Optimization of Smooth Functions with Noisy Observations:
Local Minimax Rates

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Abstract

We consider the problem of \textit{global optimization} of an unknown non-convex smooth function with zeroth-order feedback. In this setup, an algorithm is allowed to adaptively query the underlying function at different locations and receives noisy evaluations of function values at the queried points (i.e. the algorithm has access to zeroth-order information). Optimization performance is evaluated by the expected difference of function values at the estimated optimum and the true optimum. In contrast to the classical optimization setup, first-order information like gradients are not directly accessible to the optimization algorithm. We show that the classical minimax framework of analysis, which roughly characterizes the worst-case query complexity of an optimization algorithm in this setting, leads to excessively pessimistic results. We propose a \textit{local minimax} framework to study the fundamental difficulty of optimizing smooth functions with adaptive function evaluations, which provides a refined picture of the intrinsic difficulty of zeroth-order optimization. We show that for functions with fast level set growth around the global minimum, carefully designed optimization algorithms can identify a near global minimizer with many fewer queries. For the special case of strongly convex and smooth functions, our implied convergence rates match the ones developed for zeroth-order convex optimization problems \cite{1, 22}. At the other end of the spectrum, for worst-case smooth functions no algorithm can converge faster than the minimax rate of estimating the entire unknown function in the $\ell_2$-norm. We provide an intuitive and efficient algorithm that attains the derived upper error bounds. Finally, using the local minimax framework we are able to clearly dichotomize adaptive and non-adaptive algorithms by showing that non-adaptive algorithms, although optimal in a global minimax sense, do not attain the optimal local minimax rate.

1 Introduction

Global function optimization with stochastic (zeroth-order) query oracles is an important problem in optimization, machine learning and statistics. To optimize an unknown bounded function $f : \mathcal{X} \rightarrow \mathbb{R}$ defined on a known compact $d$-dimensional domain $\mathcal{X} \subseteq \mathbb{R}^d$, the data analyst makes $n$ active queries $x_1, \ldots, x_n \in \mathcal{X}$ and observes

$$y_t = f(x_t) + w_t, \quad w_t \overset{i.i.d.}{\sim} \mathcal{N}(0, 1), \quad t = 1, \ldots, n.$$  

\footnote{The exact distribution of the independent noise variables $\varepsilon_t$ is not important, and our results can be generalized to sub-Gaussian noise variables as well.}
The queries \( x_1, \ldots, x_t \) are active in the sense that the selection of \( x_t \) can depend on the previous queries and their responses \( x_1, y_1, \ldots, x_{t-1}, y_{t-1} \). After \( n \) queries, an estimate \( \hat{x}_n \in \mathcal{X} \) is produced that approximately minimizes the unknown function \( f \). Such “active query” models are relevant in a broad range of (noisy) global optimization applications, for instance in hyper-parameter tuning of machine learning algorithms [43] and sequential design in material synthesis experiments where the goal is to maximize strengths of the produced materials [37, 44]. We refer the readers to Section 2.1 for a rigorous formulation of the active query model and contrast it with the classical passive query model.

The error of the estimate \( \hat{x}_n \) is measured by the difference of \( f(\hat{x}_n) \) and the global minimum of \( f \):

\[
\mathcal{L}(\hat{x}_n; f) := f(\hat{x}_n) - f^* \quad \text{where} \quad f^* := \inf_{x \in \mathcal{X}} f(x) .
\] (2)

To simplify our presentation, throughout the paper we take the domain \( \mathcal{X} \) to be the \( d \)-dimensional unit cube \([0, 1]^d\), while our results can be easily generalized to other compact domains satisfying minimal regularity conditions.

When \( f \) belongs to a smoothness class, say the Hölder class with exponent \( \alpha \), a straightforward global optimization method is to first sample \( n \) points uniformly at random from \( \mathcal{X} \) and then construct nonparametric estimates \( \hat{f}_n \) of \( f \) using nonparametric regression methods such as (high-order) kernel smoothing or local polynomial regression [21, 49]. Classical analysis shows that the sup-norm reconstruction error \( \| \hat{f}_n - f \|_{\infty} = \sup_{x \in \mathcal{X}} |\hat{f}_n(x) - f(x)| \) can be upper bounded by \( \bar{O}_P(n^{-\alpha/(2\alpha+d)})^2 \). This global reconstruction guarantee then implies an \( \bar{O}_P(n^{-\alpha/(2\alpha+d)}) \) upper bound on \( \mathcal{L}(\hat{x}_n; f) \) by considering \( \hat{x}_n \in \mathcal{X} \) such that \( f_n(\hat{x}_n) = \inf_{x \in \mathcal{X}} \hat{f}_n(x) \) (such an \( \hat{x}_n \) exists because \( \mathcal{X} \) is closed and bounded). Formally, we have the following proposition (proved in the Appendix) that converts a global reconstruction guarantee into an upper bound on optimization error:

**Proposition 1.** Suppose \( \hat{f}_n(\hat{x}_n) = \inf_{x \in \mathcal{X}} \hat{f}_n(x) \). Then \( \mathcal{L}(\hat{x}_n; f) \leq 2\| \hat{f}_n - f \|_{\infty} \).

Typically, fundamental limits on the optimal optimization error are understood through the lens of minimax analysis where the object of study is the (global) minimax risk:

\[
\inf_{\hat{x}_n} \sup_{f \in \mathcal{F}} \mathbb{E}_f \mathcal{L}(\hat{x}_n, f) ,
\] (3)

where \( \mathcal{F} \) is a certain smoothness function class such as the Hölder class. Although optimization appears to be easier than global reconstruction, we show in this paper that the \( n^{-\alpha/(2\alpha+d)} \) rate is not improvable in the global minimax sense in Eq. (3) over Hölder classes. Such a surprising phenomenon was also noted in previous works [9, 25, 46] for related problems. On the other hand, extensive empirical evidence suggests that non-uniform/active allocations of query points can significantly reduce optimization error in practical global optimization of smooth, non-convex functions [43]. This raises the interesting question of understanding, from a theoretical perspective, under what conditions/in what scenarios is global optimization of smooth functions easier than their reconstruction, and the power of active/feedback-driven queries that play important roles in global optimization.

In this paper, we propose a theoretical framework that partially answers the above questions. In contrast to classical global minimax analysis of nonparametric estimation problems, we adopt a local analysis which characterizes the optimal convergence rate of optimization error when the underlying function \( f \) is within the neighborhood of a “reference” function \( f_0 \). (See Section 2.2 for the rigorous local minimax formulation considered in this paper.) Our main results are to characterize the local convergence rates \( R_n(f_0) \) for a wide range of reference functions \( f_0 \in \mathcal{F} \). More specifically, our contributions can be summarized as follows:

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2In the \( \bar{O}(\cdot) \) or \( \bar{O}_P(\cdot) \) notation we drop poly-logarithmic dependency on \( n \)
1. We design an iterative (active) algorithm whose optimization error \( \mathcal{O}(x_n; f) \) converges at a rate of \( R_n(f_0) \) depending on the reference function \( f_0 \). When the level sets of \( f_0 \) satisfy certain regularity and polynomial growth conditions, the local rate \( R_n(f_0) \) can be upper bounded by \( R_n(f_0) = \tilde{O}(n^{-\alpha/(2\alpha+d-\alpha\beta)}) \), where \( \beta \in [0, d/\alpha] \) is a parameter depending on \( f_0 \) that characterizes the volume growth of the level sets of the reference function \( f_0 \). (See assumption (A2), Proposition 2 and Theorem 1 for details). The rate matches the global minimax convergence \( n^{-\alpha/(2\alpha+d)} \) for worst-case \( f_0 \) where \( \beta = 0 \), but has the potential of being much faster when \( \beta > 0 \). We emphasize that our algorithm has no knowledge of the reference function \( f_0 \) and achieves this rate adaptively.

2. We prove local minimax lower bounds that match the \( n^{-\alpha/(2\alpha+d-\alpha\beta)} \) upper bound, up to logarithmic factors in \( n \). More specifically, we show that even if \( f_0 \) is known, no (active) algorithm can estimate \( f \) in close neighborhoods of \( f_0 \) at a rate faster than \( n^{-\alpha/(2\alpha+d-\alpha\beta)} \). We further show that, if active queries are not available and queries \( x_1, \ldots, x_n \) are i.i.d. uniformly sampled from \( X \), then the \( n^{-\alpha/(2\alpha+d)} \) global minimax rate also applies locally regardless of how large \( \beta \) is. Thus, there is an explicit gap between local minimax rates of active and uniform query models when \( \beta \) is large.

3. In the special case when \( f \) is convex, the global optimization problem is usually referred to as zeroth-order convex optimization and this problem has been widely studied [1, 2, 6, 22, 29, 38]. Our results imply that, when \( f_0 \) is strongly convex and smooth, the local minimax rate \( R_n(f_0) \) is on the order of \( \tilde{O}(n^{-1/2}) \), which matches the convergence rates in [1]. Additionally, our negative results (Theorem 2) indicate that the \( n^{-1/2} \) rate cannot be achieved if \( f_0 \) is merely convex, which seems to contradict \( n^{-1/2} \) results in [2, 6] that do not require strong convexity of \( f \). However, it should be noted that mere convexity of \( f_0 \) does not imply convexity of \( f \) in a neighborhood of \( f_0 \) (e.g., \( \| f - f_0 \|_\infty \leq \epsilon \)). Our results show significant differences in the intrinsic difficulty of zeroth-order optimization of convex and near-convex functions.
1.1 Related Work

Global optimization, known variously as black-box optimization, Bayesian optimization and the continuous-armed bandit, has a long history in the optimization research community [30, 31] and has also received a significant amount of recent interest in statistics and machine learning [8, 9, 25, 35, 36, 43].

Among the existing works, [35, 36] are perhaps the closest to our paper in terms of analytical perspectives. Both papers impose additional assumptions on the level sets of the underlying function to obtain an improved convergence rate. However, several important differences exist. First, the level set assumptions considered in the mentioned references are rather restrictive and essentially require the underlying function to be uni-modal, while our assumptions are much more flexible and apply to multi-modal functions as well. In addition, [35, 36] considered a noiseless setting in which exact function evaluations \( f(x) \) can be obtained, while our paper studies the noise corrupted model in Eq. (1) for which vastly different convergence rates are derived. Finally, no matching lower bounds were proved in [35, 36].

The (stochastic) global optimization problem is similar to mode estimation of either densities or regression functions, which has a rich literature [15, 32, 42]. An important difference between statistical mode estimation and global optimization is the way sample/query points \( x_1, \ldots, x_n \in \mathcal{X} \) are distributed: in mode estimation it is customary to assume the samples are independently and identically distributed, while in global optimization sequential designs of samples/queries are allowed. Furthermore, to estimate/ locate the mode of an unknown density or regression function, such a mode has to be well-defined; on the other hand, producing an estimate \( \hat{x}_n \) with small \( \mathbb{L}(\hat{x}_n, f) \) is easier and results in weaker conditions imposed on the underlying function.

Methodology-wise, our proposed algorithm is conceptually similar to the abstract Pure Adaptive Search (PAS) framework proposed and analyzed in [52]. The iterative procedure also resembles disagreement-based active learning methods [5, 16, 24] and the “successive rejection” algorithm in bandit problems [20]. The intermediate steps of candidate point elimination can also be viewed as sequences of level set estimation problems [41, 45, 47] or cluster tree estimation [4, 14] with active queries.

Another line of research has focused on first-order optimization of quasi-convex or non-convex functions [3, 11, 23, 26, 39, 53], in which exact or unbiased evaluations of function gradients are available at query points \( x \in \mathcal{X} \). [53] considered a Cheeger’s constant restriction on level sets which is similar to our level set regularity assumptions (A2 and A2’). [17, 18] studied local minimax rates of first-order optimization of convex functions. First-order optimization differs significantly from our setting because unbiased gradient estimation is generally impossible in the model of Eq. (1). Furthermore, most works on (first-order) non-convex optimization focus on convergence to stationary points or local minima, while we consider convergence to global minima.

2 Background and Notation

We first review standard asymptotic notation that will be used throughout this paper. For two sequences \( \{a_n\}_{n=1}^\infty \) and \( \{b_n\}_{n=1}^\infty \), we write \( a_n = O(b_n) \) or \( a_n \preceq b_n \) if \( \limsup_{n \to \infty} |a_n|/|b_n| < \infty \), or equivalently \( b_n = \Omega(a_n) \) or \( a_n \succeq b_n \). Denote \( a_n = \Theta(b_n) \) or \( a_n \asymp b_n \) if both \( a_n \preceq b_n \) and \( a_n \succeq b_n \) hold. We also write \( a_n = o(b_n) \) or equivalently \( b_n = o(a_n) \) if \( \limsup_{n \to \infty} |a_n|/|b_n| = 0 \). For two sequences of random variables \( \{A_n\}_{n=1}^\infty \) and \( \{B_n\}_{n=1}^\infty \), denote \( A_n = O_P(B_n) \) if for every \( \epsilon > 0 \), there exists \( C > 0 \) such that \( \limsup_{n \to \infty} \Pr[|A_n| > C|B_n|] \leq \epsilon \). For \( r > 0, 1 \leq p \leq \infty \) and \( x \in \mathbb{R}^d \), we denote \( B_r^p(x) := \{z \in \mathbb{R}^d : \|z-x\|_p \leq r \} \) as the \( d \)-dimensional \( \ell_p \)-ball of radius \( r \) centered at \( x \), where the vector \( \ell_p \) norm is defined as \( \|x\|_p := (\sum_{j=1}^d |x_j|^p)^{1/p} \) for \( 1 \leq p < \infty \) and \( \|x\|_\infty := \max_{1 \leq j \leq d} |x_j| \).
For any subset $S \subseteq \mathbb{R}^d$ we denote by $B^p_t(x; S)$ the set $B^p_t(x) \cap S$.

2.1 Passive and Active Query Models

Let $U$ be a known random quantity defined on a probability space $\mathcal{U}$. The following definitions characterize all passive and active optimization algorithms:

**Definition 1** (The passive query model). Let $x_1, \ldots, x_n$ be i.i.d. points uniformly sampled on $\mathcal{X}$ and $y_1, \ldots, y_n$ be observations from the model Eq. (1). A passive optimization algorithm $A$ with $n$ queries is parameterized by a mapping $\phi_n : (x_1, y_1, \ldots, x_n, y_n, U) \mapsto \hat{x}_n$ that maps the i.i.d. observations $\{(x_i, y_i)\}_{i=1}^n$ to an estimated optimum $\hat{x}_n \in \mathcal{X}$, potentially randomized by $U$.

**Definition 2** (The active query model). An active optimization algorithm can be parameterized by mappings $(\chi_1, \ldots, \chi_n, \phi_n)$, where for $t = 1, \ldots, n$,

$$\chi_t : (x_1, y_1, \ldots, x_{t-1}, y_{t-1}, U) \mapsto x_t$$

produces a query point $x_t \in \mathcal{X}$ based on previous observations $\{(x_i, t_i)\}_{i=1}^{t-1}$, and

$$\phi_n : (x_1, y_1, \ldots, x_n, y_n, U) \mapsto \hat{x}_n$$

produces the final estimate. All mappings $(\chi_1, \ldots, \chi_n, \phi_n)$ can be randomized by $U$.

2.2 Local Minimax Rates

We use the classical local minimax analysis [51] to understand the fundamental information-theoretical limits of noisy global optimization of smooth functions. On the upper bound side, we seek (active) estimators $\hat{x}_n$ such that

$$\sup_{f_0 \in \Theta} \sup_{f \in \Theta', |f-f_0|_{\mathcal{X}} \leq \varepsilon_n(f_0)} \Pr \left[ \mathcal{L}(\hat{x}_n; f) \geq C_1 \cdot R_n(f_0) \right] \leq 1/4, \quad (4)$$

where $C_1 > 0$ is a positive constant. Here $f_0 \in \Theta$ is referred to as the reference function, and $f \in \Theta'$ is the true underlying function which is assumed to be “near” $f_0$. The minimax convergence rate of $\mathcal{L}(\hat{x}_n; f)$ is then characterized locally by $R_n(f_0)$ which depends on the reference function $f_0$. The constant of $1/4$ is chosen arbitrarily and any small constant leads to similar conclusions. To establish negative results (i.e., locally minimax lower bounds), in contrast to the upper bound formulation, we assume the potential active optimization estimator $\hat{x}_n$ has perfect knowledge about the reference function $f_0 \in \Theta$. We then prove locally minimax lower bounds of the form

$$\inf_{\hat{x}_n} \sup_{f \in \Theta', |f-f_0|_{\mathcal{X}} \leq \varepsilon_n(f_0)} \Pr \left[ \mathcal{L}(\hat{x}_n; f) \geq C_2 \cdot R_n(f_0) \right] \geq 1/3,$$  

where $C_2 > 0$ is another positive constant and $\varepsilon_n(f_0), R_n(f_0)$ are desired local convergence rates for functions near the reference $f_0$.

Although in some sense classical, the local minimax definition we propose warrants further discussion.

1. **Roles of $\Theta$ and $\Theta'$**: The reference function $f_0$ and the true functions $f$ are assumed to belong to different but closely related function classes $\Theta$ and $\Theta'$. In particular, in our paper $\Theta \subseteq \Theta'$, meaning that less restrictive assumptions are imposed on the true underlying function $f$ compared to those imposed on the reference function $f_0$ on which $R_n$ and $\varepsilon_n$ are based.
2. Upper Bounds: It is worth emphasizing that the estimator \( \hat{x}_n \) has no knowledge of the reference function \( f_0 \). From the perspective of upper bounds, we can consider the simpler task of producing \( f_0 \)-dependent bounds (eliminating the second supremum) to instead study the (already interesting) quantity:

\[
\sup_{f_0 \in \Theta} \Pr[\mathcal{L}(\hat{x}_n; f_0) \geq C_1 R_n(f_0)] \leq 1/4.
\]

As indicated above we maintain the double-supremum in the definition because fewer assumptions are imposed directly on the true underlying function \( f \), and further because it allows to more directly compare our upper and lower bounds.

3. Lower Bounds and the choice of the “localization radius” \( \varepsilon_n(f_0) \): Our lower bounds allow the estimator knowledge of the reference function (this makes establishing the lower bound more challenging). Eq. (5) implies that no estimator \( \hat{x}_n \) can effectively optimize a function \( f \) close to \( f_0 \) beyond the convergence rate of \( R_n(f_0) \), even if perfect knowledge of the reference function \( f_0 \) is available a priori. The \( \varepsilon_n(f_0) \) parameter that decides the “range” in which local minimax rates apply is taken to be on the same order as the actual local rate \( R_n(f_0) \) in this paper. This is (up to constants) the smallest radius for which we can hope to obtain non-trivial lower-bounds: if we consider a much smaller radius than \( R_n(f_0) \) then the trivial estimator which outputs the minimizer of the reference function would achieve a faster rate than \( R_n(f_0) \). Selecting the smallest possible radius makes establishing the lower bound most challenging but provides a refined picture of the complexity of zeroth-order optimization.

3. Main Results

With this background in place we now turn our attention to our main results. We begin by collecting our assumptions about the true underlying function and the reference function in Section 3.1. We state and discuss the consequences of our upper and lower bounds in Sections 3.2 and 3.3 respectively. We defer most technical proofs to the Appendix and turn our attention to our optimization algorithm in Section 4.

3.1 Assumptions

We first state and motivate assumptions that will be used. The first assumption states that \( f \) is locally Hölder smooth on its level sets.

(A1) There exist constants \( \kappa, \alpha, M > 0 \) such that \( f \) restricted on \( \mathcal{X}_{f,\kappa} := \{x \in \mathcal{X} : f(x) \leq f^* + \kappa\} \) belongs to the Hölder class \( \Sigma_\alpha(M) \), meaning that \( f \) is \( k \)-times differentiable on \( \mathcal{X}_{f,\kappa} \) and furthermore for any \( x, x' \in \mathcal{X}_{f,\kappa} \),

\[
\sum_{j=0}^{k} \sum_{\alpha_1 + \ldots + \alpha_d = j} |f^{(\alpha,j)}(x)| + \sum_{\alpha_1 + \ldots + \alpha_d = k} \frac{|f^{(\alpha,k)}(x) - f^{(\alpha,k)}(x')|}{\|x - x'\|^{\alpha_k}} \leq M. \tag{6}
\]

Here \( k = |\alpha| \) is the largest integer lower bounding \( \alpha \) and \( f^{(\alpha,j)}(x) := \partial^j f(x) / \partial x_1^{\alpha_1} \ldots \partial x_d^{\alpha_d} \).

We use \( \Sigma_\alpha(M) \) to denote the class of all functions satisfying (A1). We remark that (A1) is weaker than the standard assumption that \( f \) on its entire domain \( \mathcal{X} \) belongs to the Hölder class \( \Sigma_\alpha(M) \). This

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3 the particular \( \ell_\infty \) norm is used for convenience only and can be replaced by any equivalent vector norms.
is because places with function values larger than \( f^* + \kappa \) can be easily detected and removed by a pre-processing step. We give further details of the pre-processing step in Section 4.3.

Our next assumption concern the “regularity” of the level sets of the “reference” function \( f_0 \).

Define \( L_{f_0}(e) := \{ x \in \mathcal{X} : f_0(x) \leq f_0^* + e \} \) as the \( \epsilon \)-level set of \( f_0 \), and \( \mu_{f_0}(e) := \lambda(L_{f_0}(e)) \) as the Lebesgue measure of \( L_{f_0}(e) \), also known as the distribution function. Define also \( N(L_{f_0}(e), \delta) \) as the smallest number of \( \ell_2 \)-balls of radius \( \delta \) that cover \( L_{f_0}(e) \).

(A2) There exist constants \( c_0 > 0 \) and \( C_0 > 0 \) such that \( N(L_{f_0}(e), \delta) \leq C_0[1 + \mu_{f_0}(e) \delta^{-d}] \) for all \( \epsilon, \delta \in (0, c_0] \).

We use \( \Theta_C \) to denote all functions that satisfy (A2) with respect to parameters \( C = (c_0, C_0) \).

At a higher level, the regularity condition (A2) assumes that the level sets are sufficiently “regular” such that covering them with small-radius balls does not require significantly larger total volumes. For example, consider a perfectly regular case of \( L_{f_0}(e) \) being the \( d \)-dimensional \( \ell_2 \) ball of radius \( \delta \): \( L_{f_0}(e) = \{ x \in \mathcal{X} : \| x - x^* \|^2 \leq r \} \). Clearly, \( \mu_{f_0}(e) \approx \pi^d / \delta^d \). In addition, the \( \delta \)-covering number in \( \ell_2 \) of \( L_{f_0}(e) \) is on the order of \( 1 + (r/\delta)^d = 1 + \mu_{f_0}(e) \delta^{-d} \), which satisfies the scaling in (A2).

When (A2) holds, uniform confidence intervals of \( f \) on its level sets are easy to construct because little statistical efficiency is lost by slightly enlarging the level sets so that complete \( d \)-dimensional cubes are contained in the enlarged level sets. On the other hand, when regularity of level sets fails to hold such nonparametric estimation can be very difficult or even impossible. As an extreme example, suppose the level set \( L_{f_0}(e) \) consists of standalone and well-spaced points in \( \mathcal{X} \): the Lebesgue measure of \( L_{f_0}(e) \) would be zero, but at least \( \Omega(n) \) queries are necessary to construct uniform confidence intervals on \( L_{f_0}(e) \). It is clear that such \( L_{f_0}(e) \) violates (A2), because \( N(L_{f_0}(e), \delta) \geq n \) as \( \delta \to 0^+ \) but \( \mu_{f_0}(e) = 0 \).

### 3.2 Upper Bound

The following theorem is our main result that upper bounds the local minimax rate of noisy global optimization with active queries.

**Theorem 1.** For any \( \alpha, M, \kappa, c_0, C_0 > 0 \) and \( f_0 \in \Sigma_\alpha^\kappa(M) \cap \Theta_C \), define

\[
\varepsilon_n(f_0) := \sup \left\{ \varepsilon > 0 : \varepsilon^{-2+\alpha/\omega} \mu_{f_0}(\varepsilon) \geq n / \log^\omega n \right\},
\]

where \( \omega > 5 + \alpha d \) is a large constant. Suppose also that \( \varepsilon_n(f_0) \to 0 \) as \( n \to \infty \). Then for sufficiently large \( n \), there exists an estimator \( \hat{x}_n \) with access to \( n \) active queries \( x_1, \ldots, x_n \in \mathcal{X} \), a constant \( C_R > 0 \) depending only on \( \alpha, M, \kappa, c_0, C_0 \) and a constant \( \gamma > 0 \) depending only on \( \alpha \) and \( d \) such that

\[
\sup_{f_0 \in \Sigma_\alpha^\kappa(M) \cap \Theta_C} \sup_{f \in \Sigma_\alpha^\kappa(M),} \Pr \left[ \Sigma(\hat{x}_n, f) > C_R \log^\gamma n \cdot (\varepsilon_n(f_0) + n^{-1/2}) \right] \leq 1/4.
\]

**Remark 1.** Unlike the (local) smoothness class \( \Sigma_\alpha^\kappa(M) \), the additional function class \( \Theta_C \) that encapsulates (A2) is imposed only on the “reference” function \( f_0 \) but not the true function \( f \) to be estimated. This makes the assumptions considerably weaker because the true function \( f \) may violate either or both (A2) while our results remain valid.
Remark 2. The estimator \( \hat{x}_n \) does not require knowledge of parameters \( \kappa, c_0, C_0 \) or \( \varepsilon_n^{U}(f_0) \), and automatically adapts to them, as shown in the next section. It however requires knowledge of \( \alpha \) and \( M \), parameters of the smooth function class. Such knowledge is unlikely to be optional, as the key step of building honest confidence intervals that adapt to \( \alpha \) and/or \( M \) is very difficult and in general not possible without additional assumptions, as shown by [10, 34].

Remark 3. When the distribution function \( \mu_{f_0}(\varepsilon) \) does not change abruptly with \( \varepsilon \) the expression of \( \varepsilon_n^{U}(f_0) \) can be significantly simplified. In particular, if for all \( \varepsilon \in (0, c_0] \) it holds that

\[
\mu_{f_0}(\varepsilon) / \log n \geq \mu_{f_0}(\varepsilon)/(\log n)^{O(1)},
\]

then \( \varepsilon_n^{U}(f_0) \) can be upper bounded as

\[
\varepsilon_n^{U}(f_0) \leq [\log n]^{O(1)} \cdot \sup \{ \varepsilon > 0 : \varepsilon^{-(2+d/\alpha)} \mu_{f_0}(\varepsilon) \geq n \}.
\]

It is also noted that if \( \mu_{f_0}(\varepsilon) \) has a polynomial behavior of \( \mu_{f_0}(\varepsilon) \leq \varepsilon^\beta \) for some constant \( \beta \geq 0 \), then Eq. (9) is satisfied and so is Eq. (10).

The quantity \( \varepsilon_n^{U}(f_0) = \inf \{ \varepsilon > 0 : \varepsilon^{-(2+d/\alpha)} \mu_{f_0}(\varepsilon) \geq n/\log^\omega n \} \) is crucial in determining the convergence rate of optimization error of \( \hat{x}_n \); locally around the reference function \( f_0 \). While the definition of \( \varepsilon_n^{U}(f_0) \) is mostly implicit and involves solving an inequality concerning the distribution function \( \mu_{f_0}(\varepsilon) \), we remark that it admits a simple form when \( \mu_{f_0}(\varepsilon) \) has a polynomial growth rate, as shown by the following proposition:

**Proposition 2.** Suppose \( \mu_{f_0}(\varepsilon) \leq \varepsilon^\beta \) for some constant \( \beta \in [0, 2+d/\alpha) \). Then \( \varepsilon_n^{U}(f_0) = \tilde{O}(n^{-\alpha/(2\alpha+d-\alpha\beta)}) \). In addition, if \( \beta \in [0, d/\alpha] \) then \( \varepsilon_n^{U}(f_0) + n^{-1/2} \leq \varepsilon_n^{U}(f_0) = \tilde{O}(n^{-\alpha/(2\alpha+d-\alpha\beta)}) \).

Proposition 2 can be easily verified by solving the system \( \varepsilon^{-(2+d/\alpha)} \mu_{f_0}(\varepsilon) \geq n/\log^\omega n \) with the condition \( \mu_{f_0}(\varepsilon) \leq \varepsilon^\beta \). We therefore omit its proof. The following two examples give some simple reference functions \( f_0 \) that satisfy the \( \mu_{f_0}(\varepsilon) \leq \varepsilon^\beta \) condition in Proposition 2 with particular values of \( \beta \).

**Example 1.** The constant function \( f_0 \equiv 0 \) satisfies (A1) through (A3) with \( \beta = 0 \).

**Example 2.** \( f_0 \in \Sigma^2_{\kappa}(M) \) that is strongly convex \(^4\) satisfies (A1) through (A3) with \( \beta = d/2 \).

Example 1 is simple to verify, as the volume of level sets of the constant function \( f_0 \equiv 0 \) exhibits a phase transition at \( \varepsilon = 0 \) and \( \varepsilon > 0 \), rendering \( \beta = 0 \) the only parameter option for which \( \mu_{f_0}(\varepsilon) \leq \varepsilon^\beta \).

Example 2 is more involved, and holds because the strong convexity of \( f_0 \) lower bounds the growth rate of \( f_0 \) when moving away from its minimum. We give a rigorous proof of Example 2 in the appendix. We also remark that \( f_0 \) does not need to be exactly strongly convex for \( \beta = d/2 \) to hold, and the example is valid for, e.g., piecewise strongly convex functions with a constant number of pieces too.

To best interpret the results in Theorem 1 and Proposition 2, it is instructive to compare the “local” rate \( n^{-\alpha/(2\alpha+d-\alpha\beta)} \) with the baseline rate \( n^{-\alpha/(2\alpha+d)} \), which can be attained by reconstructing \( f \) in sup-norm and applying Proposition 1. Since \( \beta \geq 0 \), the local convergence rate established in Theorem 1 is never slower, and the improvement compared to the baseline rate \( n^{-\alpha/(2\alpha+d)} \) is dictated by \( \beta \), which governs the growth rate of volume of level sets of the reference function \( f_0 \). In particular, for functions that grows fast when moving away from its minimum, the parameter \( \beta \) is large and therefore the local convergence rate around \( f_0 \) could be much faster than \( n^{-\alpha/(2\alpha+d)} \).

\(^4\) A twice differentiable function \( f_0 \) is strongly convex if there exists \( \sigma > 0 \) such that \( \nabla^2 f_0(x) \geq \sigma I, \forall x \in \mathcal{X}. \)
Theorem 1 also implies concrete convergence rates for special functions considered in Examples 1 and 2. For the constant reference function \( f_0 \equiv 0 \), Example 1 and Theorem 1 yield that \( R_n(f_0) \sim n^{-\alpha/(2\alpha+d)} \), which matches the baseline rate \( n^{-\alpha/(2\alpha+d)} \) and suggests that \( f_0 \equiv 0 \) is the worst-case reference function. This is intuitive, because \( f_0 \equiv 0 \) has the most drastic level set change at \( \epsilon \to 0^+ \) and therefore small perturbations anywhere of \( f_0 \) result in changes of the optimal locations. On the other hand, if \( f_0 \) is strongly smooth and convex as in Example 2, Theorem 1 suggests that \( R_n(f_0) \sim n^{-1/2} \), which is significantly better than the \( n^{-2/(4+d)} \) baseline rate \(^5\) and also matches existing works on zeroth-order optimization of convex functions \([1]\). The faster rate holds intuitively because strongly convex functions grows fast when moving away from the minimum, which implies small level set changes. An active query algorithm could then focus most of its queries onto the small level sets of the underlying function, resulting in more accurate local function reconstructions and faster optimization error rate.

Our proof of Theorem 1 is constructive, by upper bounding the local minimax optimization error of an explicit algorithm. At a higher level, the algorithm partitions the \( n \) active queries evenly into \( \log n \) epochs, and level sets of \( f \) are estimated at the end of each epoch by comparing (uniform) confidence intervals on a dense grid on \( X \). It is then proved that the volume of the estimated level sets contracts geometrically, until the target convergence rate \( R_n(f_0) \) is attained. The complete proof of Theorem 1 is placed in Section 5.2.

### 3.3 Lower Bounds

We prove local minimax lower bounds that match the upper bounds in Theorem 1 up to logarithmic terms. As we remarked in Section 2.2, in the local minimax lower bound formulation we assume the data analyst has full knowledge of the reference function \( f_0 \), which makes the lower bounds stronger as more information is available a priori.

To facilitate such a strong local minimax lower bounds, the following additional condition is imposed on the reference function \( f_0 \) of which the data analyst has perfect information.

\[
(A2') \quad \text{There exist constants } c'_0, C'_0 > 0 \text{ such that } M(L_{f_0}(\epsilon), \delta) \geq C'_0 \mu_{f_0}(\epsilon) \delta^{-d} \text{ for all } \epsilon, \delta \in (0, c'_0],
\]

where \( M(L_{f_0}(\epsilon), \delta) \) is the maximum number of disjoint \( \ell_2 \) balls of radius \( \delta \) that can be packed into \( L_{f_0}(\epsilon) \).

We denote \( \Theta'_{C'} \) as the class of functions that satisfy \( (A2') \) with respect to parameters \( C' = (c'_0, C'_0) > 0 \). Intuitively, \( (A2') \) can be regarded as the “reverse” version of \( (A2) \), which basically means that \( (A2) \) is “tight”.

We are now ready to state our main negative result, which shows, from an information-theoretical perspective, that the upper bound in Theorem 1 is not improvable.

**Theorem 2.** Suppose \( \alpha, c_0, C_0, c'_0, C'_0 > 0 \) and \( \kappa = \infty \). Denote \( C = (c_0, C_0) \) and \( C' = (c'_0, C'_0) \). For any \( f_0 \in \Theta_C \cap \Theta'_{C'} \), define

\[
\epsilon_{n}^{f_0} := \sup \left\{ \epsilon > 0 : \epsilon^{-(2+d/\alpha)} \mu_{f_0}(\epsilon) \geq n \right\}.
\]

(11)

Then there exist constant \( M > 0 \) depending on \( \alpha, d, C, C' \) such that, for any \( f_0 \in \Sigma_{\kappa}^{\alpha}(M/2) \cap \Theta_C \cap \Theta'_{C'} \),

\[
\inf_{\hat{x}_n} \sup_{f \in \Sigma_{\kappa}^{\alpha}(M)} \Pr_{f} \left[ \frac{\Omega(\hat{x}_n; f)}{\epsilon_{n}^{f_0}} \geq \epsilon_{n}^{f_0} \right] \geq \frac{1}{3}.
\]

\( ^5\)Note that \( f_0 \) being strongly smooth implies \( \alpha = 2 \) in the local smoothness assumption.
Remark 4. For any $f_0$ and $n$ it always holds that $\varepsilon_n^U(f_0) \leq \varepsilon_n^U(f_0)$.

Remark 5. If the distribution function $\mu_{f_0}(\epsilon)$ satisfies Eq. (9) in Remark 3, then $\varepsilon_n^U(f_0) = \varepsilon_n^U(f_0) / (\log n)^{O(1)}$.

Remark 4 shows that there might be a gap between the locally minimax upper and lower bounds in Theorems 1 and 2. Nevertheless, Remark 5 shows that under the mild condition of $\mu_{f_0}(\epsilon)$ does not change too abruptly with $\epsilon$, the gap between $\varepsilon_n^U(f_0)$ and $\varepsilon_n^L(f_0)$ is only a poly-logarithmic term in $n$. Additionally, the following proposition derives explicit expression of $\varepsilon_n^L(f_0)$ for reference functions whose distribution functions have a polynomial growth, which matches the Proposition 2 up to log $n$ factors. Its proof is again straightforward.

**Proposition 3.** Suppose $\mu_{f_0}(\epsilon) \geq \epsilon^\beta$ for some $\beta \in [0, 2 + d/\alpha]$. Then $\varepsilon_n^L(f_0) = \Omega(n^{-\alpha/(2\alpha + d - \alpha\beta)})$.

The following proposition additionally shows the existence of $f_0 \in \Sigma_2^M(M) \cap \Theta_C \cap \Theta_{C'}$ that satisfies $\mu_{f_0}(\epsilon) \approx \epsilon^\beta$ for any values of $\alpha > 0$ and $\beta \in [0, d/\alpha]$. Its proof is given in the appendix.

**Proposition 4.** Fix arbitrary $\alpha, M > 0$ and $\beta \in [0, d/\alpha]$. There exists $f_0 \in \Sigma_2^M(M) \cap \Theta_C \cap \Theta_{C'}$ for $\kappa = \infty$ and constants $C = (c_0, C_0)$, $C' = (c'_0, C'_0)$ that depend only on $\alpha, \beta, M$ and $d$ such that $\mu_{f_0}(\epsilon) \approx \epsilon^\beta$.

Theorem 2 and Proposition 3 show that the $n^{-\alpha/(2\alpha + d - \alpha\beta)}$ upper bound on local minimax convergence rate established in Theorem 1 is not improvable up to logarithmic factors of $n$. Such information-theoretical lower bounds on the convergence rates hold even if the data analyst has perfect information of $f_0$, the reference function on which the $n^{-\alpha/(2\alpha + d - \alpha\beta)}$ local rate is based. Our results also imply an $n^{-\alpha/(2\alpha + d)}$ minimax lower bound over all $\alpha$-Hölder smooth functions, showing that without additional assumptions, noisy optimization of smooth functions is as difficult as reconstructing the unknown function in sup-norm.

Our proof of Theorem 2 also differs from existing minimax lower bound proofs for active nonparametric models [13]. The classical approach is to invoke Fano’s inequality and to upper bound the KL divergence between different underlying functions $f$ and $g$ using $\|f - g\|_x$, corresponding to the point $x \in X$ that leads to the largest KL divergence. Such an approach, however, does not produce tight lower bounds for our problem. To overcome such difficulties, we borrow the lower bound analysis for bandit pure exploration problems in [7]. In particular, our analysis considers the query distribution of any active query algorithm $\mathcal{A} = (\varphi_1, \ldots, \varphi_n, \phi_n)$ under the reference function $f_0$ and bounds the perturbation in query distributions between $f_0$ and $f$ using Le Cam’s lemma. Afterwards, an adversarial function choice $f$ can be made based on the query distributions of the considered algorithm $\mathcal{A}$. We defer the complete proof of Theorem 2 to Section 5.3.

Theorem 2 applies to any global optimization method that makes active queries, corresponding to the query model in Theorem 2. The following theorem, on the other hand, shows that for passive algorithms (Definition 1) the $n^{-\alpha/(2\alpha + d)}$ optimization rate is not improvable even with additional level set assumptions imposed on $f_0$. This demonstrates an explicit gap between passive and adaptive query models in global optimization problems.

**Theorem 3.** Suppose $\alpha, c_0, C_0, c'_0, C'_0 > 0$ and $\kappa = \infty$. Denote $C = (c_0, C_0)$ and $C' = (c'_0, C'_0)$. Then there exist constant $M > 0$ depending on $\alpha, d, C, C'$ and $N$ depending on $M$ such that, for any $f_0 \in \Sigma_2^M(M) \cap \Theta_C \cap \Theta_{C'}$ satisfying $\varepsilon_n^L(f_0) \leq \varepsilon_n^L(f_0)$, we have:

$$\inf_{\tilde{x}_n} \sup_{f \in \Sigma_2^M(M), \|f - f_0\|_x \leq 2\varepsilon_n^L} \Pr \left[ \mathcal{L}(\tilde{x}_n; f) \geq \varepsilon_n^L \right] \geq \frac{1}{3}$$

for all $n \geq N$.
Intuitively, the apparent gap demonstrated by Theorems 2 and 3 between the active and passive query models stems from the observation that, a passive algorithm $A$ only has access to uniformly sampled query points $x_1, \ldots, x_n$ and therefore cannot focus on a small level set of $f$ in order to improve query efficiency. In addition, for functions that grow faster when moving away from their minima (implying a larger value of $\beta$), the gap between passive and active query models becomes bigger as active queries can more effectively exploit the restricted level sets of such functions.

4 Our Algorithm

In this section we describe a concrete algorithm that attains the upper bound in Theorem 1. We start with a cleaner algorithm that operates under the slightly stronger condition that $\kappa = \infty$ in (A1), meaning that $f$ is $\alpha$-Hölder smooth on the entire domain $\mathcal{X}$. The generalization to $\kappa > 0$ being a constant is given in Section 4.3 with an additional pre-processing step.

Let $G_n \subseteq \mathcal{X}$ be a finite grid of points in $\mathcal{X}$. We assume the finite grid $G_n$ satisfies the following two mild conditions:

(B1) Points in $G_n$ are sampled i.i.d. from an unknown distribution $P_X$ on $\mathcal{X}$; furthermore, the density $p_X$ associated with $P_X$ satisfies $\underline{p}_0 \leq p_X(x) \leq \overline{p}_0$ for all $x \in \mathcal{X}$, where $0 < \underline{p}_0 \leq \overline{p}_0 < \infty$ are uniform constants;

(B2) $|G_n| \geq n^{3d/\min(\alpha, 1)}$ and $\log |G_n| = O(\log n)$.

Remark 6. Although typically the choices of the grid points $G_n$ belong to the data analyst, in some applications the choices of design points are not completely free. For example, in material synthesis experiments some environment parameter settings (e.g., temperature and pressure) might not be accessible due to budget or physical constraints. Thus, we choose to consider less restrictive conditions imposed on the design grid $G_n$, allowing it to be more flexible in real-world applications.

For any subset $S \subseteq G_n$ and a “weight” function $\varrho : G_n \to \mathbb{R}^+$, define the extension $S^\varrho(\varrho)$ of $S$ with respect to $\varrho$ as

$$S^\varrho(\varrho) := \bigcup_{x \in S} B_{\varrho(x)}^\varrho(x; G_n)$$

where

$$B_{\varrho(x)}^\varrho(x; G_n) = \{z \in G_n : \|z - x\|_X \leq \varrho(x)\}. \quad (14)$$

The algorithm can then be formulated as two level of iterations, with the outer loop shrinking the “active set” $S_\tau$ and the inner loop collecting data that reduce lengths of confidence intervals on the active set. A pseudocode description of our proposed algorithm is given in Fig. 1.

4.1 Local Polynomial Regression

We use local polynomial regression [21] to obtain the estimate $\hat{f}(x)$. In particular, for any $x \in G_n$ and a bandwidth parameter $h > 0$, consider a least square polynomial estimate

$$\hat{f}_h \in \arg \min_{g \in \mathcal{P}_k} \sum_{t=1}^T \mathbb{I}[x_{t'} \in B_h^\varrho(x)] \cdot (y_{t'} - g(x_{t'}))^2,$$  

(15)

where $B_h^\varrho(x) := \{x' \in \mathcal{X} : \|x' - x\|_X \leq h\}$ and $\mathcal{P}_k$ denotes all polynomials of degree $k$ on $\mathcal{X}$.

To analyze the performance of $\hat{f}_h$ evaluated at a certain point $x \in \mathcal{X}$, define mapping $\psi_{x,h} : z \mapsto (1, \psi_{x,h}^1(z), \ldots, \psi_{x,h}^k(z))$ where $\psi_{x,h}^j : z \mapsto \left[\prod_{i=1}^d h^{-1}(z_{i,t} - x_{i,t})\right]_{i=1,\ldots,i_j=1}$ is the degree-$j$ polynomial mapping from $\mathbb{R}^d$ to $\mathbb{R}^d$. Also define $\Psi_{t,h} := (\psi_{x,h}(x_{t'}))_{1 \leq t' \leq T, x_{t'} \in B_h(x)}$ as the $m \times D$
Parameters: \(\alpha, M, \delta, n\)

Output: \(\hat{x}_n = x_n\), the final prediction

Initialization: \(S_0 = G_n, g_0(x) \equiv \infty, T = \lfloor \log_2 n \rfloor, n_0 = \lfloor n/T \rfloor\);

for \(\tau = 1, 2, \ldots, T\) do
  Compute “extended” sample set \(S_{\tau-1}^\circ(p_{\tau-1})\) defined in Eq. (14);
  for \(t = (\tau - 1)n_0 + 1\) to \(\tau n_0\) do
    Sample \(x_t\) uniformly at random from \(S_{\tau-1}^\circ(p_{\tau-1})\) and observe \(y_t = f(x_t) + w_t\);
  end
  For every \(x \in S_{\tau-1}\), find bandwidth \(h_t(x)\) and build CI \([\ell_t(x), u_t(x)]\) in Eq. (19);
  \(S_\tau := \{x \in S_{\tau-1} : \ell_t(x) \leq \min_{x' \in S_{\tau-1}} u_t(x')\}\), \(p_\tau(x) := \min\{p_{\tau-1}(x), h_t(x)\}\).
end

**Figure 1:** The main algorithm.

The aggregated design matrix, where \(m = \sum_{t' = 1}^t I[x_{t'} \in B_h^C(x)]\) and \(D = 1 + d + \ldots + d^k\), \(k = \lfloor \alpha \rfloor\). The estimate \(\hat{f}_h\) defined in Eq. (15) then admits the following closed-form expression:

\[
\hat{f}_h(z) = \psi_{x,h}(z)^\top (\Psi_{t,h}^\top \Psi_{t,h})^{-1} \Psi_{t,h}^\top Y_{t,h},
\]

where \(Y_{t,h} = (y_{t'})_{1 \leq t' \leq t, x_{t'} \in B_h^C(x)}\) and \(A^\top\) is the Moore-Penrose pseudo-inverse of \(A\).

The following lemma gives a finite-sample analysis of the error of \(\hat{f}_h(x)\):

**Lemma 1.** Suppose \(f\) satisfies Eq. (6) on \(B_h^C(x; \mathcal{X})\), \(\max_{x \in B_h^C(x; \mathcal{X})} \|\psi_{x,h}(z)\|_2 \leq b\) and \(\frac{1}{m} \Psi_{t,h}^\top \Psi_{t,h} \geq \sigma I_{D \times D}\) for some \(\sigma > 0\). Then for any \(\delta \in (0, 1/2)\), with probability \(1 - \delta\)

\[
|\hat{f}_h(x) - f(x)| \leq \frac{b^2 \ln(1/\delta)}{\sigma} M^{d^k}\alpha + b \sqrt{\frac{5D \ln(1/\delta)}{\sigma m}} =: \eta_{h,\delta}(x).
\]

**Remark 7.** \(b_{h,\delta}(x), s_{h,\delta}(x)\) and \(\eta_{h,\delta}(x)\) depend on \(x\) because \(\sigma\) depends on \(\Psi_{t,h}\), which further depends on the sample points in the neighborhood \(B_h^C(x; \mathcal{X})\) of \(x\).

In the rest of the paper we define \(b_{h,\delta}(x) := (b^2/\sigma)M^{d^k}\alpha\) and \(s_{h,\delta}(x) := b \sqrt{5D \ln(1/\delta)/\sigma m}\) as the bias and standard deviation terms in the error of \(\hat{f}_h(x)\), respectively. We also denote \(\eta_{h,\delta}(x) := b_{h,\delta}(x) + s_{h,\delta}(x)\) as the overall error in \(\hat{f}_h(x)\).

Notice that when bandwidth \(h\) increases, the bias term \(b_{h,\delta}(x)\) is likely to increase too because of the \(h^\alpha\) term; on the other hand, with \(h\) increasing the local neighborhood \(B_h^C(x; \mathcal{X})\) enlarges and would potentially contain more samples, implying a larger \(m\) and smaller standard deviation term \(s_{h,\delta}(x)\). A careful selection of bandwidth \(h\) balances \(b_{h,\delta}(x)\) and \(s_{h,\delta}(x)\) and yields appropriate confidence intervals on \(f(x)\), a topic that is addressed in the next section.

### 4.2 Bandwidth Selection and Confidence Intervals

Given the expressions of bias \(b_{h,\delta}(x)\) and standard deviation \(s_{h,\delta}(x)\) in Eq. (17), the bandwidth \(h_t(x) > 0\) at epoch \(t\) and point \(x\) is selected as

\[
h_t(x) := \frac{j_t(x)}{n^2} \quad \text{where} \quad j_t(x) := \arg\max\left\{j \in \mathbb{N}, j \leq n^2 : b_{j/n^2,\delta}(x) \leq s_{j/n^2,\delta}(x)\right\}.
\]
More specifically, $h_t(x)$ is the largest positive value in an evenly spaced grid $\{j/n^2\}$ such that the bias of $\tilde{f}_t(x)$ is smaller than its standard deviation. Such bandwidth selection is in principle similar to the Lepski’s method [33], with the exception that an upper bound on the bias for any bandwidth parameter is known and does not need to be estimated from data.

With the selection of bandwidth $h_t(x)$ at epoch $t$ and query point $x$, a confidence interval on $f(x)$ is constructed as

$$
\ell_t(x) := \max_{1 \leq t' \leq t} \left\{ \tilde{f}_{t'}(x) - \eta_{t', \delta}(x) \right\} \quad \text{and} \quad u_t(x) := \min_{1 \leq t' \leq t} \left\{ \tilde{f}_{t'}(x) + \eta_{t', \delta}(x) \right\}.
$$

Note that for any $x \in \mathcal{X}$, the lower confidence edge $\ell_t(x)$ is a non-decreasing function in $t$ and the upper confidence edge $u_t(x)$ is a non-increasing function in $t$.

### 4.3 Pre-screening

We describe a pre-screening procedure that relaxes the smoothness condition from $\kappa = \infty$ to $\kappa = \Omega(1)$, meaning that only local smoothness of $f$ around its minimum values is required. Let $n_0 = \lfloor n/\log n \rfloor$, $x_1, \ldots, x_{n_0}$ be points i.i.d. uniformly sampled from $\mathcal{X}$ and $y_1, \ldots, y_{n_0}$ be their corresponding responses. For every grid point $x \in G_n$, perform the following:

1. Compute $\bar{f}(x)$ as the average of all $y_i$ such that $\|x_i - x\|_\infty \leq n_0^{-1/2d} \log^3 n =: h_0$;

2. Remove all $x \in G_n$ from $S_0$ if $\bar{f}(x) = \min_{z \in G_n} \bar{f}(z) + 1/ \log n$.

Remark 8. The $1/ \log n$ term in removal condition $\bar{f}(x) = \min_{z \in G_n} \bar{f}(z) + 1/ \log n$ is not important, and can be replaced with any sequence $\{\omega_n\}$ such that $\lim_{n \to \infty} \omega_n = 0$ and $\lim_{n \to \infty} \omega_n n^t = \infty$ for any $t > 0$. The readers are referred to the proof of Proposition 5 in the appendix for the motivation of this term as well as the selection of the pre-screening bandwidth $h_0$.

At a high level, the pre-screening step computes local averages of $y$ and remove grid points in $S_0 = G_n$ whose estimated values are larger than the minimum in $G_n$.

To analyze the pre-screening step, we state the following proposition:

**Proposition 5.** Assume $f \in \Sigma_\kappa^\alpha(M)$ and let $S'_0$ be the screened grid after step 2 of the pre-screening procedure. Then for sufficiently large $n$, with probability $1 - O(n^{-1})$ we have

$$
\min_{x \in S'_0} f(x) = \min_{x \in G_n} f(x) \quad \text{and} \quad S'_0 \subseteq \bigcup_{x \in L_f(\kappa/2)} B^\infty_{h_0}(x; \mathcal{X}),
$$

where $L_f(\kappa/2) = \{x \in \mathcal{X} : f(x) \leq f^* + \kappa/2\}$.

To interpret Proposition 5, note that for sufficiently large $n$, $f \in \Sigma_\kappa^\alpha(M)$ implies $f$ being $\alpha$-Hölder smooth (i.e., $f$ satisfies Eq. (6)) on $\bigcup_{x \in L_f(\kappa/2)} B^\infty_{h_0}(x; \mathcal{X})$, because $\kappa > 0$ is a constant and $h_0 \to 0$ as $n \to \infty$. Subsequently, the proposition shows that with high probability, the pre-screening step will remove all grid points in $G_n$ in non-smooth regions of $f$, while maintaining the global optimal solution. This justifies the pre-processing step for $f \in \Sigma_\kappa^\alpha(M)$, because $f$ is smooth on the grid after pre-processing.

The proof of Proposition 5 uses the fact that the local mean estimation is large provided that all data points in the local mean estimator are large, regardless of their underlying smoothness. The complete proof of Proposition 5 is deferred to the appendix.
5 Proofs of main theorems

5.1 Proof of Lemma 1

Our proof closely follows the analysis of asymptotic convergence rates for series estimators in the seminal work of [40]. We further work out all constants in the error bounds to arrive at a completely finite-sample result, which is then used to construct finite-sample confidence intervals.

We start with polynomial interpolation results for all Hölder smooth functions in \( B^\alpha_h(x; \mathcal{X}) \).

**Lemma 2.** Suppose \( f \) satisfies Eq. (6) on \( B^\alpha_h(x; \mathcal{X}) \). Then there exists \( \tilde{f}_x \in \mathcal{P}_k \) such that

\[
\sup_{z \in B^\alpha_h(x; \mathcal{X})} |f(z) - \tilde{f}_x(z)| \leq Md^k h^\alpha. \tag{21}
\]

**Proof.** Consider

\[
\tilde{f}_x(z) := f(x) + \sum_{j=1}^k \sum_{\alpha_1 + \ldots + \alpha_d = j} \frac{\partial^j f(x)}{\partial x_1^{\alpha_1} \ldots \partial x_d^{\alpha_d}} \prod_{\ell=1}^d (z_\ell - x_\ell)^{\alpha_\ell}. \tag{22}
\]

By Taylor expansion with Lagrangian remainders, there exists \( \xi \in (0, 1) \) such that

\[
|\tilde{f}_x(z) - f(x)| \leq \sum_{\alpha_1 + \ldots + \alpha_d = k} |f^{(\alpha)}(x + \xi(z - x)) - f^{(\alpha)}(x)| \cdot \prod_{\ell=1}^d |z_\ell - x_\ell|^\alpha_\ell. \tag{23}
\]

Because \( f \) satisfies Eq. (6) on \( B^\alpha_h(x; \mathcal{X}) \), we have that \( |f^{(\alpha)}(x + \xi(z - x)) - f^{(\alpha)}(x)| \leq M \cdot \|z - x\|_\infty^\alpha - k \).

Also note that \( |z_\ell - x_\ell| \leq \|z - x\|_\infty \leq h \) for all \( z \in B^\alpha_h(x; \mathcal{X}) \). The lemma is thus proved.

Using Eq. (16), the local polynomial estimate \( \hat{f}_h \) can be written as \( \hat{f}_h(z) = \psi_{x,h}(z)^\top \hat{\theta}_h \), where

\[
\hat{\theta}_h = (\Psi_{t,h}^\top \psi_{t,h})^{-1} \Psi_{t,h}^\top Y_{t,h}. \tag{24}
\]

In addition, because \( \tilde{f}_x \in \mathcal{P}_h \), there exists \( \hat{\theta} \in \mathbb{R}^D \) such that \( \tilde{f}_x(z) = \psi_{x,h}(z)^\top \hat{\theta} \). Denote also that \( F_{t,h} := (f(x_{t'})_{1 \leq t' \leq t, x_{t'} \in B^\alpha_h(x)} \) and \( W_{t,h} := (w_{t'})_{1 \leq t' \leq t, x_{t'} \in B^\alpha_h(x)} \), Eq. (24) can then be re-formulated as

\[
\hat{\theta}_h = (\Psi_{t,h}^\top \psi_{t,h})^{-1} \Psi_{t,h}^\top \hat{\theta} + \Delta_{t,h} + W_{t,h}. \tag{25}
\]

Because \( \frac{1}{m} \Psi_{t,h}^\top \psi_{t,h} \geq \sigma I_{D \times D} \) and sup \( \psi_{x,h}(z) \|_2 \leq b \), we have that

\[
\|\hat{\theta}_h - \tilde{\theta}\|_2 \leq \frac{b}{\sigma} \|\Delta_{t,h}\|_\infty + \left\| \frac{1}{m} \Psi_{t,h}^\top \psi_{t,h}^{-1} \frac{1}{m} \Psi_{t,h}^\top W_t \right\|_2. \tag{27}
\]

Invoking Lemma 2 we have \( \|\Delta_{t,h}\|_\infty \leq Md^k h^\alpha \). In addition, because \( W_t \sim N_m(0, I_m \times n) \), we have that

\[
\left[ \frac{1}{m} \Psi_{t,h}^\top \psi_{t,h} \right]^{-1} \frac{1}{m} \Psi_{t,h}^\top W_t \sim N_D \left( 0, \frac{1}{m} \left[ \frac{1}{m} \Psi_{t,h}^\top \psi_{t,h} \right]^{-1} \right). \tag{28}
\]
Applying concentration inequalities for quadratic forms of Gaussian random vectors (Lemma 11), with probability $1 - \delta$ it holds that
\[
\left\| \frac{1}{m} \Psi_{t,h}^\top \Psi_{t,h} \right\|_2^{-1} \frac{1}{m} \Psi_{t,h}^\top W_t \leq \sqrt{\frac{5D \log(1/\delta)}{\sigma m}}. \tag{29}
\]

We then have that with probability $1 - \delta$ that
\[
\| \hat{\theta}_h - \tilde{\theta} \|_2 \leq \frac{b}{\sigma_h} Md^k h_i^\alpha + \sqrt{\frac{5D \log(1/\delta)}{\sigma m}}. \tag{30}
\]

Finally, noting that
\[
| \hat{f}_h(x) - f(x) | = | \hat{f}_h(x) - \bar{f}_x(x) | = | \psi(x)^\top (\hat{\theta}_h - \tilde{\theta}) | \leq b \| \hat{\theta}_h - \tilde{\theta} \|_2 \tag{31}
\]
we complete the proof of Lemma 1.

5.2 Proof of Theorem 1

In this section we prove Theorem 1. We prove the theorem by considering every reference function $f_0 \in \Sigma^3(\mathcal{X}) \cap \Theta_C$ separately. For simplicity, we assume $\kappa = \infty$ throughout the proof. The $0 < \kappa < \infty$ can be handled by replacing $\mathcal{X}$ with $S_0$ which is the grid after the pre-screening step described in Section 4.3. We also suppress dependency on $d, \alpha, M, C, p_0, \mathcal{P}_0$ in $O(\cdot), \Omega(\cdot), \Theta(\cdot), \gapprox, \lessapprox$ and $\approx$ notations. We further suppress logarithmic terms of $n$ in $\tilde{O}(\cdot)$ and $\tilde{\Omega}(\cdot)$ notations.

The following lemma is our main lemma, which shows that the active set $S_\tau$ in our proposed algorithm shrinks geometrically before it reaches a certain level. To simplify notations, denote $\tilde{c}_0 := 10c_0$ and (A2) then hold for all $\epsilon, \delta \in [0, \tilde{c}_0]$ for all $f_0 \in \Theta_C$.

Lemma 3. For $\tau = 1, \ldots, T$ define $\varepsilon_\tau := \max\{\tilde{c}_0 \cdot 2^{-\tau}, C_3[\epsilon_n^U(f_0) + n^{-1/2}] \log^2 n\}$, where $C_3 > 0$ is a constant depending only on $d, \alpha, M, p_0, \mathcal{P}_0$ and $C$. Then for sufficiently large $n$, with probability $1 - O(n^{-1})$ the following holds uniformly for all outer iterations $\tau = 1, \ldots, T$:
\[
S_{\tau} \subseteq L_f(\varepsilon_\tau). \tag{32}
\]

Lemma 3 shows that the level $\varepsilon_\tau$ in $L_f(\varepsilon_\tau)$ that contains $S_{\tau-1}$ shrinks geometrically, until the condition $\varepsilon_\tau \geq C_3[\epsilon_n^U(f_0) + n^{-1/2}] \log^2 n$ is violated. If the condition is never violated, then at the end of the last epoch $\tau^*$ we have $\varepsilon_{\tau^*} = O(n^{-1})$ because $\tau^* = \log n$, in which case Theorem 1 clearly holds. On the other hand, because $S_{\tau} \subseteq S_{\tau-1}$ always holds, we have $\varepsilon_{\tau^*} \leq [\epsilon_n^U(f_0) + n^{-1/2}] \log^2 n$ which justifies the convergence rate in Theorem 1.

In the rest of this section we prove Lemma 3. We need several technical lemmas and propositions. Except for Proposition 6 that is straightforward, the proofs of the other technical lemmas are deferred to the end of this section.

We first show that the grid $G_n$ is sufficiently dense for approximate optimization purposes. Define $x_n^* := \operatorname{argmin}_{x \in G_n} f(x)$ and $f_n^* := f(x_n^*)$. We have the following lemma:

Lemma 4. Suppose (B1) and (B2) hold. Then with probability $1 - O(n^{-1})$ the following holds:

1. $\sup_{x \in \mathcal{X}} \min_{x' \in G_n} \| x - x' \|_\infty = \tilde{O}(n^{-3/\min(\alpha, 1)})$;
2. $f_n^* - f^* = \tilde{O}(n^{-3})$. 

15
The next proposition shows that with high probability, the confidence intervals constructed in the algorithm are truthful and the successive rejection procedure will never exclude the true optimizer of $f$ on $G_n$.

**Proposition 6.** Suppose $\delta = 1/n^4|G_n|$. Then with probability $1 - O(n^{-1})$ the following holds:

1. $f(x) \in [\ell_t(x), u_t(x)]$ for all $1 \leq t \leq n$ and $x \in G_n$;

2. $x^*_n \in S_\tau$ for all $0 \leq \tau \leq n$.

**Proof.** The first property is true by applying the union bound over all $t = 1, \ldots, n$ and $x \in G_n$. The second property then follows, because $\ell_t(x^*_n) \leq f_n^*$ and $\min_{x \in S_{\tau-1}} u_t(x) \geq f_n^*$ for all $\tau$. \qed

The following lemma shows that every small box centered around a certain sample point $x \in G_n$ contains a sufficient number of sample points whose least eigenvalue can be bounded with high probability under the polynomial mapping $\psi_{x,h}$ defined in Section 3.2.

**Lemma 5.** For any $x \in G_n$, $1 \leq m \leq n$ and $h > 0$, let $K_{h,m}^1(x), \ldots, K_{h,m}^n(x)$ be $n$ independent point sets, where each point set consists of $m$ points sampled i.i.d. uniformly at random from $B_h^n(x; G_n) = G_n \cap B_h^n(x)$. With probability $1 - O(n^{-1})$ the following holds true uniformly for all $x \in G_n$.

1. $\sup_{h > 0} \sup_{x \in B_h^n(x)} \|\psi_{x,h}(z)\|_2 \approx \Theta(1)$;

2. $|B_h^n(x; G_n)| \approx h^d|G_n|$;

3. $\sigma_{\min}(K_{h,m}^\ell(x)) \approx \Theta(1)$ for all $m \geq \Omega(\log^2 n)$ and $m \leq |G_n|$, where $\sigma_{\min}(K_{h,m}^\ell(x))$ is the least eigenvalue of $\frac{1}{m} \sum_{z \in K_{h,m}^\ell(x)} \psi_{x,h}(z)\psi_{x,h}(z)^\top$.

**Remark 9.** It is possible to improve the concentration result in Eq. (51) using the strategies adopted in [14] based on sharper Bernstein type concentration inequalities. Such improvements are, however, not important in establishing the main results of this paper.

The next lemma shows that, the bandwidth $h_\tau$ selected at the end of each outer iteration $\tau$ is near-optimal, being sandwiched between two quantities determined by the size of the active sample grid $S_{\tau-1} := S_{\tau-1}(P_{\tau-1})$.

**Lemma 6.** There exist constants $C_1, C_2 > 0$ depending only on $d, \alpha, M, p, \underline{p}_0$ and $C$ such that with probability $1 - O(n^{-1})$, the following holds for every outer iteration $\tau \in \{1, \ldots, T\}$ and all $x \in S_{\tau-1}$:

$$C_1 [\tilde{U}_{\tau-1} \tilde{p}_0]^{-1/(2\alpha + d)} - \tau/n \leq h_\tau(x) \leq C_2 [\tilde{U}_{\tau-1} \tilde{p}_0]^{-1/(2\alpha + d)} \log n + \tau/n,$$

where $\tilde{U}_{\tau-1} := |G_n|/|\tilde{S}_{\tau-1}|$.

We are now ready to state the proof of Lemma 3, which is based on an inductive argument over the epochs $\tau = 1, \ldots, T$.

**Proof.** We use induction to prove this lemma. For the base case $\tau = 1$, because $\|f - f_0\|_\infty \leq \varepsilon_n^U(f_0)$ and $\varepsilon_n^U(f_0) \to 0$ as $n \to \infty$, it suffices to prove that $S_1 \subseteq L_{f_0}(\tilde{c}_0/4)$ for sufficiently large $n$. Because $\tilde{S}_0 = S_0 = G_n$, invoking Lemmas 6 and 1 we have that $|\ell_t(x) - \ell_t(x)| = \tilde{O}(n^{-\alpha/2(2\alpha + d)})$ for all $x \in G_n$ with high probability at the end of the first outer iteration $\tau = 1$. Therefore, for sufficiently large $n$ we conclude that $\sup_{x \in G_n} |\ell_t(x) - \ell_t(x)| \leq c_0/8$ and hence $S_1 \subseteq L_{f_0}(\tilde{c}_0/4)$. 

16
We now prove the lemma for $\tau \geq 2$, assuming it holds for $\tau - 1$. We also assume that $n$ (and hence $n_0$) is sufficiently large, such that the maximum CI length $\max_{x \in G} |u_t(x) - \ell_t(x)|$ after the first outer iteration $\tau - 1$ is smaller than $c_0$, where $c_0$ is a constant such that

Because $\|f - f_0\|_\infty \leq \epsilon_n(f_0)$ and $\epsilon_{\tau - 1} \geq C_3 \epsilon_n(f_0) \log^2 n$, for appropriately chosen constant $C_3$ that is not too small, we have that $\|f - f_0\|_\infty \leq \epsilon_{\tau - 1}$. By the inductive hypothesis we have

$$S_{\tau - 1} \subseteq L_f(\epsilon_{\tau - 1}) \subseteq L_{f_0}(\epsilon_{\tau - 1} + \|f - f_0\|_\infty) \subseteq L_{f_0}(2\epsilon_{\tau - 1}).$$  \hspace{1cm} (34)

Subsequently, denoting $\rho^*_\tau := \max_{x \in S_{\tau - 1}} \theta_{\tau - 1}(x)$ we have

$$\tilde{S}_{\tau - 1} = S_{\tau - 1}^0 \subseteq L_{f_0}^0(2\epsilon_{\tau - 1}, \rho^*_\tau).$$  \hspace{1cm} (35)

Let $\bigcup_{x \in H_n} B^2_{\rho^*_\tau}(x)$ be the smallest covering set of $L_{f_0}(2\epsilon_{\tau - 1})$, meaning that $L_{f_0}(2\epsilon_{\tau - 1}) \subseteq \bigcup_{x \in H_n} B^2_{\rho^*_\tau}(x)$, where $B^2_{\rho^*_\tau}(x) = \{z \in \mathcal{X} : \|z - x\|_2 \leq \rho^*_\tau\}$ is the $\ell_2$ ball of radius $\rho^*_\tau$ centered at $x$. By (A2), we know that $|H_n| \leq 1 + [\rho^*_\tau]^{-d} \mu f_0(2\epsilon_{\tau - 1})$. In addition, the enlarged level set satisfies $L_{f_0}^0(2\epsilon_{\tau - 1}, \rho^*_\tau) \subseteq \bigcup_{x \in H_n} B^2_{\rho^*_\tau}(x)$. Subsequently,

$$\mu_{f_0}^0(2\epsilon_{\tau - 1}, \rho^*_\tau) \leq |H_n| \cdot [\rho^*_\tau]^{-d} \mu f_0(2\epsilon_{\tau - 1}) + [\rho^*_\tau]^{-d}. \hspace{1cm} (36)$$

By Lemma 6, the monotonicity of $|\tilde{S}_{\tau - 1}|$ and the fact that $p_{n_0} \leq p_X(z) \leq p_0$ for all $z \in \mathcal{X}$, we have

$$\rho^*_\tau \leq \left[ \mu_{f_0}^0(2\epsilon_{\tau - 1}) \right]^{1/(2a+d)} n_0^{-1/(2a+d)} \log n \hspace{1cm} (37)$$

$$\leq \left[ \mu_{f_0}(2\epsilon_{\tau - 1}) \right]^{1/(2a+d)} n_0^{-1/(2a+d)} \log n \hspace{1cm} (38)$$

$$\leq \left( \mu f_0(2\epsilon_{\tau - 1}) + [\rho^*_\tau]^{-d} \right)^{1/(2a+d)} n_0^{-1/(2a+d)} \log n. \hspace{1cm} (39)$$

Re-arranging terms on both sides of Eq. (39) we have

$$\rho^*_\tau \leq \max \left\{ \left[ \mu f_0(2\epsilon_{\tau - 1}) \right]^{1/(2a+d)} n_0^{-1/(2a+d)} \log n, \ n_0^{1/(2a)} \log n \right\}. \hspace{1cm} (40)$$

On the other hand, according to the selection procedure of the bandwidth $h_t(x)$, we have that $\eta_{t}(x, \delta)(x) \leq b_{t}(x, \delta)(x)$. Invoking Lemma 6 we have for all $x \in S_{\tau - 1}$ that

$$\eta_{h_t(x, \delta)}(x) \leq b_{h_t(x, \delta)}(x) \leq [h_t(x)]^\alpha \hspace{1cm} (41)$$

$$\leq [\tilde{\nu}_{\tau - 1} n_0]^{-\alpha/(2a+d)} \log n \hspace{1cm} (42)$$

$$\leq [\tilde{\nu}_{\tau - 2} n_0]^{-\alpha/(2a+d)} \log n \hspace{1cm} (43)$$

$$\leq [\rho^*_\tau]^{-\alpha} \log n. \hspace{1cm} (44)$$

Here Eq. (42) holds by invoking the upper bound on $h_t(x)$ in Lemma 6, Eq. (43) holds because $\tilde{\nu}_{\tau - 1} \geq \tilde{\nu}_{\tau - 2}$, and Eq. (44) holds by again invoking the lower bound on $\rho_{\tau - 1}(x)$ in Lemma 6. Combining Eqs. (40,44) we have

$$\max_{x \in S_{\tau - 1}} \eta_{h_t(x, \delta)}(x) \leq \max \left\{ \left[ \mu f_0(2\epsilon_{\tau - 1}) \right]^{\alpha/(2a+d)} n_0^{-\alpha/(2a+d)} \log^2 n, \ n_0^{-\frac{\alpha}{2a}} \log n \right\}. \hspace{1cm} (45)$$

Recall that $n_0 = n/\log n$ and $\epsilon_n(f_0) \leq \epsilon_{\tau - 1}$, provided that $C_3$ is not too small. By definition, every $\epsilon \geq \epsilon_n(f_0)$ satisfies $\epsilon^{-(2a+d/\alpha)} \mu f_0(\epsilon) \leq n/\log^2 n$ for some large constant $\omega > 5 + d/\alpha$. Subsequently,

$$\left[ \mu f_0(2\epsilon_{\tau - 1}) \right]^{\alpha/(2a+d)} n_0^{-\alpha/(2a+d)} \log^2 n \leq 2\epsilon_{\tau - 1} n^{\alpha/(2a+d)} \log^{-\omega n} n \cdot n_0^{-\alpha/(2a+d)} \log^2 n \hspace{1cm} (46)$$
is thus proved.

Because \( \omega > 5 + d/\alpha \), the right-hand side of Eq. (47) is asymptotically dominated \(^6\) by \( \varepsilon_{\tau - 1} \). In addition, \( n_0^{-1/2} \log n \) is also asymptotically dominated by \( \varepsilon_{\tau - 1} \) because \( \varepsilon_{\tau - 1} \geq C_3 n^{-1/2} \log^2 n \). Therefore, for sufficiently large \( n \) we have

\[
\max_{x \in S_{\tau - 1}} \eta_{h_{\tau}}(x, \delta) (x) \leq \varepsilon_{\tau - 1}/4.
\] (48)

Lemma 3 is thus proved.

5.2.1 Proof of Lemma 4

Proof. Let \( H_N \subseteq \mathcal{X} \) be the finite subset of \( \mathcal{X} \) such that \( |H_N| = N \) and \( \sup_{x \in \mathcal{X}} \min_{x' \in H_n} \| x - x' \|_\infty \) is maximized. By standard results of metric entropy number of the \( d \)-dimensional unit box (see for example, \([50, \text{Lemma 2.2}]\)), we have that \( \sup_{x \in \mathcal{X}} \min_{x' \in H_n} \| x - x' \|_\infty \leq N^{-1/d} \).

For any \( x \in H_n \), consider an \( \ell_\infty \) ball \( B_{r_n}^\infty (x) \) or radius \( r_n \) centered at \( x \), with \( r_n \) to be specified later. Because the density of \( P_{\mathcal{X}} \) is uniformly bounded away from below on \( \mathcal{X} \), we have that \( P_{\mathcal{X}} (x \in B_{r_n}^\infty (x)) \geq r_n^d \). Therefore, applying union bound over all \( x \in H_n \) we have that

\[
P_{\mathcal{X}} \left( \exists x \in H_N, G_n \cap B_{r_n}^\infty (x) = \emptyset \right) \leq N (1 - r_n^d)^{|G_n|} \leq \exp \left\{ -r_n^d |G_n| + \log N \right\}.
\] (49)

Set \( N = |G_n| \) and \( r_n \asymp n^{-3/\min(\alpha,1)} \log n \). The right-hand side of the above inequality is then upper bounded by \( O(1/n^2) \), thanks to the assumption (A1) and that \( |G_n| \asymp n^{3d/\min(\alpha,1)} \). The first property is then proved by noting that

\[
\sup_{x \in \mathcal{X}} \min_{x' \in G_n} \| x - x' \|_\infty \leq \sup_{x \in \mathcal{X}} \min_{x' \in H_n} \| x - x' \|_\infty + \max_{x \in H_n} \min_{x' \in G_n} \| x - x' \|_\infty.
\] (50)

To prove the second property, note that for any \( x, x' \in \mathcal{X} \), \( |f(x) - f(x')| \leq M \cdot \| x - x' \|_\infty^{\min(\alpha,1)} \). The first property then implies that \( f_n^* - f^* = \tilde{O}(n^{-3}) \).

5.2.2 Proof of Lemma 5

Proof. We first show that the first property holds almost surely. Recall the definition of \( \psi_{x,h} \), we have that \( 1 \leq \| \psi_{x,h}(z) \|_2 \leq D \cdot \max_{1 \leq j \leq d} h^{-1} |z_j - x_j| \). Because \( \| z - x \|_\infty \leq h \) for all \( z \in B_{r_n}^\infty (x) \),

\[
\sup_{x \in B_{r_n}^\infty (x)} \| \psi_{x,h}(z) \|_2 \leq O(1) \text{ for all } h > 0.
\]

Thus, \( \sup_{h \geq 0} \sup_{x \in B_{r_n}^\infty (x)} \| \psi_{x,h}(z) \|_2 \leq \Theta(1) \text{ for all } x \in G_n \).

For the second property, by Hoeffding’s inequality (Lemma 10) and the union bound, with probability 1 \(- O(n^{-1}) \) we have that

\[
\max_{x,h} \left| \frac{B_{r_n}^\infty (x; G_n)}{|G_n|} - P_X (z \in B_{r_n}^\infty (x)) \right| \leq \sqrt{\frac{\log n}{|G_n|}}.
\] (51)

In addition, note that \( P_X (z \in B_{r_n}^\infty (x; \mathcal{X})) \geq p_{\lambda} (B_{r_n}^\infty (x; \mathcal{X})) \geq h^d \) and \( P_X (z \in B_{r_n}^\infty (x; \mathcal{X})) \leq \tau_0 \lambda (B_{r_n}^\infty (x; \mathcal{X})) \leq h^d \), where \( \lambda (\cdot) \) denotes the Lebesgue measure on \( \mathcal{X} \). Subsequently, \( |B_{r_n}^\infty (x; G_n)| \) is lower bounded by \( \Omega(h^d |G_n| - \sqrt{|G_n| \log n}) \) and upper bounded by \( O(h^d |G_n| + \sqrt{|G_n| \log n}) \). The second property is then proved by noting that \( h_d \asymp n^{-d} \) and \( |G_n| \asymp n^{3d/\min(\alpha,1)} \).

\(^6\)We say \( \{a_n\} \) is asymptotically dominated by \( \{b_n\} \) if \( \lim_{n \to \infty} |a_n|/|b_n| = 0 \).
We next prove the third property. Because $p_0 \leq p_X(z) \in \overline{p}_0$ for all $z \in \mathcal{X}$, we have that

$$P_0 \int_{B_h^\mathcal{X}(x;\mathcal{X})} \psi_{x,h}(z)\psi_{x,h}(z)^T dU_{x,h}(z) \leq \mathbb{E} \left[ \frac{1}{m} \sum_{z \in K_{h,m}^\ell} \psi_{x,h}(z)\psi_{x,h}(z)^T \right] \leq \overline{p}_0 \int_{B_h^\mathcal{X}(x;\mathcal{X})} \psi_{x,h}(z)\psi_{x,h}(z)^T dU_{x,h}(z),$$

(52)

where $U_{x,h}$ is the uniform distribution on $B_h^\mathcal{X}(x;\mathcal{X})$. Note also that

$$\int_{\mathcal{X}} \psi_{0,1}(z)\psi_{0,1}(z)^T dU(z) \leq \int_{B_h^\mathcal{X}(x;\mathcal{X})} \psi_{x,h}(z)\psi_{x,h}(z)^T dU_{x,h}(z) \leq 2^d \int_{\mathcal{X}} \psi_{0,1}(z)\psi_{0,1}(z)^T dU(z)$$

(53)

where $U$ is the uniform distribution on $\mathcal{X} = [0,1]^d$. The following proposition upper and lower bounds the eigenvalues of $\int_{\mathcal{X}} \psi_{0,1}(z)\psi_{0,1}(z)^T dU(z)$, which is proved in the appendix.

**Proposition 7.** There exist constants $0 < \psi_0 \leq \Psi_0 < \infty$ depending only on $d, D$ such that

$$\psi_0 I_{D \times D} \leq \int_{\mathcal{X}} \psi_{0,1}(z)\psi_{0,1}(z)^T dU(z) \leq \Psi_0 I_{D \times D}.$$  

(56)

Using Proposition 7 and Eqs. (54,55), we conclude that

$$\Omega(1) \cdot I_{D \times D} \leq \mathbb{E} \left[ \frac{1}{m} \sum_{z \in K_{h,m}^\ell} \psi_{x,h}(z)\psi_{x,h}(z)^T \right] \leq O(1) \cdot I_{D \times D}.  $$

(57)

Applying matrix Chernoff bound (Lemma 12) and the union bound, we have that with probability $1 - O(n^{-1}),$

$$\max_{x,h,m,\ell} \left\| \frac{1}{m} \sum_{z \in K_{h,m}^\ell(x)} \psi_{x,h}(z)\psi_{x,h}(z)^T - \mathbb{E} \left[ \psi_{x,h}(z)\psi_{x,h}(z)^T \right]_{z \in B_h(x)} \right\|_{\text{op}} \leq \sqrt{\frac{\log n}{m}}.$$  

(58)

Combining Eqs. (57,58) and applying Weyl’s inequality (Lemma 13) we have

$$\Omega(1) - O(\sqrt{\log n/m}) \leq \sigma_{\text{min}}(K_{h,m}^\ell(x)) \leq O(1) - O(\sqrt{\log n/m}).$$

(59)

The third property is therefore proved.

\[\Box\]

5.2.3 Proof of Lemma 6

**Proof.** We use induction to prove this lemma. For the base case of $\tau = 1$, we have $\tilde{S}_0 = S_0 = G_n$ and therefore $\tilde{V}_{\tau-1} = 1$. Furthermore, applying Lemma 5 we have that for all $h = \tilde{j}/n^2$,

$$b_{h,\delta}(x) \approx h^\alpha \quad \text{and} \quad s_{h,\delta}(x) \approx \frac{\log n}{h^2 n_0}.$$  

(60)

19
Thus, for $h$ selected according to Eq. (18) as the largest bandwidth of the form $j/n^2$, $j \in \mathbb{N}$ such that $b_{h,\delta}(x) \leq s_{h,\delta}(x)$, both $b_{h,\delta}(x)$, $s_{h,\delta}(x)$ are on the order of $n_0^{-1/(2\alpha+d)}$ up to logarithmic terms of $n$, and therefore one can pick appropriate constants $C_1, C_2 > 0$ such that $C_1n_0^{-1/(2\alpha+d)} \leq g_1(x) \leq C_2n_0^{-1/(2\alpha+d)} \log n$ holds for all $x \in G_n$. We next prove the lemma for $\tau > 1$, assuming it holds for $\tau - 1$. We first establish the lower bound part. Define $\rho_{\tau-1}^\ast := \min_{z \in S_{\tau-1}} \vartheta_{\tau-1}(z)$. By inductive hypothesis, $\rho_{\tau-1}^\ast \geq C_1[\tilde{\nu}_{\tau-2}n_0]^{-1/(2\alpha+d)} - (\tau - 1)/n$. Note also that $\tilde{\nu}_{\tau-1} \geq \tilde{\nu}_{\tau-2}$ because $S_{\tau-1} \subseteq S_{\tau-2}$, which holds because $S_{\tau-1} \subseteq S_{\tau-2}$ and $\vartheta_{\tau-2}(z) \leq \vartheta_{\tau-1}(z)$ for all $z$. Let $h_t^\ast$ be the smallest number of the form $j_t^\ast/n^2$, $j_t^\ast \in [n^2]$ such that $h_t^\ast \geq C_1[\tilde{\nu}_{\tau-1}n_0]^{-1/(2\alpha+d)} - \tau/n$. We then have $h_t^\ast \leq \rho_{\tau-1}^\ast$ and therefore query points in epoch $\tau$ are uniformly distributed in $B_{h_t^\ast}^\infty(x; G_n)$. Subsequently, applying Lemma 5 we have with probability $1 - O(n^{-1})$ that

$$b_{h_t^\ast,\delta}(x) \leq C'[h_t^\ast]^\alpha \quad \text{and} \quad s_{h_t^\ast,\delta}(x) \geq C'' \sqrt{\frac{\log n}{[h_t^\ast]^2 \tilde{\nu}_{\tau-1}n}},$$

(61)

where $C', C'' \geq 0$ are constants that depend on $d, \alpha, M, p_{\min}, \bar{\nu}_0$ and $\mathcal{C}$, but not $C_1, C_2, \tau$ or $h_t^\ast$. By choosing $C_1$ appropriately (depending on $C'$ and $C''$) we can make $b_{h_t^\ast,\delta}(x) \leq s_{h_t^\ast,\delta}(x)$ holds for all $x \in S_{\tau-1}$, thus establishing $\vartheta_{\tau}(x) \geq \min\{\vartheta_{\tau-1}(x), h_t^\ast\} \geq C_1[\tilde{\nu}_{\tau-1}n_0]^{-1/(2\alpha+d)} - \tau/n$.

We next prove the upper bound part. For any $h_t = j_t/n^2$ where $j_t \in [n^2]$, invoking Lemma 5 we have that

$$b_{h_t,\delta}(x) \geq \tilde{C}' h_t^\alpha \quad \text{and} \quad s_{h_t,\delta}(x) \leq \tilde{C}'' \sqrt{\frac{\log n}{\min\{h_t, \rho_{\tau-1}^\ast\}^d \cdot \tilde{\nu}_{\tau-1}n}},$$

(62)

where $\tilde{C}'$ and $\tilde{C}''$ are again constants depending on $d, \alpha, M, p_{\min}, \bar{\nu}_0$ and $\mathcal{C}$, but not $C_1, C_2$. Note also that $\rho_{\tau-1}^\ast \geq C_1[\tilde{\nu}_{\tau-2}n_0]^{-1/(2\alpha+d)} - (\tau - 1)/n \geq C_1[\tilde{\nu}_{\tau-1}n_0]^{-1/(2\alpha+d)} - \tau/n$, because $\tilde{\nu}_{\tau-1} \geq \tilde{\nu}_{\tau-2}$. By selecting constant $C_2 > 0$ carefully (depending on $\tilde{C}', \tilde{C}''$ and $C_1$), we can ensure $b_{h_t,\delta}(x) > s_{h_t,\delta}(x)$ for all $h \geq C_2[\tilde{\nu}_{\tau-1}n_0]^{-1/(2\alpha+d)} + \tau/n$. Therefore, $\vartheta_{\tau}(x) \leq h_t(x) \leq C_2[\tilde{\nu}_{\tau-1}n_0]^{-1/(2\alpha+d)} + \tau/n$. □

5.3 Proof of Theorem 2

In this section we prove the main negative result in Theorem 2. To simplify presentation, we suppress dependency on $\alpha, d, c_0$ and $C_0$ in $\lesssim, \gtrsim, =, O(\cdot)$ and $\Omega(\cdot)$ notations. However, we do not suppress dependency on $\mathcal{C}_R$ or $M$ in any of the above notations.

Let $\varphi_0 : [-2, 2]^d \to \mathbb{R}^*$ be a non-negative function defined on $\mathcal{X}$ such that $\varphi_0 \in \Sigma^{[\alpha]}(1)$ with $\kappa = \infty$, $\sup_{x \in \mathcal{X}} \varphi_0(x) = \Omega(1)$ and $\varphi_0(z) = 0$ for all $\|z\|_2 \geq 1$. Here $[\alpha]$ denotes the smallest integer that upper bounds $\alpha$. Such functions exist and are the cornerstones of the construction of information-theoretic lower bounds in nonparametric estimation problems [13]. One typical example is the “smoothstep” function (see for example [19])

$$S_N(x) := \frac{1}{Z} x^{N+1} \sum_{n=0}^{N} \binom{N+n}{n} \left( \frac{2N+1}{N-n} \right)(-x)^n, \quad N = 0, 1, 2, \ldots$$

where $Z > 0$ is a scaling parameter. The smoothstep function $S_N$ is defined on $[0, 1]$ and satisfies the Hölder condition in Eq. (6) of order $\alpha = N$ on $[0, 1]$. It can be easily extended to $\tilde{S}_{N,d} : [-2, 2]^d \to \mathbb{R}$ by considering $\tilde{S}_{N,d}(x) := 1/Z - S_N(a \|x\|_1)$ where $\|x\|_1 = |x_1| + \ldots + |x_d|$ and $a = 1/(2d)$. It is
easy to verify that, with $Z$ chosen appropriately, $\tilde{S}_{N,d} \in \Sigma^N_\infty(1)$, sup$_{x \in \mathcal{X}} \tilde{S}_{N,d}(x) = 1/Z = \Omega(1)$ and $\tilde{S}_{N,d}(z) = 0$ for all $\|z\|_2 \geq 1$, where $M > 0$ is a constant.

For any $x \in \mathcal{X}$ and $h > 0$, define $\varphi_{x,h} : \mathcal{X} \to \mathbb{R}^n$ as

$$
\varphi_{x,h}(z) := \mathbb{I}[z \in B^\infty_h(x)] \cdot \frac{Mh^\alpha}{2} \varphi_0 \left( \frac{z-x}{h} \right). \tag{63}
$$

It is easy to verify that $\varphi_{x,h} \in \Sigma^\alpha_\infty(M/2)$, and furthermore sup$_{x \in \mathcal{X}} \varphi_{x,h}(z) = M h^\alpha$ and $\varphi_{x,h}(z) = 0$ for all $z \notin B^\infty_h(x)$.

Let $L_{f_0}(\varepsilon_n^L(f_0))$ be the level set of $f_0$ at $\varepsilon_n^L(f_0)$. Let $H_n \subseteq L_{f_0}(\varepsilon_n^L(f_0))$ be the largest packing set such that $B^\infty_h(x)$ are disjoint for all $x \in H_n$, and $\bigcup_{x \in H_n} B^\infty_h(x) \subseteq L_{f_0}(\varepsilon_n^L(f_0))$. By (A2') and the definition of $\varepsilon_n^L(f_0)$, we have that

$$
|H_n| \geq M(L_{f_0}(\varepsilon_n^L(f_0)); 2\sqrt{dh}) \geq \mu_{f_0}(\varepsilon_n^L(f_0)) \cdot h^{-d} \geq [\varepsilon_n^L(f_0)]^{2+\downarrow/\alpha} \cdot nh^{-d}. \tag{64}
$$

For any $x \in H_n$, construct $f_x : \mathcal{X} \to \mathbb{R}$ as

$$
f_x(z) := f_0(z) - \varphi_{x,h}(z). \tag{65}
$$

Let $\mathcal{F}_n := \{f_x : x \in H_n\}$ be the class of functions indexed by $x \in H_n$. Let also $h = (\varepsilon_n^L(f_0)/M)^{1/\alpha}$ such that $\|\varphi_{x,h}\|_\infty = 2\varepsilon_n^L(f_0)$. We then have that $\|f_x - f_0\|_\infty \leq 2\varepsilon_n^L(f_0)$ and $f_x \in \Sigma^\alpha_\infty(M)$, because $f_0, \varphi_{x,h} \in \Sigma^\alpha_\infty(M/2)$.

The next lemma shows that, with $n$ adaptive queries to the noisy zeroth-order oracle $y_t = f(x_t) + w_t$, it is information theoretically not possible to identify a certain $f_x$ in $\mathcal{F}_n$ with high probability.

**Lemma 7.** Suppose $|\mathcal{F}_n| \geq 2$. Let $\mathcal{A}_n = (\chi_1, \ldots, \chi_n, \phi_n)$ be an active optimization algorithm operating with a sample budget $n$, which consists of samplers $\chi_n = \{(x_i, y_i)\}_{i=1}^{\ell-1} \mapsto x_t$ and an estimator $\phi_n : \{(x_i, y_i)\}_{i=1}^{\ell-1} \mapsto \hat{f}_x \in \mathcal{F}_n$, both can be deterministic or randomized functions. Then

$$
\inf_{\mathcal{A}_n} \sup_{f_x \in \mathcal{F}_n} \Pr \left[ \hat{f}_x \neq f_x \right] \geq 1 - \sqrt{\frac{n \cdot \sup_{f_x \in \mathcal{F}_n} \|f_x - f_0\|_\infty^2}{2|\mathcal{F}_n|}}. \tag{66}
$$

**Lemma 8.** There exists constant $M > 0$ depending on $\alpha, d, c_0, C_0$ such that the right-hand side of Eq. (66) is lower bounded by $1/3$.

Lemmas 7 and 8 are proved at the end of this section. Combining both lemmas and noting that for any distinct $f_x, f_{x'} \in \mathcal{F}_n$ and $z \in \mathcal{X}$, max$\{\mathcal{L}(z; f_x), \mathcal{L}(z; f_{x'})\} \geq \varepsilon_n^L(f_0)$, we proved the minimax lower bound formulated in Theorem 2.

### 5.3.1 Proof of Lemma 7

Our proof is inspired by the negative result of multi-arm bandit pure exploration problems established in [7].

**Proof.** For any $x \in H_n$, define

$$
n_x := \mathbb{E}_{f_0} \left[ \sum_{i=1}^{n} \mathbb{I}[x \in B^\infty_h(x)] \right]. \tag{67}
$$
Because $B^*_h(x)$ are disjoint for $x \in H_n$, we have $\sum_{x \in H_n} n_x \leq n$. Also define, for every $x \in H_n$,

$$\varphi_x := \Pr_{f_0} \left[ \hat{f}_x = f_x \right].$$

Because $\sum_{x \in H_n} \varphi_x = 1$, by pigeonhole principle there is at most one $x \in H_n$ such that $\varphi_x > 1/2$. Let $x_1, x_2 \in H_n$ be the points that have the largest and second largest $n_x$. Then there exists $x \in \{x_1, x_2\}$ such that $\varphi_x \leq 1/2$ and $n_x \leq 2n/|H_n|$. By Le Cam’s and Pinsker’s inequality (see, for example, [49]) we have that

$$\Pr_{f_x} \left[ \hat{f}_x = f_x \right] \leq \Pr_{f_0} \left[ \hat{f}_x = f_x \right] + d_{TV}(P_{f_0}^{A_n} \| P_{f_x}^{A_n})$$

$$\leq \Pr_{f_0} \left[ \hat{f}_x = f_x \right] + \sqrt{\frac{1}{2} \text{KL}(P_{f_0}^{A_n} \| P_{f_x}^{A_n})}$$

$$= \varphi_x + \sqrt{\frac{1}{2} \text{KL}(P_{f_0}^{A_n} \| P_{f_x}^{A_n})}$$

$$\leq \frac{1}{2} + \sqrt{\frac{1}{2} \text{KL}(P_{f_0}^{A_n} \| P_{f_x}^{A_n})}.$$ 

It remains to upper bound KL divergence of the active queries made by $A_n$. Using the standard lower bound analysis for active learning algorithms [12, 13] and the fact that $f_x \equiv f_0$ on $\mathcal{X} \setminus B^*_h(x)$, we have

$$\text{KL}(P_{f_0}^{A_n} \| P_{f_x}^{A_n}) = \mathbb{E}_{f_0, A_n} \left[ \log P_{f_0, A_n}(x_{1:n}, y_{1:n}) \right]$$

$$= \mathbb{E}_{f_0, A_n} \left[ \log \prod_{i=1}^{n} P_{f_0}(y_i|x_i) P_{A_n}(x_{i-1:i+1}, y_{i-1:i+1}) \right]$$

$$= \mathbb{E}_{f_0, A_n} \left[ \log \prod_{i=1}^{n} P_{f_0}(y_i|x_i) P_{f_0}(y_i|x_i) \prod_{i=1}^{n} P_{f_0}(y_i|x_i) \right]$$

$$= \mathbb{E}_{f_0, A_n} \left[ \sum_{x_i \in B_h(x)} \log \frac{P_{f_0}(y_i|x_i)}{P_{f_x}(y_i|x_i)} \right]$$

$$\leq n_x \cdot \sup_{x \in B^*_h(x)} \text{KL}(P_{f_0}(\cdot | y) \| P_{f_x}(\cdot | y))$$

$$\leq n_x \cdot \| f_0 - f_x \|_{\infty}^2. \tag{78}$$

Therefore,

$$\Pr_{f_x} \left[ \hat{f}_x = f_x \right] \leq \frac{1}{2} + \sqrt{\frac{1}{4} n_x \varepsilon_n^2} \leq \frac{1}{2} + \sqrt{\frac{n \| f_x - f_0 \|_{\infty}^2}{2|\mathcal{F}_n|}}. \tag{79}$$

\[ \square \]

### 5.3.2 Proof of Lemma 8

**Proof.** By construction, $n \sup_{f_x \in \mathcal{F}_n} \| f_x - f_0 \|_{\infty}^2 \leq M^2 n h^{2\alpha}$ and $|\mathcal{F}_n| = |H_n| \geq \left(\mathcal{C}_e \varepsilon_n^4(f_0)\right)^{2+d/\alpha} n h^{-d}$.

Note also that $h = \left(\varepsilon/M\right)^{1/\alpha} \approx \left(\mathcal{C}_e \varepsilon_n^4(f_0)/M\right)^{1/\alpha}$ because $\| f_x - f_0 \|_{\infty} = \varepsilon = \mathcal{C}_e \varepsilon_n^4(f_0)$. Subsequently,

$$n \sup_{f_x \in \mathcal{F}_n} \| f_x - f_0 \|_{\infty}^2 \leq \frac{n \left[ \mathcal{C}_e \varepsilon_n^4(f_0) \right]^{2+d/\alpha}}{n \left[ \mathcal{C}_e \varepsilon_n^4(f_0) \right]^2} = M^{-d/\alpha}. \tag{80}$$

By choosing the constant $M > 0$ to be sufficiently large, the right-hand side of the above inequality is upper bounded by $1/36$. The lemma is thus proved. \[ \square \]
5.4 Proof of Theorem 3

The proof of Theorem 3 is similar to the proof of Theorem 2, but is much more standard by invoking the Fano’s inequality [49]. In particular, adapting the Fano’s inequality on any finite function class $\mathcal{F}_n$ constructed we have the following lemma:

**Lemma 9** (Fano’s inequality). Suppose $|\mathcal{F}_n| \geq 2$ and $(x_i, y_i)_{i=1}^n$ are i.i.d. random variables. Then

$$\inf_{f_x} \sup_{f_x \in \mathcal{F}_n} \Pr \left[ f_x \neq f_x \right] \geq 1 - \frac{\log 2 + n \cdot \sup_{f_x, f_y \in \mathcal{F}_n} \text{KL}(P_{f_x} \| P_{f_y})}{\log |\mathcal{F}_n|},$$

where $P_{f_x}$ denotes the distribution of $(x, y)$ under the law of $f_x$.

Let $\mathcal{F}_n$ be the function class constructed in the previous proof of Theorem 2, corresponding to the largest packing set $H_n$ of $L_{f_0}(\varphi_{\alpha})$ such that $B_h^\varphi(x)$ for all $x \in H_n$ are disjoint, where $h \asymp (\varphi_{\alpha})^{1/\alpha}$ such that $\|\varphi_{x,h}\|_{\mathcal{H}} = 2\varphi_{\alpha}h$ for all $x \in H_n$. Because $f_0$ satisfies (A2'), we have that $|\mathcal{F}_n| = |H_n| \gtrsim \mu_{f_0}(\varphi_{\alpha})h^{-d}$. Under the condition that $c_n^U(f_0) \leq \varphi_{\alpha}$, it holds that $\mu_{f_0}(\varphi_{\alpha}) \gtrsim [\varphi_{\alpha}]^{2+d/\alpha}n$. Therefore,

$$|\mathcal{F}_n| \gtrsim [\varphi_{\alpha}]^{2+d/\alpha} \cdot nh^{-d} \gtrsim [\varphi_{\alpha}]^{2} \cdot nM^{d/\alpha}.$$  \hspace{1cm} (82)

Because $\log(n/\varphi_{\alpha}^n) \gtrsim \log n$ and $M > 0$ is a constant, we have that $\log |\mathcal{F}_n| \gtrsim c \log n$ for all $n \gtrsim N$, where $c > 0$ is a constant depending only on $\alpha, d$ and $N \in \mathbb{N}$ is a constant depending on $M$.

Let $U$ be the uniform distribution on $\mathcal{X}$. Because $x \sim U$ and $f_x \equiv f_{x'}$ on $\mathcal{X}\backslash B_h^\varphi(x)$, we have that

$$\text{KL}(P_{f_x} \| P_{f_{x'}}) = \frac{1}{2} \int_{\mathcal{X}} |f_x(z) - f_{x'}(z)|^2 dU(z) \hspace{1cm} (83)$$

$$\leq \frac{1}{2} \Pr \left[ z \in B_h^\varphi(x) \right] \cdot \|f_x - f_{x'}\|_{\mathcal{H}}^2 \hspace{1cm} (84)$$

$$\leq \frac{1}{2} \lambda(B_h^\varphi(x)) \cdot [\varphi_{\alpha}]^2 \hspace{1cm} (85)$$

$$\leq h^d[\varphi_{\alpha}]^{2} \leq [\varphi_{\alpha}]^{2+d/\alpha} / M^{d/\alpha}. \hspace{1cm} (86)$$

By choosing $M$ to be sufficiently large, the right-hand side of Eq. (81) can be lower bounded by an absolute constant. The theorem is then proved following the same argument as in the proof of Theorem 2.

6 Conclusion

In this paper we consider the problem of noisy zeroth-order optimization of general smooth functions. Matching lower and upper bounds on the local minimax convergence rates are established, which are significantly different from classical minimax rates in nonparametric regression problems. Many interesting future directions exist along this line of research, including exploitation of additive structures in the underlying function $f$ to completely remove curse of dimensionality, functions with spatially heterogeneous smoothness or level set growth behaviors, and to design more computationally efficient algorithms that work well in practice.

A Some concentration inequalities

**Lemma 10** ([27]). Suppose $X_1, \ldots, X_n$ are i.i.d. random variables such that $a \leq X_i \leq b$ almost surely. Then for any $t > 0$,

$$\Pr \left[ \left\lvert \frac{1}{n} \sum_{i=1}^n X_i - \mathbb{E}X \right\rvert > t \right] \leq 2 \exp \left\{ -\frac{nt^2}{2(b-a)^2} \right\}.$$
Lemma 11 ([28]). Suppose \( x \sim \mathcal{N}_d(0, I_{d \times d}) \) and let \( A \) be a \( d \times d \) positive semi-definite matrix. Then for all \( t > 0 \),
\[
\Pr \left[ x^\top Ax > \text{tr}(A) + 2\sqrt{\text{tr}(A^2)}t + 2\|A\|_{\text{op}}t \right] \leq e^{-t}.
\]

Lemma 12 ([48], simplified). Suppose \( A_1, \ldots, A_n \) are i.i.d. positive semidefinite random matrices of dimension \( d \) and \( \|A_i\|_{\text{op}} \leq R \) almost surely. Then for any \( t > 0 \),
\[
\Pr \left[ \left\| \frac{1}{n} \sum_{i=1}^n A_i - \mathbb{E}A \right\|_{\text{op}} > t \right] \leq 2 \exp \left\{ -\frac{nt^2}{8R^2} \right\}.
\]

Lemma 13 (Weyl’s inequality). Let \( A \) and \( A + E \) be \( d \times d \) matrices with \( \sigma_1, \ldots, \sigma_d \) and \( \sigma'_1, \ldots, \sigma'_d \) be their singular values, sorted in descending order. Then \( \max_{1 \leq i \leq d} |\sigma_i - \sigma'_i| \leq \|E\|_{\text{op}} \).

### B Additional proofs

**Proof of Proposition 1.** Consider arbitrary \( x^* \in \mathcal{X} \) such that \( f(x^*) = \inf_{x \in \mathcal{X}} f(x) \). Then we have that \( \mathcal{L}(\hat{x}_n; f) = f(\hat{x}_n) - f(x^*) \leq [\hat{f}_n(\hat{x}_n) + \|\hat{f}_n - f\|_\infty] - [\hat{f}_n(x^*) - \|\hat{f}_n - f\|_\infty] \leq 2\|\hat{f}_n - f\|_\infty \), where the last inequality holds because \( \hat{f}_n(\hat{x}_n) \leq \hat{f}_n(x^*) \) by optimality of \( \hat{x}_n \).

**Proof of Example 2.** Because \( f_0 \in \Sigma_n^2(M) \) is strongly convex, there exists \( \sigma > 0 \) such that \( \nabla^2 f_0(x) \succeq \sigma I \) for all \( x \in \mathcal{X}_{f_0,\kappa} \), where \( \mathcal{X}_{f_0,\kappa} := L_{f_0}(\kappa) \) is the \( \kappa \)-level set of \( f_0 \). Let \( x^* = \arg \min_{x \in \mathcal{X}} f_0(x) \), which is unique because \( f_0 \) is strongly convex. The smoothness and strong convexity of \( f_0 \) implies that
\[
f_0^* + \frac{\sigma}{2}\|x - x^*\|_2^2 \leq f_0(x) \leq f_0^* + \frac{M}{2}\|x - x^*\|_2^2 \quad \forall x \in \mathcal{X}_{f_0,\kappa}.
\]

Subsequently, there exist constants \( c_0, C_1, C_2 > 0 \) depending only on \( \sigma, M, \kappa \) and \( d \) such that for all \( \epsilon \in (0, c_0] \),
\[
B_{C_1\sqrt{\epsilon}}^\infty(x^*; \mathcal{X}) \subseteq L_{f_0}(\epsilon) \subseteq B_{C_2\sqrt{\epsilon}}^\infty(x^*; \mathcal{X}).
\]

The property \( \mu_{f_0}(\epsilon) \leq e^{\beta} \) holds because \( \mu(L_{f_0}(\epsilon)) \geq \mu(B_{C_1\sqrt{\epsilon}}^\infty(x^*; \mathcal{X})) \geq e^{\beta/2} \). To prove (A2), note that \( N(L_{f_0}(\epsilon), \delta) \leq N(B_{C_2\sqrt{\epsilon}}^\infty(x^*; \mathcal{X}), \delta) \leq 1 + \left( \sqrt{\epsilon}/\delta \right)^d \). Because \( e^{\beta/2} \geq \mu(L_{f_0}(\epsilon)) = \mu_{f_0}(\epsilon) \), we conclude that \( N(L_{f_0}(\epsilon), \delta) \leq 1 + \delta^{-d}\mu_{f_0}(\epsilon) \) and (A2) is thus proved.

**Proof of Proposition 4.** Consider \( f_0 \equiv 0 \) if \( \beta = 0 \) and \( f_0(z) := a_0 \left( z_1^n + \ldots + z_d^n \right) \) for all \( z = (z_1, \ldots, z_d) \in [0, 1]^d \), where \( a_0 > 0 \) is a constant depending on \( \alpha, M \), and \( p = d/\beta \) for \( \beta \in (0, d/\alpha] \). The \( \beta = 0 \) case where \( f_0 \equiv 0 \) trivially holds. So we shall only consider the case of \( \beta \in (0, d/\alpha] \).

We first show \( f_0 \in \Sigma_n^\alpha(M) \) with \( \kappa = \infty \), provided that \( a_0 \) is sufficiently small. For any \( j \leq k = \lfloor \alpha \rfloor \) and \( \alpha_1 + \ldots + \alpha_d = j \), we have
\[
\frac{\partial^j}{\partial x_1^{\alpha_1} \ldots \partial x_d^{\alpha_d}} f_0(z) = \begin{cases} a_0 j! \cdot z_\ell^{n-j} & \text{if } \alpha_\ell = j, \ell \in [d]; \\ 0 & \text{otherwise}. \end{cases}
\]

(89)
Because $z_1, \ldots, z_d \in [0, 1]$ and $p = d/\beta \geq \alpha \geq j$, it’s clear that $0 \leq \partial^j f_0(z)/\partial x_1^{\alpha_1} \ldots \partial x_d^{\alpha_d} \leq a_0 j!$.

In addition, for any $z, z' \in [0, 1]^d$ and $\alpha_\ell = k, \ell \in [d]$, we have

$$\left| \frac{\partial^k}{\partial x_1^{\alpha_1} \ldots \partial x_d^{\alpha_d}} f_0(z) - \frac{\partial^k}{\partial x_1^{\alpha_1} \ldots \partial x_d^{\alpha_d}} f_0(z') \right| \leq a_0 k! \cdot |z_\ell|^{p-k} - |z'_\ell|^{p-k}$$

$$\leq a_0 k! \cdot |z_\ell - z'_\ell|^{min\{p-k,1\}},$$

where the last inequality holds because $x^t$ is min\{t, 1\}-Hölder continuous on $[0, 1]$ for $t \geq 0$. The $|z_\ell - z'_\ell|^{min\{p-k,1\}}$ term can be further upper bounded by $\|z - z'|^\alpha$ because $p = d/\beta \geq \alpha$. By selecting $a_0 > 0$ to be sufficiently small (depending on $M$) we have $f_0 \in \Sigma_\alpha^0(M)$.

We next prove $f_0$ satisfies $\mu f_0(\varepsilon) \approx e^{\beta}$ with parameter $\beta$ depending on $a_0$ and $p$. For any $\varepsilon > 0$, the level set $L_{f_0}(\varepsilon)$ can be expressed as $L_{f_0}(\varepsilon) = \{z \in [0, 1]^d : z_1^p + \ldots + z_d^p \leq \varepsilon/a_0 \}$. Subsequently,

$$\left[0, \left( \frac{\varepsilon}{a_0 d} \right)^{1/p} \right]^d \subseteq L_{f_0}(\varepsilon) \subseteq \left[0, \left( \frac{\varepsilon}{a_0} \right)^{1/p} \right]^d.$$ (92)

Therefore,

$$\left[ \varepsilon/(a_0 d) \right]^{dp} \mu f_0(\varepsilon) \leq \varepsilon/a_0]^{dp}.$$ (93)

Because $a_0, d$ are constants and $dp = \beta$, we established $\mu f_0(\varepsilon) \approx e^{\beta}$ for $\beta = dp$.

Finally, note that for any $\varepsilon > 0, L_{f_0}(\varepsilon)$ is sandwiched between two cubics whose volumes only differ by a constant. This proves (A2) and (A2’). on the covering and packing numbers of $f_0(v)$. □

**Proof of Proposition 5.** By Chernoff bound and union bound, with probability $1 - O(n^{-1})$ uniformly over all $x \in G_n$, there are $\Omega(\sqrt{n_0} \log^2 n)$ uniform samples in $B_{h_0}^{\infty}(x; \mathcal{X})$. Subsequently, by standard Gaussian concentration inequality, with probability $1 - O(n^{-1})$ we have

$$\inf_{z \in B_{h_0}^{\infty}(x; \mathcal{X})} f(z) - O(n_0^{-1/4}) \leq \tilde{f}(x) \leq \sup_{z \in B_{h_0}^{\infty}(x; \mathcal{X})} f(z) + O(n_0^{-1/4}) \quad \forall x \in G_n.$$ (94)

Fix arbitrary $\tilde{x}^* \in \arg \min_{x \in G_n} f(x)$. Because $f \in \Sigma_\alpha^0(M)$ for constant $\kappa$ and $h_0 \to 0$, $f$ is smooth on $B_{h_0}^{\infty}(\tilde{x}^*; \mathcal{X})$ and therefore $\sup_{z \in B_{h_0}^{\infty}(\tilde{x}^*; \mathcal{X})} f(z) \leq f(\tilde{x}^*) + O(h_0^{min\{\alpha,1\}}) \leq f(\tilde{x}^*) + O(1/\log^2 n) \leq f^* + O(1/\log^2 n)$, where the last inequality holds due to Lemma 4. On the other hand, for all $x \in G_n$, $\tilde{f}(x) \geq f^* - O(n_0^{-1/4})$. Therefore, for sufficiently large $n$ we must have $\tilde{f}(\tilde{x}^*) \leq \min_{z \in G_n} \tilde{f}(z) + 1/\log n$ and subsequently $\tilde{x}^* \in S_0$.

We next prove the statement that $S_0 \subseteq \bigcup_{x \in L_f(\kappa/2)} B_{h_0}^{\infty}(x; \mathcal{X})$. Consider arbitrary $z \in G_n$ and $z \notin \bigcup_{x \in L_f(\kappa/2)} B_{h_0}^{\infty}(x; \mathcal{X})$. By definition, $f(z') \geq f^* + \kappa/2$ for all $z' \in B_{h_0}^{\infty}(z; \mathcal{X})$. Subsequently, $\tilde{f}(z) \geq f^* + \kappa/2 - O(n_0^{-1/4}) > f^* + 1/\log n$ for constant $\kappa > 0$ and sufficiently large $n$, which implies $z \notin S_0$. □

**Proof of Proposition 7.** The upper bound part of Eq. (56) trivially holds because the absolute values of every element in $\psi_{0,1}(z)\psi_{0,1}(z)^\top$ for $z \in \mathcal{X} = [0, 1]^d$ is upper bounded by $O(1)$. To prove the lower bound part, we only need to show $\int_{\mathcal{X}} |\psi_{0,1}(z)|^2 dU(z)$ is invertible. Assume the contrary. Then there exists $v \in \mathbb{R}^{D_1} \setminus \{0\}$ such that

$$v^\top \left[ \int_{\mathcal{X}} |\psi_{0,1}(z)|^2 dU(z) \right] v = \int_{\mathcal{X}} |\psi_{0,1}(z)^\top v|^2 dU(z) = 0.$$ (95)
Therefore, $\langle \psi_{0,1}(z), v \rangle = 0$ almost everywhere on $z \in [0, 1]^d$. Because $h > 0$, by re-scaling with constants this implies the existence of non-zero coefficient vector $\xi$ such that

$$P(z_1, \ldots, z_m) := \sum_{\alpha_1 + \ldots + \alpha_m \leq k} \xi_{\alpha_1, \ldots, \alpha_m} z_1^{\alpha_1} \ldots z_m^{\alpha_m} = 0 \text{ almost everywhere on } z \in [0, 1]^d.$$

We next use induction to show that, for any degree-$k$ polynomial $P$ of $s$ variables $z_1, \ldots, z_s$ that has at least one non-zero coefficient, the set $\{z_1, \ldots, z_s \in [0, 1]^d : P(z_1, \ldots, z_s) = 0\}$ must have zero measure. This would then result in the desired contradiction. For the base case of $s = 1$, the fundamental theorem of algebra asserts that $P(z_1) = 0$ can have at most $k$ roots, which is a finite set and of measure 0.

We next consider the case where $P(z_1, \ldots, z_s)$ takes on $s$ variables. Re-organizing the terms we have

$$P(z_1, \ldots, z_s) = P_0(z_1, \ldots, z_{s-1}) + z_s P_1(z_1, \ldots, z_{s-1}) + \ldots + z_s^k P_k(z_1, \ldots, z_{s-1}),$$

where $P_1, \ldots, P_k$ are degree-$k$ polynomials of $z_1, \ldots, z_{s-1}$. Because $P$ has a non-zero coefficient, at least one $P_j$ must also have a non-zero coefficient. By the inductive hypothesis, the set $\{z_1, \ldots, z_{s-1} : P_j(z_1, \ldots, z_{s-1}) \neq 0, \text{ for some } j\}$ has measure 0. On the other hand, if $P_j(z_1, \ldots, z_{s-1}) \neq 0$, then invoking the fundamental theorem of algebra again on $z_s$ we know that there are finitely many $z_s$ such that $P(z_1, \ldots, z_s) = 0$. Therefore, $\{z_1, \ldots, z_s : P(z_1, \ldots, z_s) = 0\}$ must also have measure zero.

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