When  $T \geq T_0 \vee \left( \exp\left(1 \vee \frac{C_{\mathcal{A}}(2\beta+d)}{4(2r_0)^{2\beta}(2\beta+d+\beta d)}\right) \vee \frac{36M_{\beta}L^2v_d^2\mu_{\max}^2C_{\mathcal{A}}(2\beta+d)}{p^2\lambda_0^2(2\beta+d+\beta d)}\right)$ , if we assume Assumptions 1 to 3, then for any  $1 \leq k \leq K-1$ ,

$$\mathbb{P}(\mathcal{G}_k^C | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_k) \leq \frac{(4+2M_{\beta}^2)|\mathcal{A}|}{T}, \quad \mathbb{P}(\mathcal{M}_k^C | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) \leq \frac{|\mathcal{A}|}{T}, \quad \mathbb{P}(\bar{\mathcal{G}}_k^C \cup \bar{\mathcal{M}}_k^C) \leq \frac{|\mathcal{A}|(5+2M_{\beta}^2)k}{T}.$$

*Proof for Theorem EC.2.* **I. Prove the bound on  $\mathbb{P}(\mathcal{G}_k^C | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_k)$ .** We note that when  $T \geq \exp\left(1 \vee \frac{36M_{\beta}L^2v_d^2\mu_{\max}^2C_{\mathcal{A}}(2\beta+d)}{p^2\lambda_0^2(2\beta+d+\beta d)}\right)$ , the proof of Theorem 1 Step I shows that all conditions in Lemma EC.7 are satisfied. We can easily revise the Step II and step III in the proof of Lemma EC.7 to show that

$$\begin{aligned} & \mathbb{P}\left(\sup_{a \in \mathcal{A}} \sup_{x \in \mathcal{R}_k(\mathcal{A}_0) \cap D_{a,k}^C} |\hat{\eta}_{k,a}(x) - \eta_{k,a}(x)| \leq \epsilon_k/2 \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}, N_{a,k} = n_{a,k}\right) \\ & \leq \delta^{-d} |\mathcal{A}| (4+2M_{\beta}^2) \exp(-C_{\mathcal{A}} n_{a,k}^{\frac{2\beta}{2\beta+d}} \epsilon_k^2). \end{aligned}$$

where  $C_0$  is given in Lemma EC.9.

Then we can prove the conclusion by following Step I in the proof of Theorem 1.

**II. Prove the bound on  $\mathbb{P}(\mathcal{M}_k^C | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1})$ .** We first note that for any  $a \in \mathcal{A}$

$$\begin{aligned} \mathbb{E}(N_{a,k} | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) &= \mathbb{E}\left(\sum_{t \in \mathcal{T}_k} \mathbb{I}\{X_t \in \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_k(\mathcal{A}_0)\} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}\right) \\ &= n_k \mathbb{P}(X_t \in \bigcup_{\mathcal{A}_0: a \in \mathcal{A}_0} \mathcal{R}_k(\mathcal{A}_0) \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) \\ &\geq \frac{1}{|\mathcal{A}|} n_k \mathbb{P}(X_t \in \mathcal{Q}_a \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) \geq \frac{p}{|\mathcal{A}|} n_k. \end{aligned}$$

where the inequality follows from Lemma EC.1 statement iv.

By Hoeffding's inequality,

$$\begin{aligned} & \mathbb{P}\left(N_{a,k} < \left(\frac{\log(T\delta^{-d})}{C_{\mathcal{A}}\epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}\right) \\ & \leq \mathbb{P}\left(\mathbb{E}(N_{a,k} | \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}) - N_{a,k} > \frac{p}{|\mathcal{A}|} n_k - \left(\frac{\log(T\delta^{-d})}{C_{\mathcal{A}}\epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}\right) \\ & \leq \exp\left(-\frac{2}{n_k} \left[\frac{p}{|\mathcal{A}|} n_k - \left(\frac{\log(T\delta^{-d})}{C_{\mathcal{A}}\epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}}\right]^2\right). \end{aligned}$$

$$\text{When } n_k \geq \frac{2|\mathcal{A}|}{p} \left(\frac{\log(T\delta^{-d})}{C_{\mathcal{A}}\epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} + \frac{|\mathcal{A}|^2}{2p^2} \log T$$

$$\frac{2}{n_k} \left[\frac{p}{|\mathcal{A}|} n_k - \left(\frac{\log(T\delta^{-d})}{C_{\mathcal{A}}\epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}}\right]^2 \geq 2 \frac{p^2}{|\mathcal{A}|^2} n_k - \frac{4}{|\mathcal{A}|} p \left(\frac{\log(T\delta^{-d})}{C_{\mathcal{A}}\epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} \geq \log T.$$

Thus

$$\mathbb{P}\left(N_{a,k} < \left(\frac{\log(T\delta^{-d})}{C_{\mathcal{A}}\epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}\right) \leq \frac{1}{T}.$$

Accordingly,

$$\mathbb{P}\left(\min_{a \in \mathcal{A}} N_{a,k} < \left(\frac{\log(T\delta^{-d})}{C_{\mathcal{A}}\epsilon_k^2}\right)^{\frac{2\beta+d}{2\beta}} \mid \bar{\mathcal{G}}_{k-1}, \bar{\mathcal{M}}_{k-1}\right) \leq \frac{|\mathcal{A}|}{T}.$$

**III. Prove the bound on  $\mathbb{P}(\bar{\mathcal{G}}_k^C \cup \bar{\mathcal{M}}_k^C)$ .** We can follow the proof of Theorem 1 and note that

$$\begin{aligned} \mathbb{P}(\bar{\mathcal{G}}_k^C \cup \bar{\mathcal{M}}_k^C) &\leq \sum_{j=0}^{k-1} \mathbb{P}(\mathcal{G}_{j+1}^C \cap \bar{\mathcal{M}}_{j+1} \cap \bar{\mathcal{G}}_j) + \sum_{j=0}^{k-1} \mathbb{P}(\mathcal{M}_{j+1}^C \cap \bar{\mathcal{G}}_j \cap \bar{\mathcal{M}}_j) \\ &\leq \sum_{j=0}^{k-1} \mathbb{P}(\mathcal{G}_{j+1}^C \mid \bar{\mathcal{G}}_j, \bar{\mathcal{M}}_{j+1}) + \sum_{j=0}^{k-1} \mathbb{P}(\mathcal{M}_{j+1}^C \mid \bar{\mathcal{G}}_j, \bar{\mathcal{M}}_j) \\ &\leq \sum_{j=0}^{k-1} \frac{(4+2M_{\beta}^2)|\mathcal{A}|}{T} + \frac{|\mathcal{A}|}{T} = \frac{(5+2M_{\beta}^2)k|\mathcal{A}|}{T}. \end{aligned}$$

*Proof for Theorem EC.1:*

$$\begin{aligned} R_T(\hat{\pi}) &= \sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{E}[Y_t(\pi^*(X_t)) - Y_t(A_t)] \\ &\leq \sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{E}[Y_t(\pi^*(X_t)) - Y_t(A_t) \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}] + \sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C). \end{aligned}$$

Here

$$\begin{aligned} &\sum_{t \in \mathcal{T}_k} \mathbb{E}[Y_t(\pi^*(X_t)) - Y_t(A_t) \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}] \\ &\leq \sum_{t \in \mathcal{T}_k} \sum_{\mathcal{A}_0: \emptyset \neq \mathcal{A}_0 \subseteq \mathcal{A}} \mathbb{E} \left[ \max_{a \in \mathcal{A}} \eta_a(X_t) - \min_{a \in \mathcal{A}_0} \eta_a(X_t) \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}, X_t \in \mathcal{R}_k(\mathcal{A}_0) \right] \mathbb{P}(X_t \in \mathcal{R}_k(\mathcal{A}_0) \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \end{aligned}$$

Note that by Lemma EC.1 statement ii, we never delete optimal arm from the active arm sets, i.e.,  $\max_{a \in \mathcal{A}} \eta_a(X_t) - \min_{a \in \mathcal{A}_0} \eta_a(X_t) = \max_{a \in \mathcal{A}_0} \eta_a(X_t) - \min_{a \in \mathcal{A}_0} \eta_a(X_t)$ . Moreover, if  $|\mathcal{A}_0| = 1$ , then trivially  $\mathbb{E}[\max_{a \in \mathcal{A}} \eta_a(X_t) - \min_{a \in \mathcal{A}_0} \eta_a(X_t) \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}, X_t \in \mathcal{R}_k(\mathcal{A}_0)] = 0$ , and if  $|\mathcal{A}_0| > 1$ , by Lemma EC.1 statement iii,  $\max_{a \in \mathcal{A}} \eta_a(X_t) - \min_{a \in \mathcal{A}_0} \eta_a(X_t) \leq 2\epsilon_{k-1}$  for  $X_t \in \mathcal{R}_k(\mathcal{A}_0)$ . We further define  $\bar{\mathcal{R}}_k = \bigcup_{\mathcal{A}_0: \mathcal{A}_0 \subseteq \mathcal{A}, |\mathcal{A}_0| > 1} \mathcal{R}_k(\mathcal{A}_0)$  as the region where more than one arm is pulled with positive probability. Obviously, Lemma EC.1 statement iii and the fact that any hypercube in  $\bar{\mathcal{R}}_k$  explores more than one arm together imply that  $\bar{\mathcal{R}}_k \subseteq \{x \in \mathcal{X}: \exists a \neq a' \in \mathcal{A}, |\eta_a(x) - \eta_{a'}(x)| \leq 2\epsilon_{k-1}\}$ . Combining all these facts, we get

$$\begin{aligned} &\sum_{t \in \mathcal{T}_k} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t) \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \\ &= \sum_{t \in \mathcal{T}_k} \sum_{\mathcal{A}_0: \mathcal{A}_0 \subseteq \mathcal{A}, |\mathcal{A}_0| > 1} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t) \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}, X_t \in \mathcal{R}_k(\mathcal{A}_0)) \mathbb{P}(X_t \in \mathcal{R}_k(\mathcal{A}_0) \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \\ &\leq \sum_{t \in \mathcal{T}_k} \sum_{\mathcal{A}_0: \mathcal{A}_0 \subseteq \mathcal{A}, |\mathcal{A}_0| > 1} 2\epsilon_{k-1} \mathbb{P}(X_t \in \mathcal{R}_k(\mathcal{A}_0) \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \\ &= \sum_{t \in \mathcal{T}_k} 2\epsilon_{k-1} \mathbb{P}(X_t \in \bar{\mathcal{R}}_k \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \\ &\leq \sum_{t \in \mathcal{T}_k} 2\epsilon_{k-1} \sum_{a, a' \in \mathcal{A}} \mathbb{P}(0 < |\eta_a(x) - \eta_{a'}(x)| \leq 2\epsilon_{k-1} \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) \\ &\leq \gamma |\mathcal{A}|^2 2^{1+\alpha} \epsilon_{k-1}^{1+\alpha} n_k, \end{aligned}$$

where the second last inequality follows from the margin condition (condition iv in Assumption EC.1). This implies that

$$\sum_{t \in \mathcal{T}_k} \mathbb{E}(Y_t(\pi^*(X_t)) - Y_t(A_t) \mid \bar{\mathcal{G}}_{k-1} \cap \bar{\mathcal{M}}_{k-1}) = \tilde{O}(|\mathcal{A}|^3 T^{\frac{\beta+d-\alpha\beta}{2\beta+d}}).$$

Moreover, we can follow the proof of Theorem 2 to show that the conclusions of Theorem EC.2 imply

$$\sum_{k=1}^K \sum_{t \in \mathcal{T}_k} \mathbb{P}(\bar{\mathcal{G}}_{k-1}^C \cup \bar{\mathcal{M}}_{k-1}^C) = \tilde{O}(1).$$

**CornellEngineering**  
Operations Research and Information Engineering

Frank H.T. Rhodes Hall  
Ithaca, New York  
14853-3901  
t: 607.255.4856

June 20, 2020

Dear APS Best Student Paper Competition Committee,

I would like to nominate my students, Yichun Hu and Xiaojie Mao, for the APS Best Student Paper Competition for our paper entitled "Smooth Contextual Bandits: Bridging the Parametric and Non-differentiable Regret Regimes."

As their advisor, I certify that both Yichun and Xiaojie meet the eligibility criteria for the prize. In particular, I verify that:

1. Both are currently PhD students at Cornell University;
2. The research was conducted while both were students at Cornell University;
3. They are the major contributors to this work;
4. They are not co-authors on any other entry this year;
5. The paper presents original research results;
6. The paper has not won or selected a finalist in a previous INFORMS competition;
7. They are available to present the work at the INFORMS annual meeting.

Please let us know if you have any further questions. We look forward to hearing back from you soon.

Sincerely,



Nathan Kallus

Assistant Professor

School of Operations Research and Information Engineering and Cornell Tech

Cornell University

kallus@cornell.edu

We confirm our eligibility as above.



Xiaojie Mao  
Cornell University  
xm77@cornell.edu



Yichun Hu  
Cornell University  
yh767@cornell.edu