
Nonparametric Indirect Active Learning

Shashank Singh

Max Planck Institute for Intelligent Systems, Tübingen, Germany

Abstract

Typical models of active learning assume a learner can directly manipulate or query a covariate X to study its relationship with a response Y . However, if X is a feature of a complex system, it may be possible only to indirectly influence X by manipulating a control variable Z , a scenario we refer to as Indirect Active Learning. Under a nonparametric fixed-budget model of Indirect Active Learning, we study minimax convergence rates for estimating a local relationship between X and Y , with different rates depending on the complexities and noise levels of the relationships between Z and X and between X and Y . We also derive minimax rates for passive learning under comparable assumptions, finding in many cases that, while there is an asymptotic benefit to active learning, this benefit is fully realized by a simple two-stage learner that runs two passive experiments in sequence.

1 INTRODUCTION

Traditional models of active learning and experimental design assume a learner can directly manipulate, query, or design a covariate X in order to probe its influence on a response Y . In many cases, however, a learner’s ability to *control* X may be much more limited than its ability to *observe* X . A well-studied example is the case of treatment noncompliance, in which an experimenter can prescribe a treatment to a participant (and later ask whether they took the prescribed treatment), but not force them to take the treatment (Zelen, 1979, 1990; Pearl, 1995). More generally, the covariate X might be the result of a complex process that the learner can influence and measure but not completely control. For example, genetic modifications intended to target specific genes often have limited precision,

causing unintended random or systematic (but measurable) changes in other off-target genes and making it challenging to measure the effect of the intended modification (Cellini et al., 2004; Hendel et al., 2015; Wang and Wang, 2019). Similarly, it is often unclear whether manipulations conducted in psychological experiments reliably induce a desired psychological state in a participant, necessitating the use of manipulation checks (Festinger, 1953; Lench et al., 2014). In the most general case, studied here, the learner’s influence over X might be governed by an unknown black-box function and subject to noise.

This paper analyzes nonparametric regression under an *Indirect Active Learning* model, illustrated in Figure 1, in which, rather than specifying the covariate X , the learner specifies a control variable Z and then observes both a resulting covariate value $X = g(Z) + \sigma_X \varepsilon_X$ and a resulting response $Y = f(X) + \sigma_Y \varepsilon_Y$. Here, f and g are unknown functions, ε_X is unobserved centered additive *covariate noise* of level $\sigma_X \geq 0$, and ε_Y is unobserved centered additive *response noise* of level $\sigma_Y \geq 0$. This generalizes the usual setup of (homoskedastic) regression, in which $g(z) = z$, $\varepsilon_X = 0$, $f(x) = \mathbb{E}[Y|X = x]$, $\varepsilon_Y = Y - \mathbb{E}[Y|X = x]$ (Wasserman, 2006; Tsybakov, 2008). The learner repeats this process iteratively, using

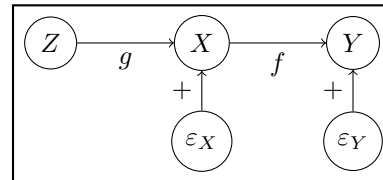


Figure 1: Graphical model of Indirect Active Learning.

past observations of (X, Y, Z) to select a new value for the control variable Z in each iteration, until a prespecified learning budget has been met. The learner’s goal is to estimate the expected response $f(x_0)$ corresponding to a prespecified target covariate value x_0 .¹ To do this efficiently, the learner must query “informative” values of Z , i.e., those such that $g(Z) + \sigma_X \varepsilon_X$ is likely to be near to x_0 . Thus, in contrast to traditional active learning, which involves

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¹Our results extend easily to estimating a contrast, i.e., a difference $f(x_1) - f(x_0)$ at two covariate values x_0 and x_1 .

only exploitation (selecting the most informative values of X), Indirect Active Learning involves an exploration-exploitation trade-off, as the learner must both search for the most informative choices of Z and query these choices repeatedly to mitigate noise.

The present paper begins to characterize the statistical properties of optimal learning under this Indirect Active Learning model. Specifically, in Section 6, we study minimax convergence rates under a nonparametric model of Indirect Active Learning with a fixed budget, obtaining different rates depending on the complexities of the functions f and g and the noise levels σ_X and σ_Y . Our upper bounds utilize an algorithm (Algorithm 1 in Section 6) consisting of two passive learning stages, a “pure exploration” stage followed by a “pure exploitation” stage. We derive high-probability upper bounds on the error of this algorithm as well as minimax lower bounds (on the error of any algorithm) that match our upper bounds in most, though not all, cases. Because passive experiments are typically much easier to carry out (and parallelize) than sequential active experiments, the optimality of this simple two-stage algorithm in many settings has important practical implications for optimal experimental design.

To understand the specific benefits of active learning under indirect control, Section 5 derives minimax rates for passive learning under comparable assumptions, which differ from those of typical nonparametric regression. In the passive case, the standard k -nearest neighbor (k -NN) regressor turns out to be minimax rate-optimal. However, in many cases, the two-stage learner described above asymptotically outperforms the k -NN regressor, demonstrating an advantage of (even a very limited form of) active learning over passive learning.

Finally, Section 8 presents experiments validating our theoretical results and comparing the performance of active and passive learning in both simple synthetic data and in a more complex epidemiological forecasting application.

2 NOTATION & DEFINITIONS

For positive real sequences $\{a_n\}_{n=1}^\infty$ and $\{b_n\}_{n=1}^\infty$, we write $a_n \lesssim b_n$ if $\limsup_{n \rightarrow \infty} a_n/b_n < \infty$, $a_n \gtrsim b_n$ if $b_n \lesssim a_n$, and $a_n \asymp b_n$ if both $a_n \gtrsim b_n$ and $a_n \lesssim b_n$. When ignoring polylogarithmic factors, we write $a_n \lesssim_{\log} b_n$ (to mean $a_n \lesssim b_n (\log b_n)^p$ for some $p > 0$), etc. For positive integers n , $[n] = \{1, \dots, n\}$ is the set of positive integers at most n . For $x \in \mathbb{R}$, $\lfloor x \rfloor = \max\{z \in \mathbb{Z} : z \leq x\}$ is the greatest integer at most x . For $x \in \mathbb{R}^d$, $\|x\| = \max_j |x_j|$ and $\|x\|_2 = \sqrt{\sum_j x_j^2}$ are ℓ_∞ - and ℓ_2 -norms of x .

We now define three regularity conditions needed for our learning problem. The first is *local Hölder smoothness*, used to measure the complexities of the functions f and g :

Definition 1 (Local Hölder Seminorm, Space, and Ball). *For any $s \in (0, 1]$ and metric spaces (\mathcal{Z}, ρ_Z) and (\mathcal{X}, ρ_X) , the local Hölder seminorm $\|\cdot\|_{\mathcal{C}^s(\mathcal{Z}, z_0; \mathcal{X})}$ around a point $z_0 \in \mathcal{Z}$ is defined for $f : \mathcal{Z} \rightarrow \mathcal{X}$ by*

$$\|f\|_{\mathcal{C}^s(\mathcal{Z}, z_0; \mathcal{X})} := \sup_{z \neq z_0 \in \mathcal{Z}} \frac{\rho_X(f(z), f(z_0))}{\rho_Z^s(x, y)},$$

the local Hölder space $\mathcal{C}^s(\mathcal{Z}, z_0; \mathcal{X})$ around $z_0 \in \mathcal{Z}$ is

$$\mathcal{C}^s(\mathcal{Z}, z_0; \mathcal{X}) := \{f : \mathcal{Z} \rightarrow \mathcal{X} \text{ s.t. } \|f\|_{\mathcal{C}^s(\mathcal{Z}, z_0; \mathcal{X})} < \infty\}.$$

For $L \geq 0$, the local Hölder ball $\mathcal{C}^s(\mathcal{Z}; \mathcal{X}; L)$ is

$$\mathcal{C}^s(\mathcal{Z}, z_0; \mathcal{X}; L) := \{f : \mathcal{Z} \rightarrow \mathcal{X} \text{ s.t. } \|f\|_{\mathcal{C}^s(\mathcal{Z}, z_0; \mathcal{X})} \leq L\}.$$

Local Hölder continuity is much weaker than the more common notion *global Hölder continuity* (defined in Appendix B). To prove the most general possible bounds, our upper bounds assume only local Hölder continuity around particular points, while matching lower bounds are given under global Hölder continuity.

We next provide a definition of *local dimension* that will be used to measure intrinsic complexities of the random variables Z and ε_X :

Definition 2 (Local Dimension). *A random variable X taking values in a metric space (\mathcal{X}, ρ) has local dimension d around a point $x \in \mathcal{X}$ if*

$$\liminf_{r \downarrow 0} \frac{\mathbb{P}[\rho(X, x) \leq r]}{r^d} > 0.$$

This notion of local dimension can be thought of as a local version of Frostman Dimension (Frostman, 1935), and is closely related to the Hausdorff and (lower) box counting or Minkowski dimensions of the underlying space \mathcal{X} (see Corollary 4.12 of Falconer (2014) and Chapter 8 of Mattila (1999)).

Finally, we state a *sub-Gaussian tail condition*, used to control the noise variables ε_X and ε_Y :

Definition 3 (Sub-Gaussian Random Variable). *For any integer $d > 0$, an \mathbb{R}^d -valued random variable ε is said to be sub-Gaussian if, for all $t \in \mathbb{R}^d$, $\mathbb{E}[e^{\langle \varepsilon, t \rangle}] \leq e^{\|t\|_2^2/2}$.*

Sub-Gaussianity is usually defined with a parameter $\sigma \geq 0$ indicating the scale of ε . In this work, to be consistent with other assumptions (namely, the local dimension assumption on ε_X), we separate the scale parameter σ , explicitly writing $\sigma\varepsilon$ as needed.

3 PROBLEM SETUP

We now describe our passive and active learning problems.

Passive Setting In the passive setting, for some known $x_0 \in \mathcal{X} \subseteq \mathbb{R}^d$, the learner must estimate $f(x_0)$ from pre-collected IID data $\{(X_i, Y_i, Z_i)\}_{i=1}^n \in (\mathcal{X} \times \mathbb{R} \times \mathcal{Z})^n$, assuming:

- A1) Data are drawn from the model $X = g(Z) + \sigma_X \varepsilon_X$, $Y = f(X) + \sigma_Y \varepsilon_Y$, as illustrated in Figure 1.
- A2) The marginal distribution P_Z of Z has dimension d_Z around some $z_0 \in \mathcal{Z}$ with $g(z_0) = x_0$.
- A3) The distribution of ε_X has dimension d_X around 0.
- A4) g and f lie in local Hölder balls $\mathcal{C}^{s_g}(\mathcal{Z}, z_0; \mathcal{X}; L_g)$ and $\mathcal{C}^{s_f}(\mathcal{X}, x_0; \mathbb{R}; L_f)$, respectively.
- A5) ε_X and ε_Y are sub-Gaussian.

Note that our bounds will depend on the intrinsic dimensions d_Z of Z and d_X of ε_X , but not on the extrinsic dimension d of X . Assumptions A2), A3), A4), and A5) are quite mild, comparable to the weakest assumptions typically made in nonparametric regression. The strongest assumption is the heteroscedastic additive error model in A1), but this is primarily for convenience and can also be weakened substantially; for example, our upper bounds hold even if σ_Y is a sufficiently smooth function of X around x_0 ; see Remark 12 in the Appendix for details.

Active Setting In the active setting, at each time step i , the learner must select a new sample Z_i based on the past data $\{(X_j, Y_j, Z_j)\}_{j=1}^{i-1}$. The learner may also utilize the “prior” distribution P_Z of Z from the passive case.² After selecting Z_i , the learner observes the covariate-response pair (X_i, Y_i) , and the process repeats. After n iterations of this process, the learner must estimate $f(x_0)$ (for some $x_0 \in \mathcal{X}$ known in advance), using the dataset $\{(X_i, Y_i, Z_i)\}_{i=1}^n$. The learner may also assume A1)-A5) from the passive setting.

4 RELATED WORK

Several models of active learning have been previously considered (Settles, 2009), including Query Synthesis (Angelescu, 1988; Wang et al., 2015) or Adaptive Sampling (Castro et al., 2005), in which the learner can request a label for any desired query $x \in \mathcal{X}$, Pool-Based Sampling (Lewis, 1995; Hanneke, 2014), in which the learner can request a label for any $x \in S$ given a finite “data pool” $S \subseteq \mathcal{X}$, and Stream-Based Selective Sampling (Atlas et al., 1989), in which a learner can request labels for individual data points as they appear sequentially. Although assumed in many theoretical analyses (Burnashev and Zigangirov, 1974; Sung and Niyogi, 1994; Castro et al., 2005), Query Synthesis can often be impractical, as generating arbitrary $x \in \mathcal{X}$ to query may be difficult (although progress is being made on this front, for example using modern genera-

²Although not a prior on z_0 in the typical Bayesian sense, P_Z plays a similar role in that the estimators’ performance will depend on how concentrated P_Z is around z_0 .

tive models (Zhu and Bento, 2017)). Indirect Active Learning can be viewed as a significant relaxation of Query Synthesis, under which the learner generates new queries with only limited control over the content of the query. Indirect Active Learning can also be related to Pool-Based Sampling, e.g., if g maps x to its nearest neighbor in a fixed data pool $S \subseteq \mathcal{X}$; however, such a formulation violates the Hölder smoothness assumption we make on g , and we do not pursue this here.

While we are not aware of prior research within the Indirect Active Learning paradigm, several closely related paradigms have been studied previously:

Active Nonparametric Regression Within the Query Synthesis paradigm, Castro et al. (2005) showed that, in the standard nonparametric regression setting (i.e., fixing $g(z) = z$), considering globally Hölder-smooth f , active learning provides no asymptotic advantages over passive learning. This contrasts with our results under Indirect Active Learning, where we show that active learning often asymptotically improves over passive learning (by leveraging an estimate of g to better select informative queries).

Active Learning with Feature Noise Our generative model (Figure 1) generalizes the Berkson errors-in-variables regression model (Berkson, 1950), the special case when $\mathcal{X} = \mathcal{Z}$ and g is known to be the identity function. The Berkson model, which has been studied extensively in passive supervised learning (Buonaccorsi, 2010; Carroll et al., 2006), was used by Ramdas et al. (2014) to study the effects of feature noise in active binary nonparametric classification. To the best of our knowledge, this is the only prior work generalizing Query Synthesis such that the learner cannot exactly select the covariate.

Note that the Berkson model is distinct from the classical errors-in-variables regression model (Fuller, 2009), in which noise would be applied *after* observing X (i.e., we would have $X = g(Z)$ and $Y = f(X + \sigma_X \varepsilon_X) + \sigma_Y \varepsilon_Y$); the Berkson model is appropriate in our setting where noise affects the learner’s ability to *control* X rather than to *measure* X . One could additionally consider noise in the measurement of X , which has the effect of smoothing the observed relationship between X and Y ; however, this additional bias often makes the learning problem statistically intractable, with optimal convergence rates decaying only polylogarithmically with the sample size n under common (e.g., Gaussian) noise models (Fan and Truong, 1993). Measurement error in X could potentially be mitigated using knowledge of Z (e.g., using two-stage regression, as in instrumental variable methods; Sargan, 1958), which we leave as a direction for future work.

Active Learning on Manifolds When the dimension d_Z of Z is smaller than that of X and g is sufficiently smooth,

the model $X = g(Z) + \sigma_X \varepsilon_X$ implies that X lies near a low-dimensional manifold in \mathcal{X} . This is a natural model under which to study active learning on an unknown manifold (i.e., in the presence of unknown structural constraints on the covariate \mathcal{X}). To the best of our knowledge, no statistical theory has been developed for this problem, although a number of practical methods have been proposed (Zhou and Sun, 2014; Li et al., 2020; Huang et al., 2020; Sreenivasaiah et al., 2021). Our results show that, whereas rates for passive learning often depend on the total intrinsic dimension $d_X + d_Z/s_g$ of the distribution of X , rates for active learning depend mostly on the smaller dimension d_X of the noise ε_X in X . Note that both of these intrinsic dimensions may be much smaller than the extrinsic dimension of X , which does not appear in our rates.

Approximate Bayesian Computation Approximate Bayesian Computation (ABC) is an approach to estimating a posterior distribution for parameters of a complex model that avoids explicit computation of a likelihood function by using a simulation to relate the parameter to measurable data (Csilléry et al., 2010; Sunnåker et al., 2013). The two-stage Algorithm 1 we propose is similar in spirit to the rejection algorithm typically used in ABC (Csilléry et al., 2010), in that different values of the input parameter Z are first sampled randomly and then evaluated in terms of similarity between experimental and target measurements X . However, rather than to construct a posterior distribution for the “true value” of the input parameters Z of a simulation, our goal is to estimate an outcome Y of the simulation. Moreover, our formulation and analysis of Indirect Active Learning is completely frequentist, although, as noted previously, the distribution P_Z can be regarded as a prior on z_0 .

Instrumental Variables Methods Our model of Indirect Active Learning (Figure 1) assumes that the relationship between X and Y is unconfounded given Z , i.e., that ε_Y is independent of X and that Y is conditionally independent of ε_X given X . In general, as illustrated in Figure 2, there may exist unobserved confounders that affect both X and Y , leading to the causal model assumed by instrumental variable methods, which attempt to use an unconfounded *instrumental variable* Z to deconfound the relationship between X and Y , typically by projecting X onto its variation caused by Z (Baiocchi et al., 2014). In the

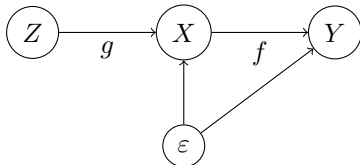


Figure 2: Structural causal model assumed by instrumental variable methods.

passive case, Singh et al. (2019) provided minimax rates for nonparametric instrumental variable regression, but we are not aware of work characterizing the potential benefits of actively manipulating the instrumental variable Z . Indeed, as we discuss further in Section 9, one motivation for the present work is to provide a foundation for such work by first characterizing minimax-optimal learning in the absence of confounders.

5 BOUNDS FOR PASSIVE LEARNING

To provide an appropriate baseline for performance in Indirect Active Learning, we first consider the problem of *passively* estimating $f(x_0)$ from an IID dataset $\{(X_i, Y_i, Z_i)\}_{i=1}^n$. Upon first glance, since observations of Z provide no information about the relationship between X and Y , one might suppose that this passive problem reduces to standard passive regression, in which we have only IID observations of (X, Y) . However, while observations of Z are indeed uninformative here, the assumption $X = g(Z) + \sigma_X \varepsilon_X$ imposes constraints on the distribution of X that differ from the standard passive regression setting, resulting in significantly different convergence rates. Obtaining minimax rates for the passive case will therefore facilitate interpretation of our main results for the active case, especially to understand the benefit of active learning over passive learning.

In the passive case, we consider a k -nearest neighbor (k -NN) regression estimate of $f(x_0)$:

Definition 4 (Nearest-Neighbor Order and k -Nearest Neighbor Regressor). Given a point x_0 lying in a metric space (\mathcal{X}, ρ) and a finite dataset $X_1, \dots, X_n \in \mathcal{X}$, the nearest-neighbor order $\pi(x_0; \{X_1, \dots, X_n\})$ is a permutation of $[n]$ such that

$$\begin{aligned} \rho(x_0, X_{\pi_1(x_0; \{X_1, \dots, X_n\})}) &\leq \rho(x_0, X_{\pi_2(x_0; \{X_1, \dots, X_n\})}) \\ &\leq \dots \\ &\leq \rho(x_0, X_{\pi_n(x_0; \{X_1, \dots, X_n\})}), \end{aligned}$$

with ties broken arbitrarily. The k -nearest neighbor regressor $\hat{f}_{x_0, k}$ of f at x_0 is defined by

$$\hat{f}_{x_0, k} := \frac{1}{k} \sum_{i=1}^k Y_{\pi_i(x_0; \{X_1, \dots, X_n\})}, \quad (1)$$

Crucially, in contrast to most other approaches to nonparametric regression, k -NN regression automatically adapts to unknown low-dimensional structure in the distribution of X_1, \dots, X_n (Kpotufe, 2011), which is important in our setting because the model $X = g(Z) + \sigma_X \varepsilon_X$ can constrain the intrinsic dimension of X . In contrast, we expect many methods, such as kernel methods with uniform bandwidth, to be sub-optimal in our setting. The following re-

sult, proven in Appendix A, bounds the error of the k -NN estimate (1):

Theorem 5 (Passive Upper Bound). *Let $\delta \in (0, 1)$ and let $\hat{f}_{x_0, k}$ denote the k -NN regression from Eq. (1) with k chosen according to Eq. (6) in Appendix A. Under Assumptions A1)-A5), there exists a constant $C > 0$, depending only on $L_g, s_g, L_f, s_f, d_X, d_Z$, such that*

$$\Pr \left[\left| \hat{f}_{x_0, k} - f(x_0) \right| > C\Phi_P \log^{1/\delta} \right] \leq \delta,$$

where

$$\Phi_P = \max \left\{ \left(\frac{1}{n} \right)^{\frac{s_f s_g}{d_Z}}, \left(\frac{\sigma_X^{d_X}}{n} \right)^{\frac{s_f}{d_X + d_Z / s_g}}, \left(\frac{\sigma_Y^2}{n} \right)^{\frac{s_f}{2s_f + d_Z / s_g}}, \left(\frac{\sigma_X^{d_X} \sigma_Y^2}{n} \right)^{\frac{s_f}{2s_f + d_X + d_Z / s_g}} \right\}. \quad (2)$$

Before discussing this result further, we present a matching lower bound, proven in Appendix B, showing that the rate Φ_P in Theorem 5 is the optimal in the passive case:

Theorem 6 (Passive Lower Bound). *There exist constants $c_1, c_2, n_0 > 0$, depending only on $L_g, s_g, L_f, s_f, d_X, d_Z$, such that, for all $n \geq n_0$, for any passive estimator \hat{f}_{x_0} ,*

$$\sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_D \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq c_1 \Phi_P \right] \geq c_2, \quad (3)$$

where Φ_P is the passive minimax rate defined in Eq. (2) and the supremum is taken over all $g, f, P_Z, \varepsilon_X, \varepsilon_Y$ satisfying Assumptions A1)-A5).

Comparing Theorems 5 and 6, we see that the k -NN regressor in Eq. (1) achieves the minimax optimal rate Φ_P , given in Eq. (2), for the passive case. Each of the terms in Φ_P can dominate, depending on the relative magnitudes of σ_X, σ_Y , and n . If the covariate noise level σ_X is sufficiently small, one can show that the distribution of X concentrates near a manifold of dimension d_Z/s_g within \mathcal{X} . Hence, depending on the response noise level σ_Y , we obtain the rate $\asymp n^{-\frac{s_f s_g}{d_Z}}$ or $\asymp n^{-\frac{s_f}{2s_f + d_Z / s_g}}$, corresponding to the rate of nonparametric regression over a covariate space of dimension d_Z/s_g , in the absence of response noise (Kohler, 2014) or the presence of response noise (Tsybakov, 2008), respectively. Increasing the level σ_X of covariate noise leads to slower rates, respectively $\asymp n^{-\frac{s_f}{d_X + d_Z / s_g}}$ or $\asymp n^{-\frac{s_f}{2s_f + d_X + d_Z / s_g}}$, equivalent to increasing the dimension of the covariate space by d_X . An alternative interpretation is as a multi-resolution bound: fixing $\sigma_X > 0$ and $\sigma_Y > 0$, the convergence rate slows as $n \rightarrow \infty$, initially from $n^{-s_f s_g / d_Z}$ to $n^{-\frac{s_f}{d_X + d_Z / s_g}}$ (if $d_X \geq 2s_f$) or $n^{-\frac{s_f}{2s_f + d_Z / s_g}}$ (if $d_X \leq 2s_f$), and then further to $n^{-\frac{s_f}{2s_f + d_X + d_Z / s_g}}$.

6 BOUNDS FOR ACTIVE LEARNING

We now turn to the active case. Our upper bounds use a “two-stage” algorithm, detailed in Algorithm 1, which sequentially performs two passive experiments, a “pure exploration” experiment followed by a “pure exploitation” experiment. In the first stage, the algorithm randomly samples the control variable Z according to the given “prior” distribution P_Z (as in the passive algorithm). Each sample value of Z is repeated several times, and the resulting values of X are averaged to determine which observed value of Z is most likely to return a value of X near x_0 . The algorithm then repeatedly samples this value of Z (hopefully obtaining a large number of samples with X near x_0), and finally applies the k -NN regressor from Eq. (1) over the resulting dataset.

Algorithm 1: Two-stage active learning algorithm.

Input: Budget n , integers $\ell, k \in [1, n/2]$, distribution P_Z on \mathcal{Z} , target point $x_0 \in \mathcal{X}$

Output: Estimate \hat{f}_{x_0} of x_0

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1  $m \leftarrow \lfloor n/2 \rfloor$ 
2 for  $i \in [\lfloor m/\ell \rfloor]$  do // exploration stage
3   Draw  $Z_i \sim P_Z$ 
4   for  $l \in [\ell]$  do
5     Observe  $X_{i,l} = g(Z_i) + \sigma_X \varepsilon_{X,i,l}$  and
6      $Y_{i,l} = f(X_{i,l}) + \sigma_Y \varepsilon_{Y,i,l}$ 
7     Compute  $\bar{X}_i = \sum_{l=1}^{\ell} X_{i,l}$ 
8    $i^* \leftarrow \operatorname{argmin}_{i \in [\lfloor m/\ell \rfloor]} \|\bar{X}_i - x_0\|$ 
9 for  $i \in [n - m]$  do // exploitation stage
10  Sample  $X_{m+i} = g(Z_{i^*}) + \sigma_X \varepsilon_{X,m+i}$  and
11   $Y_{m+i} = f(X_{m+i}) + \sigma_Y \varepsilon_{Y,m+i}$ 
12 return  $\hat{f}_{x_0} = \frac{1}{k} \sum_{j=1}^k Y_{\pi_j(x_0; \{X_1, \dots, X_n\})}$ 

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Because passive experiments are often much easier to carry out (and parallelize) than sequential active experiments, this two-stage design may be practical in many settings where a fully iterative procedure would be expensive or time-consuming to implement. Nevertheless, Algorithm 1 achieves the optimal convergence rate in most, though not all, experimental settings, and typically converges faster than the passive minimax rate. In particular, we have the following upper bound, proven in Appendix C:

Theorem 7 (Active Upper Bound). *Let $\delta \in (0, 1)$, and let \hat{f}_{x_0} denote the estimator proposed in Algorithm 1, with k and ℓ chosen according to Eqs. (33) and (34) in Appendix C. Then, under Assumptions A1)-A5), for some constant $C > 0$ depending only on L_g, s_g, L_f, s_f, d_X , and d_Z , with probability $\geq 1 - \delta$, $\left| \hat{f}_{x_0} - f(x_0) \right| \leq C\Phi_A^* \log^{1/\delta}$,*

where

$$\Phi_A^* := \max \left\{ \left(\frac{1}{n} \right)^{\frac{s_f s_g}{d_Z}}, \left(\frac{\sigma_X^{d_X}}{n} \right)^{\frac{s_f}{d_X}}, \frac{\sigma_Y}{\sqrt{n}}, \left(\frac{\sigma_Y^2 \sigma_X^{d_X}}{n} \right)^{\frac{s_f}{2s_f + d_X}}, \left(\frac{\sigma_X^2 \log n}{n} \right)^{\frac{s_f s_g}{2s_g + d_Z}} \right\}. \quad (4)$$

Meanwhile, we have the following minimax lower bound, proven in Appendix D, on the error of any active learner:

Theorem 8 (Lower Bounds for the Active Case). *There exist constants $c_1, c_2 > 0$, depending only on L_g, s_g, L_f, s_f, d_X , and d_Z , such that, for any active estimator \widehat{f}_{x_0}*

$$\sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_{\{(Z_i, X_i, Y_i)\}_{i=1}^n} \left[\left| \widehat{f}_{x_0} - f(x_0) \right| \geq c_1 \Phi_{A,*} \right] \geq c_2,$$

where the supremum is over all g, f, P_Z, ε_X , and ε_Y satisfying Assumptions A1)-A5), and

$$\Phi_{A,*} = \max \left\{ \left(\frac{1}{n} \right)^{\frac{s_f s_g}{d_Z}}, \left(\frac{\sigma_X^{d_X}}{n} \right)^{\frac{s_f}{d_X}}, \frac{\sigma_Y}{\sqrt{n}}, \left(\frac{\sigma_X^{d_X} \sigma_Y^2}{n} \right)^{\frac{s_f}{2s_f + d_X}} \right\}. \quad (5)$$

Comparing the upper bound Φ_A^* (Eq. (4)) and lower bound $\Phi_{A,*}$ (Eq. (5)), we can write

$$\Phi_A^* = \max \left\{ \Phi_{A,*}, \left(\frac{\sigma_X^2 \log n}{n} \right)^{\frac{s_f s_g}{2s_g + d_Z}} \right\};$$

i.e., the first four terms in Φ_A^* match the corresponding terms in $\Phi_{A,*}$, while the fifth term in Φ_A^* may be sub-optimal. Hence, Algorithm 1 is optimal whenever σ_Y is sufficiently large or both d_X and σ_X are sufficiently small; specifically, for σ_Y small, the fifth term $\left(\frac{\sigma_X^2 \log n}{n} \right)^{\frac{s_f s_g}{2s_g + d_Z}}$ dominates Φ_A^* only when $1 \lesssim_{\log} \sigma_X n^{\frac{s_g}{d_Z}} \lesssim_{\log} n^{\frac{2s_g + d_Z}{d_X d_Z}}$.

7 DISCUSSION

Comparison of Active and Passive Bounds The first terms of the passive minimax rate Φ_P (Eq. (2)) and our upper bound rate Φ_A^* (Eq. (4)) match, while, Φ_A^* strictly improves on the second, third, and fourth terms of Φ_P by removing d_Z/s_g from the exponents. Meanwhile, the last term of Φ_A^* dominates Φ_P only if σ_Y is sufficiently small and both $d_X \leq 2$ and $\sigma_X \gtrsim_{\log} n^{-d_Z/s_g}$. In particular, whenever σ_Y is sufficiently large or both $d_X > 2$ and

$\sigma_X \gtrsim_{\log} n^{-d_Z/s_g}$, (i.e., whenever the response or covariate noise is sufficiently large), Algorithm 1 strictly outperforms the best passive algorithm. Intuitively, the advantage of active learning comes from the ability to learn the structure of g and thereby remove the degrees of freedom in X that come from variation in Z .

Two-Stage vs. Fully Active Algorithms Our proposed two-stage Algorithm 1 utilizes active learning in only a very limited way, as prior information from preceding iterations is used only once, in between exploration and exploitation stages, rather than in each iteration. Practically, this demonstrates that running a pilot experiment to optimize free parameters of a main experiment can provide a dramatic improvement in the utility of data from the main experiment. That is, Algorithm 1 may be useful not only in the specific setting of Active Learning, but also in the more general setting of Experimental Design, where one wishes to design an optimal experiment before collecting (most of) the data. Moreover, when possible, data collection within each of the two stages can be trivially parallelized. On the other hand, sequentially optimizing these parameters separately before collecting each sample may be prohibitively complex, laborious, or time-consuming.

One may speculate that this simplicity causes the gap between our upper and lower bounds for the active case (Theorems 7 and 8), and that a more sophisticated algorithm might iteratively utilize all of the past information to inform each future decision. On the other hand, the evaluation function, namely the error of the final estimate, is more comparable to the notion of Simple Regret, rather than Cumulative Regret, used to evaluate many active algorithms (Slivkins, 2019). For example, in our problem, an algorithm can afford to perform $\Omega(n)$ steps of pure exploration (as in Algorithm 1), whereas any such algorithm necessarily exhibits linear cumulative regret. Since, in many problems (e.g., multi-armed bandits), simple two-stage algorithms can be optimal under Simple Regret, it remains unclear whether the gap between Theorems 7 and 8 is inherent to two-stage algorithms such as Algorithm 1 or is an artifact of our (upper or lower) bounds.

8 EXPERIMENTAL RESULTS

In this section, we present the results of two numerical experiments designed to numerically validate our theoretical findings. The main goal was to investigate whether the theoretical performance advantages of the two-stage algorithm (over the Passive algorithm) predicted by our theoretical results translate into apparent practical advantages, and to shed light on how these performance advantages scale with various parameters of the data-generating process. Python code and instructions for replicating our results are available at <https://gitlab.tuebingen.mpg.de/shashank/indirect-active-learning>.

8.1 Experiment 1: Synthetic Data

We first consider a setting with simple synthetic data where we can directly manipulate features of the data-generating process, such as the dimensions d_Z of P_Z and d_X of ε_X , the smoothness s_g of g , and the noise levels σ_X and σ_Y .

Algorithms As our Passive algorithm, we utilized standard k -NN regression, as in Theorem 5. As our Active algorithm, we used the two-stage algorithm presented in Algorithm 1. For comparison, we also evaluated an ‘‘Oracle’’ estimator that always samples (X, Y, Z) conditional on $Z = z_0$ and then runs a k -NN regression of Y over X . Since this relies on knowledge of z_0 , this is not feasible in practice, but comparing the performance of the Active estimator to this ideal estimator will allow us to discern how much of the Active estimator’s error comes from learning f versus learning g .

Although Theorems 5 and 7 specify optimal values of the hyperparameters k and ℓ of the active and passive estimators, respectively, these optimal values depend on parameters, such as the local smoothness of g and f around z_0 and x_0 , that are typically unknown in practice. We therefore considered two versions of each algorithm: a version utilizing the theoretically optimal values of each parameter (according to Eqs. (6), (33), and (34)) and a fully data-dependent version that used 4-fold cross-validation to select each hyperparameter.

Hence, in total, we compared 6 algorithms, namely Passive, Active, and Oracle algorithms with theoretically optimal hyperparameter values, as well as their cross-validated counterparts Passive CV, Active CV, and Oracle CV.

Data Generating Process Synthetic data was generated as follows. P_Z was uniform on $[0, 1]^{d_Z}$, $\varepsilon_X \sim \mathcal{N}(0, I_{d_X})$, $\varepsilon_Y \sim \mathcal{N}(0, 1)$, $g : \mathbb{R}^{d_Z} \rightarrow \mathbb{R}^{d_X}$ defined by $g_1(z) = \dots = g_{d_X}(z) = \sum_{j=1}^{d_Z} |z_j|^{s_g}$ for all $z \in \mathbb{R}^{d_Z}$, and $f : \mathbb{R}^{d_X} \rightarrow \mathbb{R}$ defined by $f(x) = \|x\|_2$ for all $x \in \mathbb{R}^{d_X}$. One can then check that $g \in \mathcal{C}^{s_g}(\mathcal{Z}, z_0; \mathcal{Z}; 1)$ and $f \in \mathcal{C}^1(\mathcal{X}, x_0; \mathcal{Y}; 1)$.

In the default setup, we set $n = 2^{10}$, $s_g = 1$, $d_Z = d_X = 3$, and $\sigma_X = \sigma_Y = 1$. We then varied each of these parameters to demonstrate its effect on the performance of each estimator. Specifically, we varied:

- $n \in \{2^4, 2^5, \dots, 2^{12}\}$
- $s_g \in \{0.1, 0.2, \dots, 1.0\}$
- $d_Z, d_X \in \{1, 2, \dots, 10\}$
- $\sigma_X, \sigma_Y \in \{10^{-1}, 10^{-0.8}, 10^{-0.6}, \dots, 10^{0.8}, 10^1\}$

Results Each experiment was replicated independently 2^{10} times. Figure 3 displays means and standard errors (across IID replicates) of the mean squared error of each algorithm. Unsurprisingly, Passive estimators consistently exhibit the largest error, with Passive CV typically outper-

forming Passive, and the Oracle estimators consistently exhibit the smallest error, with Oracle typically slightly outperforming Oracle CV. Meanwhile, performance of the Active estimators lies between those of the corresponding Passive and Oracle estimators.

Whether Active estimators perform more like corresponding Passive estimators or corresponding Oracle estimators depends primarily on how easy it is to learn the function g and thereby select values of $Z \approx z_0$. Hence, the advantage of Active estimators over their Passive counterparts increases with sample size n and smoothness s_g , decreases with intrinsic dimension d_Z and covariate noise level σ_X , and is essentially unaffected by covariate noise dimension d_X and response noise level σ_Y .

The performances of the Active and Active CV estimators are generally quite similar. This is encouraging, as Active CV, though computationally more demanding, is more practical in most real applications where the smoothness levels of g and f are unknown. Since the Active estimator is minimax optimal in most settings, we may similarly expect Active CV to be minimax optimal in most settings.

8.2 Experiment 2: Epidemiological Forecasting

We now consider a more realistic data-generating process based on a stochastic SIRD model, a system of discrete-time stochastic differential equations (SDEs) that forms the basis for many models of infectious disease spread used in epidemiology (Bailey et al., 1975; Arik et al., 2020). Given a fixed population of individuals the SIRD model tracks the number of individuals in each of four states: individuals (S)usceptible to contracting the disease, (I)nfectious individuals who carry the disease and may infect others, (R)ecovered individuals who are assumed to be immune to the disease, and (D)eceased individuals who died from the disease. Given SIRD counts at a point in time, a system of SDEs (given in Appendix F.2) determines how SIRD compartment counts change at the next time step, allowing one to simulate SIRD compartment counts over time.

Problem Setup We consider the common epidemiological challenge of predicting the outcome of an epidemic disease outbreak, using only data from the beginning of the outbreak (Brooks et al., 2015; Desai et al., 2019; Arik et al., 2020). Specifically, in a population of $N = 1000$ individuals, given SIRD counts from the first 20 of a simulation ($X = (S_{1:20}, I_{1:20}, R_{1:20}, D_{1:20}) \in \mathbb{N}^{80}$), we aim to predict the total number $Y = D_{100} \in \mathbb{N}$ of deaths by day $T = 100$.

Since key parameters $Z = (\beta, \gamma, \delta) \in [0, 1]^3$ determining the rates at which individuals transition between SIRD compartments are unknown, one cannot simply propagate SDEs starting from the given measurement data. One can, however, use this simulation to generate a dataset of

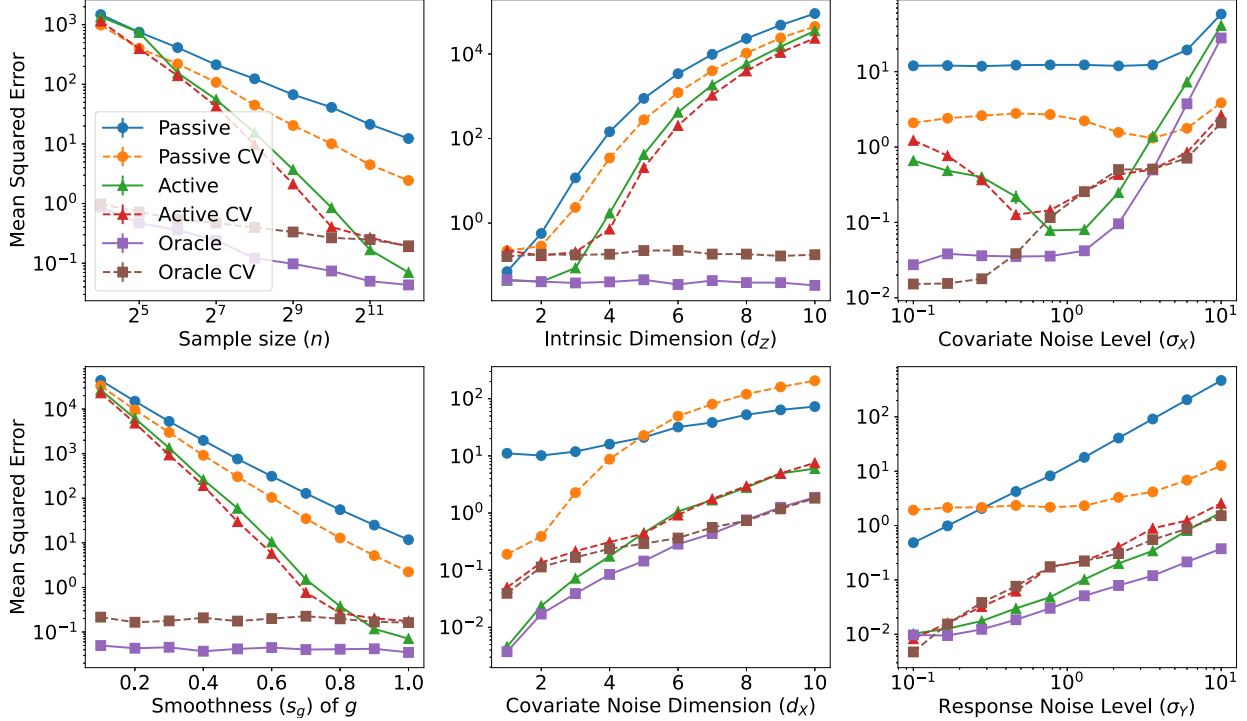


Figure 3: Experiment 1: Mean (over 2^{10} IID replicates) squared error of each estimator, over parameters of the data-generating process. Error bars denoting standard errors over replicates are too small to be visible. Note logarithmic y -axes.

(X, Y, Z) triples for various values of Z and then train a machine learning model to predict Y from X . This can be compared to the approach of Brooks et al. (2015), who forecast current seasonal influenza epidemics based on outcomes from historical epidemic seasons exhibiting greatest similarity to data collected so far in the current season. Since we have access to a simulation, we can try to improve forecasts by selecting values of Z intelligently, rather than completely randomly. This is precisely what Indirect Active Learning attempts to do (in a similar spirit as Approximate Bayesian Computation).

Results We evaluated the performance of both our two-stage Active learning Algorithm 1 and the Passive k -NN regressor on this task, for various sample sizes (i.e., simulation budgets) n . Since we do not know the true smoothness levels s_g and s_f in this scenario, we selected estimator hyperparameters using 4-fold cross-validation, as in the previous experiment. As shown in Figure 4, as sample size n increases from 2^4 to 2^{14} , mean absolute error of the Active estimate decreases. Meanwhile, the error of the Passive estimator fails to improve perceptibly. Figure 5 visualizes why the Active algorithm outperforms the Passive algorithm, namely that it preferentially samples simulated scenarios that are similar to, and therefore useful for predicting, the test scenario.

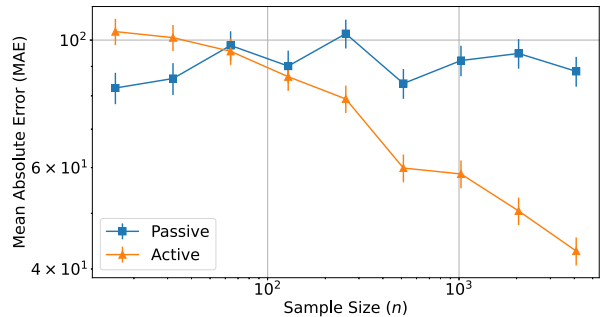


Figure 4: Experiment 2: Mean absolute error of Active and Passive estimates of D_{100} , as a function of sample size n .

9 CONCLUSIONS & FUTURE WORK

This paper studied the nonparametric minimax theory of Indirect Active Learning and a corresponding passive baseline. We showed that active learning asymptotically outperforms passive learning in many cases, and that most of this improvement is realized by a two-stage algorithm using only a very limited form of active learning, which may be easier to implement than fully active algorithms. Finally, we illustrated how behaviors of these algorithms change with parameters of a synthetic data-generating process and demonstrated benefits of two-stage active learning in an epidemiological forecasting application.

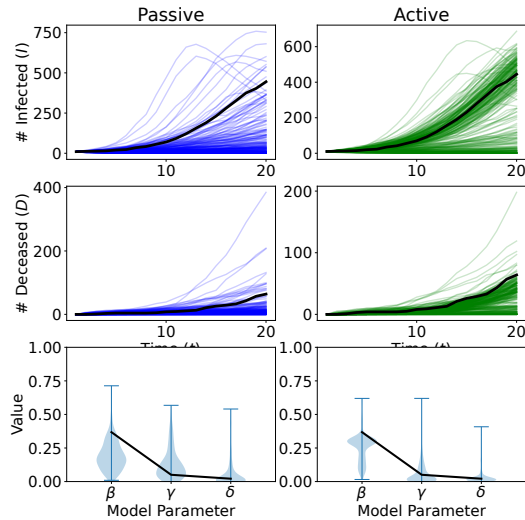


Figure 5: Experiment 2: Example distributions of Infected ($I_{1:20}$) and Deceased ($D_{1:20}$) trajectories over the first 20 days of the outbreak, as well as underlying $Z = (\beta, \gamma, \delta)$ parameters, sampled according to the Passive and Active algorithms. Black lines indicate the test scenario (x_0, z_0) being queried.

Besides closing the gap between our active upper and lower bounds, several interesting directions remain for future work. First, we focused here on a local nonparametric problem of estimating $f(x_0)$ at a single point x_0 . In many cases, it may be more useful or tractable to estimate a global parametric relationship, such as a linear relationship $f(x) = \beta^\top x$. One could additionally assume that g is linear or that either or both of f and g depend sparsely on their inputs, allowing for results that scale better with dimensions d_Z and d_X than our nonparametric results.

Second, as discussed in Section 4, our model of indirect learning assumes the relationship between X and Y is unconfounded given Z , while introducing confounding leads to the instrumental variable setting. When Z is actively manipulated, the relationship between Z and Y is automatically likely to be unconfounded, satisfying a key assumption of instrumental variable methods. Furthermore, we conjecture that active learning approaches such as ours could help address the *problem of weak instruments* (Stock et al., 2002; Murray, 2006; Olea and Pflueger, 2013) by selecting values of Z that induce maximal variation in X .

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A Upper Bound for the Passive Case (Theorem 5)

In this Appendix, we prove our main upper bound for the passive case. We begin by reiterating the result:

Theorem 5 (Main Passive Upper Bound). *Suppose that Z has dimension d_Z around some $z_0 \in \mathcal{Z}$ with $g(z_0) = x_0$. Suppose ε_X is sub-Gaussian and has dimension d_X around 0. Suppose that the response noise ε_Y is sub-Gaussian. Suppose that $g \in \mathcal{C}^{s_g}(\mathcal{Z}, \mathcal{X})$ and $f \in \mathcal{C}^{s_f}(\mathcal{X}, \mathcal{Y})$. Then, there exists a constant $C > 0$ such that, for any $\delta \in (0, 1)$, with probability at least $1 - \delta/2 - 2e^{-k/4}$,*

$$\left| \widehat{f}_{x_0, k} - f(x_0) \right| \leq C \left(\sigma_Y \sqrt{\frac{\log 1/\delta}{k}} + \max \left\{ \left(\left(\frac{k}{n} \right)^{\frac{s_g}{d_Z}} \sqrt{\log \frac{n}{\delta}} \right)^{s_f}, \left(\frac{k \sigma_X^{d_X}}{n} \right)^{\frac{s_f}{d_X + d_Z/s_g}} \right\} \right).$$

In particular, setting

$$k = \max \left\{ 4 \log \frac{4}{\delta}, \min \left\{ \sigma_Y^{\frac{2(d_X + d_Z/s_g)}{2s_f + d_X + d_Z/s_g}} \left(\frac{n}{\sigma_X^{d_X}} \right)^{\frac{2s_f}{2s_f + d_X + d_Z/s_g}}, \sigma_Y^{\frac{2d_Z}{2s_f s_g + d_Z}} n^{\frac{2s_f s_g}{2s_f s_g + d_Z}} \right\} \right\}, \quad (6)$$

gives, with probability $\geq 1 - \delta$, $\left| \widehat{f}_{x_0, k} - f(x_0) \right| \lesssim \Phi_P \log \frac{1}{\delta}$, where

$$\Phi_P = \max \left\{ \left(\frac{1}{n} \right)^{\frac{s_f s_g}{d_Z}}, \left(\frac{\sigma_X^{d_X}}{n} \right)^{\frac{s_f}{d_X + d_Z/s_g}}, \left(\frac{\sigma_Y^2}{n} \right)^{\frac{s_f}{2s_f + d_Z/s_g}}, \left(\frac{\sigma_X^{d_X} \sigma_Y^2}{n} \right)^{\frac{s_f}{2s_f + d_X + d_Z/s_g}} \right\}.$$

Before proving this theorem, we state and prove a few useful lemmas. Our first lemma shows that, under the Local Dimension assumption (Definition 2), the distribution of k -NN distances is tightly concentrated. Such results are commonly used in the analysis of k -NN methods (Kpotufe, 2011; Chaudhuri and Dasgupta, 2014; Biau and Devroye, 2015; Singh and Póczos, 2016; Singh and Khim, 2021):

Lemma 9 (Convergence of k -NN Distance). *Let X be a random variable taking values in a metric space (\mathcal{X}, ρ) , and let X_1, \dots, X_n be IID observations of X . Suppose X has local dimension d around a point $x \in \mathcal{X}$. Then there exist constants $C, \kappa > 0$ such that, whenever $k/n \leq \kappa$, with probability at least $1 - e^{-k/4}$, the distance $\rho(x, X_{\pi_k(x; \{X_1, \dots, X_n\})})$ from x to its k -nearest neighbor in $\{X_1, \dots, X_n\}$ is at most*

$$\rho(x, X_{\pi_k(x; \{X_1, \dots, X_n\})}) \leq C \left(\frac{k}{n} \right)^{1/d}.$$

Proof. By definition of local dimension, there exist $c, r^* > 0$ such that, for all $r \in (0, r^*)$, $\mathbb{P}[\rho(X, x) \leq r] \geq cr^d$. Suppose $\frac{k}{n} \leq \frac{c(r^*)^d}{2}$, so that, for $r := \left(\frac{2k}{cn} \right)^{1/d}$, $r \leq r^*$. Then,

$$\mathbb{P}[\rho(X, x) \leq r] \geq \frac{2k}{n}.$$

Since, for each $i \in [n]$, $1\{\rho(X_i, x) \leq r\} \sim \text{Bernoulli}(\mathbb{P}[\rho(X, x) \leq r])$, by a multiplicative Chernoff bound, with probability at least $1 - e^{-k/4}$,

$$\sum_{i=1}^n 1\{\rho(X_i, x) \leq r\} \geq k,$$

which implies $\rho(x, X_{\pi_k(x; \{X_1, \dots, X_n\})}) \leq r$. □

Our next lemma shows that local dimension is (sub-)additive:

Lemma 10. *Consider two independent \mathbb{R}^d -valued random variables X_1 and X_2 . Under any norm $\|\cdot\| : \mathbb{R}^d \rightarrow \mathbb{R}$, suppose X_1 has local dimension d_1 around x_1 and X_2 has local dimension d_2 around x_2 . Then, $X_1 + X_2$ has local dimension $d_1 + d_2$ around $x_1 + x_2$.*

Proof of Lemma 10. By the triangle inequality and independence of X and ε ,

$$\begin{aligned} \Pr[\|X_1 + X_2 - (x_1 + x_2)\| \leq r] &\geq \Pr[\|X_1\| \leq r/2 \text{ AND } \|X_2\| \leq r/2] \\ &= \Pr[\|X_1\| \leq r/2] \Pr[\|X_2\| \leq r/2]. \end{aligned}$$

The result follows from the definition of local dimension. \square

Finally, the following lemma shows how local dimension of a random variable changes when applying a Hölder-smooth function:

Lemma 11 (Dimension of Pushforward). *Let $(\mathcal{X}, \rho_{\mathcal{X}})$ and $(\mathcal{Y}, \rho_{\mathcal{Y}})$ be metric spaces. Let X be a random variable taking values in \mathcal{X} , and let $f \in \mathcal{C}^s(\mathcal{X}, x; \mathcal{Y})$ be a map from \mathcal{X} to \mathcal{Y} that is locally Hölder continuous around a point $x \in \mathcal{X}$. If X has local dimension d around x in $(\mathcal{X}, \rho_{\mathcal{X}})$, then $f(X)$ has local dimension d/s around $f(x)$ in $(\mathcal{Y}, \rho_{\mathcal{Y}})$.*

Proof. If $\|f\|_{\mathcal{C}^s(\mathcal{X}, x; \mathcal{Y})} = 0$, then f is constant and the result follows trivially. Otherwise, by definition of Hölder continuity,

$$\begin{aligned} \liminf_{r \downarrow 0} \frac{\mathbb{P}[\rho_{\mathcal{Y}}(f(X), f(x)) \leq r]}{r^{d/s}} &= \|f\|_{\mathcal{C}^s(\mathcal{X}, x; \mathcal{Y})}^{-d} \liminf_{r \downarrow 0} \frac{\mathbb{P}[\rho_{\mathcal{Y}}(f(X), f(x)) \leq Lr^s]}{r^d} \\ &\geq \|f\|_{\mathcal{C}^s(\mathcal{X}, x; \mathcal{Y})}^{-d} \liminf_{r \downarrow 0} \frac{\mathbb{P}[\rho_{\mathcal{X}}(X, x) \leq r]}{r^d} > 0, \end{aligned}$$

since X has dimension d around x . \square

We are now ready to prove Theorem 5. The key idea of the proof is that, combining Lemmas 10 and 11, X has dimension $d_X + d_Z/s_g$ around x_0 . Together with Lemma 9, this implies that the distance between x and its k -nearest neighbor among $\{X_1, \dots, X_n\}$ is of order $\left(\frac{k}{n}\right)^{\frac{1}{d_X + d_Z/s_g}}$, determining the bias due to smoothing implicit in the k -NN regressor. The full proof is as follows:

Proof of Theorem 5. For any $X_1, \dots, X_n \in \mathcal{X}$, let

$$\tilde{f}_{x_0, X_1, \dots, X_n, k} = \frac{1}{k} \sum_{i=1}^k f(X_{\pi_i(x; \{X_1, \dots, X_n\})})$$

denote the conditional expectation of $\hat{f}_{x_0, k}$ given X_1, \dots, X_n . By the triangle inequality,

$$\left| \hat{f}_{x_0, k} - f(x_0) \right| \leq \left| \hat{f}_{x_0, k} - \tilde{f}_{x_0, X_1, \dots, X_n, k} \right| + \left| \tilde{f}_{x_0, X_1, \dots, X_n, k} - f(x_0) \right|, \quad (7)$$

where the first term captures stochastic error due to the response noise ε_Y and the second term captures smoothing bias.

For the first term in Eq. (7), since the response noise $\{\varepsilon_{Y, i}\}_{i=1}^n$ is assumed to be additive,

$$\left| \hat{f}_{x_0, k} - \tilde{f}_{x_0, X_1, \dots, X_n, k} \right| = \left| \frac{1}{k} \sum_{i=1}^k \sigma_Y \varepsilon_{Y, \pi_i(x_0; \{X_1, \dots, X_n\})} \right|. \quad (8)$$

Hence, noting that the response noise $\{\varepsilon_{Y, i}\}_{i=1}^n$ is independent of the covariates $\{X_i\}_{i=1}^n$, by a standard concentration inequality for sub-Gaussian random variables (e.g., Lemma 24 in Appendix E), with probability at least $1 - \delta/2$,

$$\left| \hat{f}_{x_0, k} - \tilde{f}_{x_0, X_1, \dots, X_n, k} \right| \leq \sigma_Y \sqrt{\frac{2}{k} \log \frac{4}{\delta}}. \quad (9)$$

For the second term in Eq. (7), by the triangle inequality and local Hölder smoothness of f around x_0 , for some constant

$C_1 > 0$,

$$\begin{aligned}
\left| \tilde{f}_{x_0, X_1, \dots, X_n, k} - f(x_0) \right| &= \left| \frac{1}{k} \sum_{i=1}^k f(X_{\pi_i(x_0; \{X_1, \dots, X_n\})}) - f(x_0) \right| \\
&\leq \frac{1}{k} \sum_{i=1}^k |f(X_{\pi_i(x_0; \{X_1, \dots, X_n\})}) - f(x_0)| \\
&\leq C_1 \frac{1}{k} \sum_{i=1}^k \|x_0 - X_{\pi_i(x_0; \{X_1, \dots, X_n\})}\|^{s_f} \\
&\leq C_1 \|x_0 - X_{\pi_k(x_0; \{X_1, \dots, X_n\})}\|^{s_f}.
\end{aligned} \tag{10}$$

Hence, the remainder of this proof is devoted to bounding the distance $\|x_0 - X_{\pi_k(x_0; \{X_1, \dots, X_n\})}\|$ from x_0 to its k -nearest neighbor in X_1, \dots, X_n .

Combining Lemmas 9, 10, and 11 gives, for some constant $C_2 > 0$, with probability at least $1 - e^{-k/4}$,

$$\|x_0 - X_{\pi_k(x_0; \{X_1, \dots, X_n\})}\| \leq C_2 \left(\frac{k\sigma_X^{d_X}}{n} \right)^{\frac{1}{d_X + d_Z/s_g}}. \tag{11}$$

Now suppose that $(k/n)^{s_g/d_Z} \geq \sigma_X$. By the triangle inequality,

$$\|x_0 - X_{\pi_k(x_0; \{X_1, \dots, X_n\})}\| \leq \|x_0 - X_{\pi_k(x_0; \{g(Z_1), \dots, g(Z_n)\})}\| + \max_{i \in [n]} \|\varepsilon_{X,i}\|. \tag{12}$$

Combining Lemmas 9 and 11, there exists a constant $C_4 > 0$ such that

$$\|x_0 - X_{\pi_k(x_0; \{g(Z_1), \dots, g(Z_n)\})}\| \leq C_4 \left(\frac{k}{n} \right)^{\frac{s_g}{d_Z}}. \tag{13}$$

Meanwhile, by a standard maximal inequality for sub-Gaussian random variables (Lemma 23 in Appendix E), for some constant $C_3 > 0$, with probability at least $1 - \delta/2$,

$$\max_{i \in [n]} \|\varepsilon_i\| \leq \sigma_X \sqrt{2 \log \frac{4n}{\delta}} \leq C_3 \left(\frac{k}{n} \right)^{s_g/d_Z} \sqrt{\log \frac{n}{\delta}}. \tag{14}$$

Plugging Inequalities (13) and (14) into Inequality (12) gives, with probability at least $1 - e^{-k/4}$,

$$\|x_0 - X_{\pi_k(x_0; \{X_1, \dots, X_n\})}\| \leq (C_3 + C_4) \left(\frac{k}{n} \right)^{\frac{s_g}{d_Z}} \sqrt{\log \frac{n}{\delta}}. \tag{15}$$

One can check that, whenever $(k/n)^{s_g/d_Z} < \sigma_X$, the bound (11) dominates the bound (15). Hence, can take the maximum of these two bounds and omit the condition $(k/n)^{s_g/d_Z} \geq \sigma_X$; i.e., for some constant $C_5 > 0$, we always have

$$\|x_0 - X_{\pi_k(x_0; \{X_1, \dots, X_n\})}\| \leq C_5 \max \left\{ \left(\frac{k\sigma_X^{d_X}}{n} \right)^{\frac{1}{d_X + d_Z/s_g}}, \left(\frac{k}{n} \right)^{\frac{s_g}{d_Z}} \sqrt{\log \frac{n}{\delta}} \right\}.$$

plugging this into Inequality (10) gives the desired result. \square

Remark 12 (Heteroscedastic Errors). As noted in Section 3 of the main paper, we can dramatically weaken the assumptions of homoscedastic additive errors. In particular, suppose that the response noise level $\sigma_Y : \mathcal{X} \rightarrow [0, \infty)$ varies as a function of x , so that $Y = f(X) + \sigma_Y(X)\varepsilon_Y$. This difference affects the above proof only in bounding Equation (8).

Specifically, we instead have

$$\begin{aligned} \left| \widehat{f}_{x_0, k} - \widetilde{f}_{x_0, X_1, \dots, X_n, k} \right| &= \left| \frac{1}{k} \sum_{i=1}^k \sigma_Y(X_{\pi_i(x_0; \{X_1, \dots, X_n\})}) \varepsilon_{Y, \pi_i(x_0; \{X_1, \dots, X_n\})} \right| \\ &\leq \left| \frac{1}{k} \sum_{i=1}^k \sigma_Y(x_0) \varepsilon_{Y, \pi_i(x_0; \{X_1, \dots, X_n\})} \right| \\ &\quad + \left| \frac{1}{k} \sum_{i=1}^k (\sigma_Y(X_{\pi_i(x_0; \{X_1, \dots, X_n\})}) - \sigma_Y(x_0)) \varepsilon_{Y, \pi_i(x_0; \{X_1, \dots, X_n\})} \right|. \end{aligned}$$

For the first term above, we get the same bound

$$\left| \frac{1}{k} \sum_{i=1}^k \sigma_Y(x_0) \varepsilon_{Y, \pi_i(x_0; \{X_1, \dots, X_n\})} \right| \leq \sigma_Y(x_0) \sqrt{\frac{2}{k} \log \frac{4}{\delta}}$$

as in the homoscedastic case. Additionally, if the function σ_Y is smooth near x_0 , the second term will be small. Specifically, suppose σ_Y lies in a local Hölder ball $\mathcal{C}^{s_{\sigma_Y}}(\mathcal{X}, x_0; \mathcal{Y}; L_{\sigma_Y})$. Then, Hölder's inequality, a standard maximal inequality for sub-Gaussian random variables (Lemma 23 in Appendix E), and Eq. (11) give, with high probability,

$$\begin{aligned} &\left| \frac{1}{k} \sum_{i=1}^k (\sigma_Y(X_{\pi_i(x_0; \{X_1, \dots, X_n\})}) - \sigma_Y(x_0)) \varepsilon_{Y, \pi_i(x_0; \{X_1, \dots, X_n\})} \right| \\ &\leq |\sigma_Y(X_{\pi_k(x_0; \{X_1, \dots, X_n\})}) - \sigma_Y(x_0)| \max_{i \in [k]} |\varepsilon_{Y, \pi_i(x_0; \{X_1, \dots, X_n\})}| \in O \left(L_{\sigma_Y} \left(\frac{k \sigma_X^{d_X}}{n} \right)^{\frac{s_{\sigma_Y}}{d_X + d_Z / s_g}} \sqrt{\log k} \right). \end{aligned}$$

As long as $s_{\sigma_Y} > s_f$, this additional error is asymptotically negligible compared to the smoothing bias term in Eq. (11).

B Lower Bounds for the Passive Case (Theorem 6)

In this section, we prove our lower bounds on minimax risk in the passive case. Throughout this section, we assume $\mathcal{Z} = [0, 1]^{d_Z}$ and $\mathcal{X} = \mathbb{R}^{d_X}$.

While, in the main paper, we assumed local Hölder continuity of g and f around specific points, we can actually prove stronger lower bounds over *globally* Hölder continuous g and f . Global Hölder continuity is defined as follows:

Definition 13 (Global Hölder Seminorm, Space, and Ball). *For any $s \in [0, 1]$ and metric spaces (\mathcal{Z}, ρ_Z) and (\mathcal{X}, ρ_X) , the global Hölder seminorm $\|\cdot\|_{\mathcal{C}^s(\mathcal{Z}, z_0; \mathcal{X})}$ is defined for $f : \mathcal{Z} \rightarrow \mathcal{X}$ by*

$$\|f\|_{\mathcal{C}^s(\mathcal{Z}; \mathcal{X})} := \sup_{z \in \mathcal{Z}} \|f\|_{\mathcal{C}^s(\mathcal{Z}, z; \mathcal{X})},$$

the global Hölder space $\mathcal{C}^s(\mathcal{Z}; \mathcal{X})$ is

$$\mathcal{C}^s(\mathcal{Z}; \mathcal{X}) := \bigcap_{z \in \mathcal{Z}} \mathcal{C}^s(\mathcal{Z}, z; \mathcal{X}) = \{f : \mathcal{Z} \rightarrow \mathcal{X} \text{ such that } \|f\|_{\mathcal{C}^s(\mathcal{Z}; \mathcal{X})} < \infty\}.$$

For $L \geq 0$, the global Hölder ball $\mathcal{C}^s(\mathcal{Z}; \mathcal{X}; L)$ is

$$\mathcal{C}^s(\mathcal{Z}; \mathcal{X}; L) := \bigcap_{z \in \mathcal{Z}} \mathcal{C}^s(\mathcal{Z}, z_0; \mathcal{X}; L) = \{f : \mathcal{Z} \rightarrow \mathcal{X} \text{ such that } \|f\|_{\mathcal{C}^s(\mathcal{Z}; \mathcal{X})} \leq L\}.$$

Comparing Definition 13 with Definition 1 (local Hölder continuity), one can easily see that global Hölder continuity implies Local Hölder continuity. Therefore, minimax lower bounds under global Hölder continuity immediately imply identical lower bounds under local Hölder continuity.

We can now state our main lower bound for the Passive case:

Theorem 6 (Main Passive Lower Bound). *In the passive case, there exist constants $c_1, c_2, n_0 > 0$, depending only on L_g, s_g, L_f, s_f, d_X , and d_Z , such that, for all $n \geq n_0$,*

$$\sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_D \left[\left| \widehat{f}_{x_0} - f(x_0) \right| \geq c_1 \Phi_P \right] \geq c_2, \quad (16)$$

where

$$\Phi_P = \max \left\{ \left(\frac{1}{n} \right)^{\frac{s_f s_g}{d_Z}}, \left(\frac{\sigma_X^{d_X}}{n} \right)^{\frac{s_f}{d_X + d_Z / s_g}}, \left(\frac{\sigma_Y^2}{n} \right)^{\frac{s_f s_g}{2s_f s_g + d_Z}}, \left(\frac{\sigma_X^{d_X} \sigma_Y^2}{n} \right)^{\frac{s_f}{2s_f + d_X + d_Z / s_g}} \right\}. \quad (17)$$

The remainder of this section is devoted to proving Theorem 6. Since Inequality (16) is a maximum of four lower bounds, we can prove each of these lower bounds separately. Proposition 17 will provide the two terms depending on σ_Y . Proposition 18 will provide the $n^{-\frac{s_f s_g}{d_Z}}$ term. Finally, Proposition 19 will provide the term depending on σ_X but not on σ_Y .

We begin by construct a family $\Theta_{g, M}$ of functions $g : \mathcal{Z} \rightarrow \mathcal{X}$ that will be used throughout the proofs:

Lemma 14. *For any $M \in \mathbb{N}$, $s_g, L_g > 0$, there exists a family $\Theta_{g, M} \subseteq \mathcal{C}^{s_g}(\mathcal{Z}; \mathcal{X}; L_g)$ of globally s_g -Hölder continuous functions from \mathcal{Z} to \mathcal{X} such that:*

1. $|\Theta_{g, M}| = M^{d_Z}$.
2. for each $g \in \Theta_{g, M}$, there exists $z_g \in \mathcal{Z}$ with $g(z_g) = x_0$.
3. for some $g_0 \in \mathcal{X}$ and some constant $C_{d_Z, s_g} > 0$ depending only on d_Z and s_g ,
 - (a) $\|g_0 - x_0\|_\infty = C_{d_Z, s_g} L_g M^{-s_g}$.
 - (b) for $g \neq g' \in \Theta_{g, M}$, the functions $x \mapsto 1\{g(x) \neq g_0\}$, $x \mapsto 1\{g'(x) \neq g_0\}$ have disjoint supports in \mathcal{Z} .

Intuitively, the family $\Theta_{g, M}$ is constructed such that, for any $z \in \mathcal{Z}$, there is no more than one $g \in \Theta_{g, M}$ such that $\|g(z) - x_0\|_\infty \lesssim M^{-s_g}$; hence, for the typical $g \in \Theta_{g, M}$, $\lesssim 1/|\Theta_{g, M}|$ of the samples X_1, \dots, X_n will lie within $\asymp M^{-s_g}$ of x_0 . The formal construction of $\Theta_{g, M}$ is as follows:

Proof. For any positive integer d , let $K_d : \mathbb{R}^d \rightarrow \mathbb{R}$ denote the standard d -dimensional ‘‘bump function’’ defined by

$$K_d(x) = \exp \left(1 - \frac{1}{1 - \|x\|_2^2} \right) 1\{\|x\|_2 \leq 1\} \quad \text{for all } x \in \mathbb{R}^d. \quad (18)$$

Note in particular that K_d satisfies the following:

1. $K_d \in \mathcal{C}^\infty(\mathbb{R}^d)$; i.e., K_d is infinitely differentiable.
2. For all $x \notin (-1, 1)^d$, $K_d(x) = 0$.
3. $\|K_d\|_\infty = K(0) = 1$.

For any $m \in [M]^{d_Z}$, define $g_m : \mathcal{Z} \rightarrow \mathcal{X}$ by

$$g_m(z) = x_0 + \frac{L_g}{M^{s_g} \|K_{d_Z}\|_{\mathcal{C}^{s_g}}} (K_{d_Z}(0) - K_{d_Z}((M+1)z - m)) v, \quad \text{for all } z \in \mathcal{Z}, \quad (19)$$

where v is an arbitrary unit vector in \mathbb{R}^{d_X} . Then, define $\Theta_{g, M} := \{g_m : m \in [M]^{d_Z}\}$. Clearly, $|\Theta_{g, M}| = M^{d_Z}$. By Eq. (19), $\Theta_{g, M} \subseteq \mathcal{C}^{s_g}(\mathcal{Z}; \mathcal{X}; L_g)$. Moreover, for each $m \in [M]^{d_Z}$, $g_m(m/(M+1)) = x_0$, while, whenever $\|(M+1)z - m\|_\infty \geq 1$, $g_m(z) = g_0 := x_0 + \frac{L_g}{\|K_{d_Z}\|_{\mathcal{C}^{s_g}}} M^{-s_g} v$. \square

Next, we present a general information-theoretic lower bound in the ‘‘stochastic case’’, i.e., in the presence of response noise ($\sigma_Y > 0$). Together with the construction of the family $\Theta_{g, M}$ in Lemma 14, this lemma will be the basis for our lower bounds depending on σ_Y , in both the active and passive cases:

Lemma 15 (General Lower Bound with Response Noise). *Suppose $Y_i|X_i \sim \mathcal{N}(f(X_i), \sigma_Y^2)$, and suppose that the distribution of (Z_i, X_i) depends only on the preceding observations $\{(Z_j, X_j, Y_j)\}_{j=1}^{i-1}$. Let $h > 0$, and let P_g be any probability distribution over $\mathcal{C}^{s_g}(\mathcal{Z}; \mathcal{X}; L_g)$. Then, there exist $f_0, f_1 \in \mathcal{C}^{s_f}(\mathcal{X}; \mathcal{Y}; L_f)$ such that, if $P_0 = P_g \times \delta_{f_0}$ is the product distribution of P_g and a unit mass on f_0 , and P_1 is the product distribution of P_g and a unit mass on f_1 , for some constant $C_{d_X, s_f} > 0$ depending only on d_X and s_f ,*

$$\begin{aligned} & \inf_{\widehat{f}_{x_0}} \sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_D \left[|\widehat{f}_{x_0} - f(x_0)| \geq C_{d_X, s_f} L_f h^{s_f} \right] \\ & \geq \frac{1}{2} \left(1 - C_{d_X, s_f} \frac{L_f h^{s_f}}{\sigma_Y} \sqrt{\sum_{i=1}^n \mathbb{E}_{D, g \sim P_0} [1\{\|X_i - x_0\|_\infty < h\}]} \right). \end{aligned} \quad (20)$$

Here, the infimum is taken over all estimators \widehat{f}_{x_0} (i.e., all functions $\widehat{f}_{x_0} : (\mathcal{Z} \times \mathcal{X} \times \mathcal{Y})^n \rightarrow \mathcal{Y}$), the supremum is taken over all $g \in \mathcal{C}^{s_g}(\mathcal{Z}; \mathcal{X}; L_g)$, $f \in \mathcal{C}^{s_f}(\mathcal{X}; \mathcal{Y}; L_f)$, sub-Gaussian covariate noise random variables ε_X with dimension d_X around 0, and sub-Gaussian response noise random variables ε_Y , and we used the shorthand $D := \{(Z_i, X_i, Y_i)\}_{i=1}^n$ to denote the entire dataset.

Intuitively, Lemma 15 provides a lower bound in terms of the expected number of covariate observations X_i that are “informative” about $f(x_0)$, i.e., those that lie sufficiently near x_0 . The family $\Theta_{g, M}$ was constructed in Lemma 14 such that Hence, it remains only to bound the expected number of such X_i , which will be small for g lying in the family $\Theta_{g, M}$. Note that inequality (20) applies in both active and passive settings. However, in the passive setting, the distribution of each Z_i will be independent of g , whereas, in the active setting, Z_i may depend on g through the preceding observations (specifically, $(Z_1, X_1), \dots, (Z_{i-1}, X_{i-1})$).

The proof of Lemma 15 is based on the method of two fuzzy hypotheses, specifically the following lemma:

Lemma 16 (Theorem 2.15 of Tsybakov (2008), Total Variation Case). *Let P_0 and P_1 be probability distributions over Θ , and let $F : \Theta \rightarrow \mathbb{R}$. Suppose*

$$\sup_{\theta \in \text{supp}(P_0)} F(\theta) \leq 0, \quad \text{and} \quad s := \inf_{\theta \in \text{supp}(P_1)} F(\theta) > 0. \quad (21)$$

Then,

$$\inf_{\widehat{F}} \sup_{\theta \in \Theta} \Pr_{\theta} \left[|\widehat{F} - F(\theta)| \geq s/2 \right] \geq \frac{1 - D_{TV}(P_0, P_1)}{2}.$$

The method of two fuzzy hypotheses is one of several standard methods for deriving minimax lower bounds on statistical estimation error (see Chapter 2 of Tsybakov (2008) for further discussion of this and other methods). The method of two fuzzy hypotheses, in particular, is typically used in semiparametric problems where one wishes to estimate a parametric quantity (here, $\widehat{f}(x_0)$) that is subject to variation in a nonparametric “nuisance” quantity (here, g). The key idea of the method is to lower bound the supremum over the nuisance quantity (here, \sup_g) by in terms of an appropriate information-theoretic measure (here D_{TV}) computed over an appropriately chosen distribution of the nuisance variable (here, P_g). By choosing this distribution carefully (as we will do later in this section, using the family $\Theta_{g, M}$ constructed in Lemma 14), the information-theoretic measure will give a tight lower bound on the probability of error.

We now present the proof of Lemma 15.

Proof. Let $h > 0$. Define $f_0, f_1 : \mathcal{X} \rightarrow \mathcal{Y}$ by

$$f_0(x) = 0 \quad \text{and} \quad f_1(x) = \frac{L_f h^{s_f}}{\|K_{d_X}\|_{\mathcal{C}^{s_f}}} K_{d_X} \left(\frac{x - x_0}{h} \right) \quad \text{for all } x \in \mathcal{X}, \quad (22)$$

where K_{d_X} is as defined in Eq. (18). Clearly,

$$\sup_{(g, f) \in \text{supp}(P_0)} f(x_0) = 0,$$

while

$$s := \inf_{(g, f) \in \text{supp}(P_1)} f(x_0) = \frac{L_f h^{s_f}}{\|K_{d_X}\|_{\mathcal{C}^{s_f}}} K_{d_X}(0) = \frac{L_f h^{s_f}}{\|K_{d_X}\|_{\mathcal{C}^{s_f}}}, \quad (23)$$

satisfying the condition (21). It remains only to bound $D_{\text{TV}}(P_0, P_1)$. For each $i \in [n]$, let $P_{0,i}$ and $P_{1,i}$ denote the conditional distributions of

$$(Z_i, X_i, Y_i) \quad \text{given} \quad (Z_1, X_1, Y_1), \dots, (Z_{i-1}, X_{i-1}, Y_{i-1})$$

under P_0 and P_1 , respectively, and let $P_{Y,0,i}$ and $P_{Y,1,i}$ denote the conditional distributions of

$$Y_i \quad \text{given} \quad (Z_1, X_1, Y_1), \dots, (Z_{i-1}, X_{i-1}, Y_{i-1}), (Z_i, X_i)$$

under P_0 and P_1 , respectively. By a standard formula for the KL divergence between two Gaussian random variables,

$$D_{\text{KL}}(P_{Y,0,i} \| P_{Y,1,i}) = \frac{f_1^2(X_i)}{2\sigma_Y^2}.$$

Moreover, by construction of P_0 and P_1 , the conditional distributions of

$$(Z_i, X_i) \quad \text{given} \quad (Z_1, X_1, Y_1), \dots, (Z_{i-1}, X_{i-1}, Y_{i-1})$$

are identical under P_0 and P_1 . Therefore, by the chain rule for KL divergence,

$$\begin{aligned} D_{\text{KL}}(P_0, P_1) &= \sum_{i=1}^n \mathbb{E}_{D, g \sim P_0} [D_{\text{KL}}(P_{0,i} \| P_{1,i})] \\ &= \sum_{i=1}^n \mathbb{E}_{D, g \sim P_0} [D_{\text{KL}}(P_{Y,0,i} \| P_{Y,1,i})] \\ &= \frac{1}{2\sigma_Y^2} \sum_{i=1}^n \mathbb{E}_{D, g \sim P_0} [f_1^2(X_i)] \\ &\leq \frac{\|f_1\|_\infty^2}{2\sigma_Y^2} \sum_{i=1}^n \mathbb{E}_{D, g \sim P_0} [1\{f_1(X_i) \neq 0\}] \\ &= \frac{L_f^2 h^{2s_f}}{2\sigma_Y^2 \|K_{d_X}\|_{\mathcal{C}^{s_f}}^2} \sum_{i=1}^n \mathbb{E}_{D, g \sim P_0} [1\{f_1(X_i) \neq 0\}] \\ &\leq \frac{L_f^2 h^{2s_f}}{2\sigma_Y^2 \|K_{d_X}\|_{\mathcal{C}^{s_f}}^2} \sum_{i=1}^n \mathbb{E}_{D, g \sim P_0} [1\{\|X_i - x_0\|_\infty < h\}], \end{aligned}$$

where the last inequality follows from the fact that f_1 is non-zero only on the open ℓ_∞ ball of radius h centered at x_0 (see Eq. (22)). Thus, by Pinsker's Inequality,

$$D_{\text{TV}}(P_0, P_1) \leq \sqrt{2D_{\text{KL}}(P_0, P_1)} \leq \frac{L_f h^{s_f}}{\sigma_Y \|K_{d_X}\|_{\mathcal{C}^{s_f}}} \sqrt{\sum_{i=1}^n \mathbb{E}_{D, g \sim P_0} [1\{\|X_i - x_0\|_\infty < h\}]}$$

The result now follows by plugging this bound on $D_{\text{TV}}(P_0, P_1)$ into Lemma 16. \square

We now utilize Lemma 15 to prove the following minimax lower bound for the passive case under response noise:

Proposition 17 (Minimax Lower Bound, Passive Case, σ_Y large). *In the passive case, there exists a constant $C > 0$ depending only on $d_Z, d_X, s_g, L_g, s_f, L_f$ such that*

$$\sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_D \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq C \max \left\{ \left(\frac{\sigma_Y^2}{n} \right)^{\frac{s_f s_g}{2s_f s_g + d_Z}}, \left(\frac{\sigma_X^2 \sigma_Y^2}{n} \right)^{\frac{s_f}{2s_f + d_X + d_Z/s_g}} \right\} \right] \geq \frac{1}{4}.$$

Proof. Consider the case in which $\sigma_{X \in X_i}$ is uniformly distributed over the cube $[-\frac{\sigma_X}{\sqrt{d_X}}, \frac{\sigma_X}{\sqrt{d_X}}]^{d_X}$. Let

$$h := \begin{cases} \left(\frac{\|K_{d_X}\|_{\mathcal{C}^{s_f}}^2 L_g^{d_Z/s_g} \sigma_Y^2}{2^{2+d_Z/s_g} L_f^2 n} \right)^{\frac{1}{2s_f + d_Z/s_g}} & \text{if } \sigma_X \leq d_X^{-1/2} \left(\frac{\|K_{d_X}\|_{\mathcal{C}^{s_f}}^2 L_g^{d_Z/s_g} \sigma_Y^2}{2^{2+d_Z/s_g} L_f^2 n} \right)^{\frac{1}{2s_f + d_Z/s_g}} \\ \left(\frac{\|K_{d_X}\|_{\mathcal{C}^{s_f}}^2 L_g^{d_Z/s_g} \sigma_X^2 \sigma_Y^2}{2^{2+d_Z/s_g} d_X^{d_X/2} L_f^2 n} \right)^{\frac{1}{2s_f + d_X + d_Z/s_g}} & \text{else} \end{cases} \quad (24)$$

and

$$M := \left(\frac{L_g}{\|K_{d_Z}\|_{C^{s_g}} \left(h + \frac{\sigma_X}{\sqrt{d_X}} \right)} \right)^{1/s_g}. \quad (25)$$

Suppose P_g is the uniform distribution over $\Theta_{g,M}$, given in Lemma 14.

By the Law of Total Probability,

$$\begin{aligned} \mathbb{E}_{D,g \sim P_0} [1\{\|X_i - x_0\|_\infty < h\}] &= \Pr_{D,g \sim P_0} [\|g(Z_i) + \sigma_X \varepsilon_{X,i} - x_0\|_\infty < h] \\ &\leq \Pr_{D,g \sim P_0} [\|g(Z_i) + \sigma_X \varepsilon_{X,i} - x_0\|_\infty < h | g(Z_i) \neq g_0] \Pr_{D,g \sim P_0} [g(Z_i) \neq g_0] \\ &\quad + \Pr_{D,g \sim P_0} [\|g(Z_i) + \sigma_X \varepsilon_{X,i} - x_0\|_\infty < h | g(Z_i) = g_0] \end{aligned} \quad (26)$$

Since in the passive case, g is uniformly distributed over $\Theta_{g,M}$ independently of Z_i and the elements of $\Theta_{g,M}$ have disjoint supports,

$$\Pr_{D,g \sim P_0} [g(Z_i) \neq g_0] \leq \frac{1}{|\Theta_{g,M}|} = M^{-d_Z} = \left(\frac{\|K_{d_Z}\|_{C^{s_g}}}{L_g} \left(h + \frac{\sigma_X}{\sqrt{d_X}} \right) \right)^{d_Z/s_g}.$$

Since $\varepsilon_{X,i}$ has a uniform distribution with mean 0, the function $x \mapsto \Pr[\|\sigma_X \varepsilon_{X,i} + x\| \leq h]$ is maximized at $x = 0$, and so, similar to Inequality (42),

$$\begin{aligned} \Pr_{D,g \sim P_0} [\|g(Z_i) + \sigma_X \varepsilon_{X,i} - x_0\|_\infty < h | g(Z_i) \neq g_0] &\leq \Pr_{D,g \sim P_0} [\|\sigma_X \varepsilon_{X,i}\|_\infty < h | g(Z_i) \neq g_0] \\ &= \min \left\{ 1, \left(\frac{h\sqrt{d_X}}{\sigma_X} \right)^{d_X} \right\}. \end{aligned}$$

Finally, since $\sigma_X \varepsilon_{X,i}$ is uniformly distributed over the cube $[-\frac{\sigma_X}{\sqrt{d_X}}, \frac{\sigma_X}{\sqrt{d_X}}]^{d_X}$, by our choice (Eq. (25)) of M , if $g(Z_i) = g_0$, then there is no overlap between the supports of X_i and f_1 ; formally,

$$\begin{aligned} \Pr_{D,g \sim P_0} [\|g(Z_i) + \sigma_X \varepsilon_{X,i} - x_0\|_\infty < h | g(Z_i) = g_0] &= \left(\max \left\{ 0, x_0 + h - g_0 + \frac{\sigma_X}{\sqrt{d_X}} \right\} \right)^{d_X} \\ &= \left(\max \left\{ 0, h + \frac{\sigma_X}{\sqrt{d_X}} - \frac{L_g}{M^{s_g} \|K_{d_Z}\|_{C^{s_g}}} \right\} \right)^{d_X} = 0. \end{aligned}$$

Plugging these into Inequality (26) gives

$$\mathbb{E}_{D,g \sim P_0} [1\{\|X_i - x_0\|_\infty < h\}] \leq \min \left\{ 1, \left(\frac{h\sqrt{d_X}}{\sigma_X} \right)^{d_X} \right\} \left(\frac{\|K_{d_Z}\|_{C^{s_g}}}{L_g} \left(h + \frac{\sigma_X}{\sqrt{d_X}} \right) \right)^{d_Z/s_g}, \quad (27)$$

and plugging this into Lemma (15) gives

$$\begin{aligned} \inf_{\hat{f}_{x_0}} \sup_{g,f,P_Z,\varepsilon_X,\varepsilon_Y} \Pr_D [|\hat{f}_{x_0} - f(x_0)| \geq Ch^{s_f}] \\ \geq \frac{1}{2} \left(1 - C \frac{h^{s_f}}{\sigma_Y} \sqrt{n \min \left\{ 1, \left(\frac{h\sqrt{d_X}}{\sigma_X} \right)^{d_X} \right\} \left(h + \frac{\sigma_X}{\sqrt{d_X}} \right)^{d_Z/s_g}} \right), \end{aligned}$$

where $C > 0$ is a constant depending only on d_X, L_f, s_f, d_Z, L_g , and s_g . Plugging in the appropriate value of h , according to Eq. (24), depending on whether σ_X is greater or less than $h/\sqrt{d_X}$, gives

$$\inf_{\hat{F}} \sup_{\theta \in \Theta} \Pr_\theta [|\hat{F} - F(\theta)| \geq s/2] \geq \frac{1}{4},$$

where

$$s \asymp \begin{cases} \left(\frac{\sigma_Y^2}{n} \right)^{\frac{s_f s_g}{2s_f s_g + d_Z}} : & \text{if } \sigma_X \sqrt{d_X} \leq \left(\frac{1}{2^{2+d_Z/s_g}} \frac{L_g^{d_Z/s_g}}{L_f^2} \frac{\|K_{d_X}\|_{C^{s_f}}^2 \sigma_Y^2}{\|K_{d_Z}\|_{C^{s_g}}^{s_f/s_g} n} \right)^{\frac{1}{2s_f + d_Z/s_g}} \\ \left(\frac{\sigma_X^{d_X} \sigma_Y^2}{n} \right)^{\frac{s_f}{2s_f + d_X + d_Z/s_g}} : & \text{else} \end{cases}$$

□

Proposition 17 provided minimax lower bounds for the passive case under response noise of scale $\sigma_Y > 0$, based on information-theoretic bounds showing that the information obtainable from a single pair (X_i, Y_i) decays as σ_Y^{-2} ; hence, a different approach is needed to obtain tight bounds when σ_Y is very small or 0. Our next results provide tight lower bounds for the case when σ_Y is small or 0 using a combinatorial, rather than information-theoretic, approach. In particular, we show that, given a sufficiently large family $\Theta_{g,M}$ of functions g with $x \mapsto 1\{g(x) \neq g_0\}$ having disjoint supports, the probability of observing any X_i with $g(X_i) \neq g_0$ is small.

Proposition 18 (Minimax Lower Bound, Active and Passive Case, σ_X small, σ_Y small). *In both active and passive cases,*

$$\inf_{\hat{f}_{x_0}} \sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_D \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq C \left(\frac{1}{n} \right)^{\frac{s_f s_g}{d_Z}} \right] \geq \frac{1}{4}, \quad (28)$$

where C is a constant (given in Eq. (29)) depending only on L_g, s_g, L_f, s_f, d_X , and d_Z .

We note that, in contrast to other the other lower bounds in this section, Proposition 18 applies to to both the active and passive settings, as its proof makes no assumptions on the distribution of the control variables Z_1, \dots, Z_n .

Proof. Let $\Theta_{g,M}$ be as given in Lemma 14, with $M := \lceil (2n)^{1/d_Z} \rceil$. Additionally, let f_0 and f_1 be as in Eq. (22). For each $g \in \Theta_{g,M}$, let E_g denote the event $g(Z_1) = g(Z_2) = \dots = g(Z_n) = g_0$. Since, for any $g_1 \neq g_2 \in \Theta_{g,M}$, the functions $z \mapsto 1\{g_1(z) \neq g_0\}$ and $z \mapsto 1\{g_2(z) \neq g_0\}$ have disjoint support, for any Z_1, \dots, Z_n ,

$$\sum_{g \in \Theta_{g,M}} 1 - 1_{E_g} \leq n.$$

Since, by our choice of M , $|\Theta_{g,M}| = M^{d_Z} \geq 2n$, for any (potentially randomized) estimator \hat{f}_{x_0} ,

$$\begin{aligned} |\Theta_{g,M}| \max_{g \in \Theta_{g,M}} \Pr[E_g] &\geq \sum_{g \in \Theta_{g,M}} \Pr[E_g] \\ &= \mathbb{E} \left[\sum_{g \in \Theta_{g,M}} 1_{E_g} \right] \\ &= \mathbb{E} \left[\sum_{g \in \Theta_{g,M}} 1 - (1 - 1_{E_g}) \right] \geq |\Theta_{g,M}| - n \geq n, \end{aligned}$$

and so there exists $g_{\hat{f}_{x_0}} \in \Theta_{g,M}$ such that

$$\Pr \left[E_{g_{\hat{f}_{x_0}}} \mid g = g_{\hat{f}_{x_0}} \right] \geq \frac{n}{|\Theta_{g,M}|} \geq \frac{n}{((2n)^{1/d_Z} + 1)^{d_Z}} \geq 2^{-d_Z - 1}.$$

For $h := \|x_0 - g_0\|_\infty = \frac{L_g}{M^{s_g} \|K_{d_Z}\|_{C^{s_g}}}$, under the event E_g , the distribution of the data $\{(X_i, Y_i, Z_i)\}_{i=1}^n$ is independent of whether $f = f_0$ or $f = f_1$. In particular, either

$$\Pr \left[\hat{f}_{x_0} \geq \frac{f_0(x_0) + f_1(x_0)}{2} \mid f = f_0 \right] \geq \frac{1}{2} \quad \text{or} \quad \Pr \left[\hat{f}_{x_0} \leq \frac{f_0(x_0) + f_1(x_0)}{2} \mid f = f_1 \right] \geq \frac{1}{2},$$

and so

$$\max_{g \in \Theta_{g,M}, f \in \{f_0, f_1\}} \Pr \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq \frac{|f_1(x_0) - f_0(x_0)|}{2} \right] \geq \frac{1}{2} \Pr[E_{g_{\hat{f}_{x_0}}}] \geq 2^{-d_Z - 2}.$$

By construction of f_0 and f_1 ,

$$|f_1(x_0) - f_0(x_0)| = \frac{L_f h^{s_f}}{\|K_{d_X}\|_{C^{s_f}}},$$

and so plugging in our choices of M and h gives

$$\max_{g \in \Theta_{g,M}, f \in \{f_0, f_1\}} \Pr \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq \frac{L_f L_g^{s_f}}{2 \|K_{d_X}\|_{C^{s_f}} \|K_{d_Z}\|_{C^{s_g}}^{s_f} ((2n)^{s_f s_g / d_Z} + 1)} \right] \geq 2^{-d_Z - 2}. \quad (29)$$

□

Proposition 19 (Minimax Lower Bound, Passive Case, σ_X large, σ_Y small). *In the passive case, for some constant $C > 0$, whenever $n \geq C\sigma_X^{-d_Z/s_g}$,*

$$\inf_{\hat{f}_{x_0}} \sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_D \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq C \left(\frac{\sigma_X^{d_X}}{n} \right)^{\frac{s_f}{d_X + d_Z/s_g}} \right] \geq \frac{1}{2e} > 0, \quad (30)$$

where $C > 0$ (given below in Eq. (32)) depends only on L_g, s_g, L_f, s_f, d_X , and d_Z .

We note that the condition $n \gtrsim \sigma_X^{-d_Z/s_g}$ is precisely when the rate $\left(\sigma_X^{d_X}/n\right)^{\frac{s_f}{d_X + d_Z/s_g}}$ in Proposition 19 dominates the rate $n^{-\frac{s_f s_g}{d_Z}}$ obtained earlier in Proposition 18; hence, this condition can be omitted when we take the maximum of these lower bounds in Theorem 6.

Proof. Suppose Z is uniformly distributed over \mathcal{Z} and $\sigma_X \varepsilon_{X,i}$ is uniformly distributed on the set $\{0\} \times [-\frac{\sigma_X}{\sqrt{d_X}}, \frac{\sigma_X}{\sqrt{d_X}}]^{d_X} \subseteq \mathbb{R}^{d_X+1}$ (i.e., the first coordinate of $\varepsilon_{X,i}$ is always 0 and the remaining d_X coordinates are uniformly random). Define $g : \mathcal{Z} \rightarrow \mathcal{X}$ by $g(z) = L_g \|z\|_\infty^{s_g} e_1$, where $e_1 \in \mathbb{R}^{d_X+1}$ denotes the first canonical basis vector. It is straightforward to verify that (a) Z has dimension d_Z around 0, (b) $\varepsilon_{X,i}$ is sub-Gaussian, (c) $\varepsilon_{X,i}$ has dimension d_X around 0, and (d) $g \in \mathcal{C}^{s_g}(\mathcal{Z}; \mathcal{X})$. Let f_0 and f_1 be as in Eq. (22) with $x_0 = 0$.

Let $r^* := \min\{L_g, \frac{\sigma_X}{\sqrt{d_X}}\}$. Then, for each $i \in [n]$ and any $r \in [0, r^*]$, since Z_i and $\varepsilon_{X,i}$ are independent,

$$\begin{aligned} \Pr[\|X_i\|_\infty \leq r] &= \Pr[\max\{\|g(Z_i)\|, \|\varepsilon_i\|_\infty\} \leq r] \\ &= \Pr[\|Z_i\|_\infty \leq (r/L_g)^{1/s_g}] \Pr[\|\varepsilon_i\|_\infty \leq r] \\ &= \left(\frac{r}{L_g}\right)^{d_Z/s_g} \left(\frac{r\sqrt{d_X}}{\sigma_X}\right)^{d_X}. \end{aligned}$$

Since, in the passive case, X_1, \dots, X_n are IID,

$$\begin{aligned} \Pr\left[\min_{i \in [n]} \|X_i\|_\infty \geq r\right] &= (\Pr[\|X_i\|_\infty \geq r])^n \\ &= (1 - \Pr[\|X_i\|_\infty \leq r])^n \\ &= \left(1 - \left(\frac{r}{L_g}\right)^{d_Z/s_g} \left(\frac{r\sqrt{d_X}}{\sigma_X}\right)^{d_X}\right)^n. \end{aligned}$$

For n sufficiently large that $r \leq r^*$ (i.e., $n \geq C\sigma_X^{-d_Z/s_g}$, as assumed), plugging in

$$r = \left(\left(\frac{\sigma_X}{\sqrt{d_X}}\right)^{d_X} \frac{L_g^{d_Z/s_g}}{n}\right)^{\frac{1}{d_X + d_Z/s_g}} \quad (31)$$

gives

$$\Pr\left[\min_{i \in [n]} \|X_i\|_\infty \geq \left(\left(\frac{\sigma_X}{\sqrt{d_X}}\right)^{d_X} \frac{L_g^{d_Z/s_g}}{n}\right)^{\frac{1}{d_X + d_Z/s_g}}\right] = \left(1 - \frac{1}{n}\right)^n \geq 1/e > 0,$$

since $(1 - \frac{1}{n})^n$ approaches $1/e$ from above as $n \rightarrow \infty$.

Now let f_0 and f_1 be as in Eq. (22), with $h = r$ above. Given the event $\min_{i \in [n]} \|X_i\|_\infty \geq h$, the distribution of the data $\{(X_i, Y_i, Z_i)\}_{i=1}^n$ is independent of whether $f = f_0$ or $f = f_1$. Hence, as argued in the proof of the previous Proposition (18),

$$\max_{f \in \{f_0, f_1\}} \Pr\left[\left|\hat{f}_{x_0} - f(x_0)\right| \geq \frac{|f_1(x_0) - f_0(x_0)|}{2}\right] \geq \frac{1}{2} \Pr\left[\min_{i \in [n]} \|X_i\|_\infty \leq h\right] \geq \frac{1}{2e}.$$

Since, by construction of f_0 and f_1 ,

$$|f_1(x_0) - f_0(x_0)| = \frac{L_f h^{s_f}}{\|K_{d_X}\|_{\mathcal{C}^{s_f}}},$$

it follows that

$$\max_{f \in \{f_0, f_1\}} \Pr \left[\left| \widehat{f}_{x_0} - f(x_0) \right| \geq \frac{L_f h^{s_f}}{2\|K_{d_X}\|_{\mathcal{C}^{s_f}}} \right] \geq \frac{1}{2e}.$$

Plugging in our choice of $h = r$ from Eq (31) above gives

$$\max_{f \in \{f_0, f_1\}} \Pr \left[\left| \widehat{f}_{x_0} - f(x_0) \right| \geq C \left(\frac{\sigma_X}{n} \right)^{\frac{s_f}{d_X + d_Z/s_g}} \right] \geq \frac{1}{2e},$$

where

$$C = \frac{L_f \left(d_X^{-d_X/2} L_g^{d_Z/s_g} \right)^{\frac{s_f}{d_X + d_Z/s_g}}}{2\|K_{d_X}\|_{\mathcal{C}^{s_f}}}. \quad (32)$$

□

C Upper Bound for the Active Case (Theorem 7)

In this section, we state and prove our main upper bound for the two-stage active learner presented in Algorithm 1. We first state the full result:

Theorem 7 (Main Active Upper Bound). *Let $\delta \in (0, 1)$. Let \widehat{f}_{x_0} denote the estimator proposed in Algorithm 1, with $k, \ell \geq 4 \log \frac{6}{\delta}$. Then, for some constant $C > 0$ depending only on L_g, s_g, L_f, s_f, d_X , and d_Z , with probability at least $1 - \delta$,*

$$\left| \widehat{f}_{x_0, k} - f(x_0) \right| \leq C_4 \left(\sigma_Y \sqrt{\frac{1}{k} \log \frac{1}{\delta}} + \sigma_X^{s_f} \left(\frac{k}{n} \right)^{\frac{s_f}{d_X}} + \left(\frac{\ell}{n} \right)^{\frac{s_f s_g}{d_Z}} + \left(\sigma_X \sqrt{\frac{1}{\ell} \log \frac{n}{\delta}} \right)^{s_f} \right),$$

In particular, setting

$$k \asymp \max \left\{ \log \frac{1}{\delta}, \min \left\{ n, \left(\frac{\sigma_Y}{\sigma_X^{s_f}} \right)^{\frac{2d_X}{2s_f + d_X}} n^{\frac{2s_f}{2s_f + d_X}} \right\} \right\} \quad (33)$$

and

$$\ell \asymp \max \left\{ \log \frac{1}{\delta}, \min \left\{ n, \sigma_X^{\frac{2d_Z}{2s_g + d_Z}} n^{\frac{2s_g}{2s_g + d_Z}} (\log n)^{\frac{d_Z}{2s_g + d_Z}} \right\} \right\}, \quad (34)$$

we have, with probability at least $1 - \delta$, $\left| \widehat{f}_{x_0} - f(x_0) \right| \leq C \Phi_A^* \log \frac{1}{\delta}$, where

$$\Phi_A^* := \max \left\{ \left(\frac{1}{n} \right)^{\frac{s_f s_g}{d_Z}}, \left(\frac{\sigma_X^{d_X}}{n} \right)^{\frac{s_f}{d_X}}, \frac{\sigma_Y}{\sqrt{n}}, \left(\frac{\sigma_Y^2 \sigma_X^{d_X}}{n} \right)^{\frac{s_f}{2s_f + d_X}}, \left(\frac{\sigma_X^2 \log n}{n} \right)^{\frac{s_f s_g}{2s_g + d_Z}} \right\}.$$

We now prove the result, utilizing several lemmas and key steps from the Passive upper bound in Appendix A.

Proof. As in the proof of the Passive Upper Bound (Theorem 5), for any $X_1, \dots, X_n \in \mathcal{X}$, let

$$\widetilde{f}_{x_0, X_1, \dots, X_n, k} = \frac{1}{k} \sum_{i=1}^k f(X_{\pi_i(x_0; \{X_1, \dots, X_n\})})$$

denote the conditional expectation of $\widehat{f}_{x_0, k}$ given X_1, \dots, X_n . By the triangle inequality,

$$\left| \widehat{f}_{x_0, k} - f(x_0) \right| \leq \left| \widehat{f}_{x_0, k} - \widetilde{f}_{x_0, X_1, \dots, X_n, k} \right| + \left| \widetilde{f}_{x_0, X_1, \dots, X_n, k} - f(x_0) \right|, \quad (35)$$

where the first term captures stochastic error due to the response noise ε_Y and the second term captures smoothing bias.

For the first term in Eq. (35), as argued in the passive case (see Eq. (36)), since the response noise ε_Y is sub-Gaussian, with probability at least $1 - \delta/2$,

$$\left| \widehat{f}_{x_0, k} - \widetilde{f}_{x_0, X_1, \dots, X_n, k} \right| \leq \sigma_Y \sqrt{\frac{2}{k} \log \frac{4}{\delta}}. \quad (36)$$

For the second term in Eq. (35), by the triangle inequality and local Hölder continuity of f around x_0 , for some constant $C_1 > 0$,

$$\begin{aligned} \left| \widetilde{f}_{x_0, X_1, \dots, X_n, k} - f(x_0) \right| &\leq \frac{1}{k} \sum_{i=1}^k \left| f(X_{\pi_i(x_0; \{X_1, \dots, X_n\})}) - f(x_0) \right| \\ &\leq \frac{C_1}{k} \sum_{i=1}^k \left\| X_{\pi_i(x_0; \{X_1, \dots, X_n\})} - x_0 \right\|^{s_f} \\ &\leq C_1 \left\| X_{\pi_k(x_0; \{X_1, \dots, X_n\})} - x_0 \right\|^{s_f}. \end{aligned} \quad (37)$$

By Lemmas 9 and 11, for some constant $C_2 > 0$, with probability at least $1 - \delta/6$, if $\ell \geq 4 \log \frac{6}{\delta}$,

$$\left\| g(Z_{\pi_\ell(x_0, \{g(Z_1), \dots, g(Z_\ell)\})}) - x_0 \right\| \leq C_2 \left(\frac{\ell}{m} \right)^{s_g/d_Z}, \quad (38)$$

where $m = \lfloor n/2 \rfloor$ as in Algorithm 1. Meanwhile, by a standard maximal inequality for sub-Gaussian random variables (Lemma 23 in Appendix E), with probability at least $1 - \delta/6$,

$$\max_{i \in \llbracket \lfloor m/\ell \rfloor \rrbracket} \left\| g(Z_i) - \bar{X}_i \right\| \leq \sigma_X \sqrt{\frac{2}{\ell} \log \frac{12m}{\delta}}. \quad (39)$$

By Inequality 39 and Inequality 38, with probability at least $1 - 2\delta/6$,

$$\begin{aligned} \left\| g(Z_{\pi_\ell(x_0, \{\bar{X}_1, \dots, \bar{X}_{\lfloor m/\ell \rfloor})})} - x_0 \right\| &\leq \left\| \bar{X}_{\pi_\ell(x_0, \{\bar{X}_1, \dots, \bar{X}_{\lfloor m/\ell \rfloor})} - x_0 \right\| + \sigma_X \sqrt{\frac{2}{\ell} \log \frac{8m}{\delta}} \\ &\leq \left\| \bar{X}_{\pi_\ell(x_0, \{\bar{X}_1, \dots, \bar{X}_{\lfloor m/\ell \rfloor})} - x_0 \right\| + \sigma_X \sqrt{\frac{2}{\ell} \log \frac{8m}{\delta}} \\ &\leq C_2 \left(\frac{\ell}{m} \right)^{s_g/d_Z} + \sigma_X \sqrt{\frac{2}{\ell} \log \frac{8m}{\delta}}. \end{aligned}$$

Since $Z_{m+1} = \dots = Z_n = Z_{\pi_\ell(x_0, \{\bar{X}_1, \dots, \bar{X}_{\lfloor m/\ell \rfloor})}$, by Lemma 9, for some constant $C_3 > 0$, with probability at least $1 - \delta/6$, if $k \geq 4 \log \frac{6}{\delta}$,

$$\left\| X_{\pi_k(x; \{X_{m+1}, \dots, X_n\})} - g(Z_{\pi_\ell(x_0, \{\bar{X}_1, \dots, \bar{X}_{\lfloor m/\ell \rfloor})})} \right\| \leq C_3 \sigma_X \left(\frac{k}{n-m} \right)^{1/d_X},$$

and it follows from the triangle inequality and the preceding inequality, with probability at least $1 - \delta/2$,

$$\begin{aligned} &\left\| X_{\pi_k(x_0; \{X_1, \dots, X_n\})} - x_0 \right\| \\ &\leq \left\| X_{\pi_k(g(Z_{\pi_\ell(x_0, \{\bar{X}_1, \dots, \bar{X}_{\lfloor m/\ell \rfloor})}); \{X_{m+1}, \dots, X_n\})} - g(Z_{\pi_\ell(x_0, \{\bar{X}_1, \dots, \bar{X}_{\lfloor m/\ell \rfloor})})} \right\| \\ &\quad + \left\| g(Z_{\pi_\ell(x_0, \{\bar{X}_1, \dots, \bar{X}_{\lfloor m/\ell \rfloor})})} - x_0 \right\| \\ &\leq C_3 \sigma_X \left(\frac{k}{n-m} \right)^{1/d_X} + C_2 \left(\frac{\ell}{m} \right)^{s_g/d_Z} + \sigma_X \sqrt{\frac{2}{\ell} \log \frac{12m}{\delta}}. \end{aligned}$$

Combining this with inequalities (37), (36), and (35) gives, with probability at least $1 - \delta$, as long as $k, \ell \geq 4 \log \frac{6}{\delta}$,

$$\left| \widehat{f}_{x_0, k} - f(x_0) \right| \leq C_4 \left(\sigma_Y \sqrt{\frac{1}{k} \log \frac{1}{\delta}} + \left(\sigma_X^{d_X} \frac{k}{n} \right)^{\frac{s_f}{d_X}} + \left(\frac{\ell}{n} \right)^{\frac{s_f s_g}{d_Z}} + \left(\sigma_X \sqrt{\frac{1}{\ell} \log \frac{n}{\delta}} \right)^{s_f} \right),$$

for some constant $C_4 > 0$, since $m = \lfloor n/2 \rfloor$. □

D Lower Bounds for the Active Case (Theorem 8)

In this section, we state and prove our main lower bounds for the Active case. As in the Passive case, our lower bounds will be given under global Hölder continuity (see Definition 13). We first state the main (overall) bound:

Theorem 8 (Main Active Lower Bound). *In the active case, there exist constants $C, c > 0$, depending only on L_g, s_g, L_f, s_f, d_X , and d_Z , such that, for any estimator \hat{f}_{x_0}*

$$\inf_{\hat{f}_{x_0}} \sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_D \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq C \Phi_{A,*} \right] \geq c,$$

where

$$\Phi_{A,*} = \max \left\{ \left(\frac{1}{n} \right)^{\frac{s_f s_g}{d_Z}}, \left(\frac{\sigma_X^{d_X}}{n} \right)^{s_f/d_X}, \frac{\sigma_Y}{\sqrt{n}}, \left(\frac{\sigma_X^{d_X} \sigma_Y^2}{n} \right)^{\frac{s_f}{2s_f + d_X}} \right\}.$$

Since this lower bound is the maximum of four terms, it suffices to prove each of these four lower bounds separately. Recall that the $\asymp n^{-s_f s_g/d_Z}$ term was proven in Proposition 18, which holds in both the Passive and Active cases. The remaining three lower bounds are prove in the the following three Propositions 20, 21, and 22.

Proposition 20 (Minimax Lower Bound, Active Case, σ_X large, σ_Y large). *In the active case,*

$$\inf_{\hat{f}_{x_0}} \sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_D \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq C \left(\frac{\sigma_X^{d_X} \sigma_Y^2}{n} \right)^{\frac{s_f}{2s_f + d_X}} \right] \geq \frac{1}{4}, \quad (40)$$

where $C > 0$ (given in Eq. (43)) depends only on L_f, s_f , and d_X .

Proof. As in the proofs of Propositions 17 and 19, consider the case in which $\sigma_X \varepsilon_{X,i}$ is uniformly distributed on the cube $[-\frac{\sigma_X}{\sqrt{d_X}}, \frac{\sigma_X}{\sqrt{d_X}}]^{d_X}$. Let

$$h := \left(\frac{\|K_{d_X}\|_{C^{s_f}}^2 \sigma_X^{d_X} \sigma_Y^2}{4d_X^{d_X/2} L_f^2 n} \right)^{\frac{1}{2s_f + d_X}}. \quad (41)$$

Since $\varepsilon_{X,i}$ has a uniform conditional distribution independent of Z_i and g , the function

$$x \mapsto \mathbb{E}_{D, g \sim P_0} [1\{\|x + \sigma_X \varepsilon_{X,i}\|_\infty < h\}]$$

is maximized over $x \in \mathbb{R}^{d_X}$ when $x = 0$. Note that, since this bound depends *only* on the distribution of $\varepsilon_{X,i}$, and not on the distribution of Z_i or g , this applies even in the active case.

$$\begin{aligned} \mathbb{E}_{D, g \sim P_0} [1\{\|X_i - x_0\|_\infty < h\}] &= \mathbb{E}_{D, g \sim P_0} [1\{\|g(Z_i) + \sigma_X \varepsilon_{X,i} - x_0\|_\infty < h\}] \\ &\leq \mathbb{E}_{D, g \sim P_0} [1\{\|\sigma_X \varepsilon_{X,i}\|_\infty < h\}] = \min \left\{ 1, \left(\frac{h\sqrt{d_X}}{\sigma_X} \right)^{d_X} \right\}. \end{aligned} \quad (42)$$

where ϕ_{d_X} denotes the d_X -dimensional standard normal density. Plugging this into Lemma 15 gives

$$\sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_D \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq C_{d_X, s_f} L_f h^{s_f} \right] \geq \frac{1}{2} \left(1 - \frac{L_f h^{s_f}}{\sigma_Y \|K_{d_X}\|_{C^{s_f}}} \sqrt{n \left(\frac{h\sqrt{d_X}}{\sigma_X} \right)^{d_X}} \right).$$

Plugging in our choice (Eq. (41)) of h gives

$$\inf_{\hat{F}} \sup_{\theta \in \Theta} \Pr_\theta \left[|\hat{F} - F(\theta)| \geq s \right] \geq \frac{1}{4},$$

for

$$s = \frac{1}{2} \left(\frac{L_f}{\|K_{d_X}\|_{C^{s_f}}} \right)^{\frac{d_X}{2s_f + d_X}} \left(4\sqrt{d_X} \right)^{\frac{-s_f}{2s_f + d_X}} \left(\frac{\sigma_X^{d_X} \sigma_Y^2}{n} \right)^{\frac{s_f}{2s_f + d_X}}. \quad (43)$$

□

Next, we prove a tight lower bound for the case that the covariate noise level σ_X is large but the response noise level σ_Y is small. This proof is quite similar to that of Proposition 19 for the passive case, except that, (a) rather than considering Z uniformly distributed on \mathcal{Z} , we make no assumptions on Z and utilize only randomness coming from ε_X , and (b) we must reason somewhat more carefully about the interdependence between samples.

Proposition 21 (Minimax Lower Bound, Active Case, σ_X large, σ_Y small). *In the active case,*

$$\inf_{\hat{f}_{x_0}} \sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_D \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq C \left(\frac{\sigma_X^{d_X}}{n} \right)^{s_f/d_X} \right] \geq \frac{1}{2e} \approx 0.18, \quad (44)$$

where $C > 0$ (given below in Eq. (46)) depends only on L_g, s_g, L_f, s_f, d_X , and d_Z .

Proof. Suppose $\sigma_X \varepsilon_{X,i}$ is uniformly distributed on $[-\frac{\sigma_X}{\sqrt{d_X}}, \frac{\sigma_X}{\sqrt{d_X}}]^{d_X} \subseteq \mathbb{R}^{d_X+1}$. It is straightforward to verify that $\varepsilon_{X,i}$ is sub-Gaussian with and that $\varepsilon_{X,i}$ has dimension d_X around 0. Let $r^* := \frac{\sigma_X}{\sqrt{d_X}}$. For any $r \in [0, r^*]$, since each ε_i is independent of the preceding data $\{(X_j, Y_j, Z_j)\}_{j=1}^n$, and since the function $x \mapsto \Pr[\|x + \varepsilon_i\|_\infty \leq r]$ is maximized at $x = 0$,

$$\begin{aligned} \Pr \left[\min_{i \in [n]} \|X_i\|_\infty \geq r \right] &= \prod_{i=1}^n \Pr \left[\|X_i\|_\infty \geq r \mid \min_{j \in [i-1]} \|X_j\|_\infty \geq r \right] \\ &= \prod_{i=1}^n \left(1 - \Pr \left[\|X_i\|_\infty \leq r \mid \min_{j \in [i-1]} \|X_j\|_\infty \geq r \right] \right) \\ &= \prod_{i=1}^n \left(1 - \Pr \left[\|g(Z_i) + \varepsilon_i\|_\infty \leq r \mid \min_{j \in [i-1]} \|X_j\|_\infty \geq r \right] \right) \\ &\geq \prod_{i=1}^n \left(1 - \Pr \left[\|\varepsilon_i\|_\infty \leq r \mid \min_{j \in [i-1]} \|X_j\|_\infty \geq r \right] \right) \\ &= \prod_{i=1}^n (1 - \Pr[\|\varepsilon_i\|_\infty \leq r]) \\ &= \left(1 - \left(\frac{r\sqrt{d_X}}{\sigma_X} \right)^{d_X} \right)^n. \end{aligned}$$

For n sufficiently large that $r \leq r^*$, plugging in

$$r = \frac{\sigma_X}{\sqrt{d_X}} n^{-1/d_X}. \quad (45)$$

gives

$$\Pr \left[\min_{i \in [n]} \|X_i\|_\infty \geq \frac{\sigma_X}{\sqrt{d_X}} n^{-1/d_X} \right] = \left(1 - \frac{1}{n} \right)^n \geq 1/e > 0,$$

since $(1 - \frac{1}{n})^n$ approaches $1/e$ from above as $n \rightarrow \infty$.

Now let f_0 and f_1 be as in Eq. (22), with $h = r$ above. Given the event $\min_{i \in [n]} \|X_i\|_\infty \geq h$, the distribution of the data $\{(X_i, Y_i, Z_i)\}_{i=1}^n$ is independent of whether $f = f_0$ or $f = f_1$. Hence, as argued in the proof of Proposition (18),

$$\max_{f \in \{f_0, f_1\}} \Pr \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq \frac{|f_1(x_0) - f_0(x_0)|}{2} \right] \geq \frac{1}{2} \Pr \left[\min_{i \in [n]} \|X_i\|_\infty \leq h \right] \geq \frac{1}{2e}.$$

Since, by construction of f_0 and f_1 ,

$$|f_1(x_0) - f_0(x_0)| = \frac{L_f h^{s_f}}{\|K_{d_X}\|_{C^{s_f}}},$$

it follows that

$$\max_{f \in \{f_0, f_1\}} \Pr \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq \frac{L_f h^{s_f}}{2\|K_{d_X}\|_{C^{s_f}}} \right] \geq \frac{1}{2e}.$$

Plugging in our choice of $h = r$ from Eq (45) above gives

$$\max_{f \in \{f_0, f_1\}} \Pr \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq C \left(\frac{\sigma_X^{d_X}}{n} \right)^{s_f/d_X} \right] \geq \frac{1}{2e},$$

where

$$C = \frac{L_f d_X^{-s_f/2}}{2 \|K_{d_X}\|_{C^{s_f}}}. \quad (46)$$

□

Finally, we prove a lower bound for the Active case that is tight when σ_X is small but σ_Y is large:

Proposition 22 (Minimax Lower Bound, Active Case, σ_X small, σ_Y large). *In the active case,*

$$\inf_{\hat{f}_{x_0}} \sup_{g, f, P_Z, \varepsilon_X, \varepsilon_Y} \Pr_D \left[\left| \hat{f}_{x_0} - f(x_0) \right| \geq \frac{\sigma_Y}{4\sqrt{n}} \right] \geq \frac{1}{4}. \quad (47)$$

Proof. Plugging the trivial bound

$$\sum_{i=1}^n \mathbb{E}_{D, g \sim P_0} [1\{\|X_i - x_0\|_\infty < h\}] \leq n \quad \text{and} \quad h = \left(\frac{\sigma_Y \|K_{d_X}\|_{C^{s_f}}}{2L_f \sqrt{n}} \right)^{1/s_f}$$

into Lemma 15 gives

$$\inf_{\hat{F}} \sup_{\theta \in \Theta} \Pr_\theta \left[\left| \hat{F} - F(\theta) \right| \geq \frac{\sigma_Y}{4\sqrt{n}} \right] \geq \frac{1}{4}.$$

□

E Supplementary Lemmas

For the reader's convenience, here we state two standard concentration inequalities for sub-Gaussian random variables, used in our upper bounds.

Lemma 23 (Theorem 1.14 of Rigollet (2015)). *Suppose that X_1, \dots, X_n are IID observations of a sub-Gaussian random variable. Then, for any $\delta \in (0, 1)$,*

$$\Pr_{X_1, \dots, X_n} \left[\max_{i \in [n]} |X_i| \leq \sqrt{2 \log \left(\frac{2n}{\delta} \right)} \right] \leq \delta.$$

Lemma 24 (Proposition 2.1 of Wainwright (2019)). *Suppose that X_1, \dots, X_n are IID observations of a sub-Gaussian random variable. Then, for any $\delta \in (0, 1)$,*

$$\Pr_{X_1, \dots, X_n} \left[\frac{1}{n} \sum_{i=1}^n X_i \leq \sqrt{\frac{2}{n} \log \frac{1}{\delta}} \right] \leq \delta.$$

F Details of Experimental Results

This section provides further details regarding the experimental results reported in the main paper. Python code and instructions for reproducing Figures 3, 4, and 5 of the main paper are available at <https://gitlab.tuebingen.mpg.de/shashank/indirect-active-learning>. Experiments we run in Python 3.9, on an Ubuntu laptop with Intel Core i7-10750H CPU.

Code In the code included in the supplementary material:

- `README.md` explains how to set up and run the code.
- `knn_regressors.py` implements the Passive, Passive CV, Active, Active CV, Oracle, and Oracle CV estimators used in Experiments 1 and 2 of the main paper.

F.1 Synthetic Data

Code In the code included in the supplementary material:

- `sampler.py` produces joint samples of (X, Y, Z) , as well as conditional samples of (X, Y, Z) given Z .
- `figure_3.py` carries out Experiment 1 described in Section 8.1 of the main paper. It also generates Figure 3.

F.2 Epidemiological Forecasting Application

SIRD Simulation The stochastic SIRD simulation was run for $T = 100$ time steps over a total population of $N = 1000$, beginning with 10 initially infected individuals ($I_0 = 10$), 990 susceptible individuals ($S_0 = 990$), and no deceased or recovered individuals ($R_0 = D_0 = 0$). The simulation takes in three $[0, 1]$ -valued hyperparameters, an infection rate β , a recovery rate γ , and a death rate δ .

Given these inputs and initial conditions, the stochastic SIRD simulation proceeds as follows. At each timepoint t , a random number of individuals from the Susceptible compartment is newly infected, according to

$$S_{t-1} - S_t \sim \text{Binomial}(S_{t-1}, \beta I/N),$$

where the rate $\beta I/N$ of new infections is proportional to the proportion I/N of infected individuals in the population. Meanwhile, members of the Infected compartment either (i) recover, (ii) die, or (iii) stay infected according to

$$(R_t - R_{t-1}, D_t - D_{t-1}, \text{---}) \sim \text{Multinomial}(I_{t-1}, (\gamma, \delta, 1 - (\gamma + \delta)))$$

distribution. The new number of infected individuals is then updated according to

$$I_t = N - (S_t + R_t + D_t).$$

This process was iterated for $t \in \{1, \dots, T\}$.

Hyperparameters Distributions The first component of the distribution P_Z on $[0, 1]^3$ was a Beta(2, 8) distribution, while the second and third components were the first two components of a Dirichlet(1.0, 0.3, 8.7) distribution, reflecting plausible ranges for these parameters in recent COVID-19 outbreaks (Calafiore et al., 2020; Bousquet et al., 2022).

Code In the code included in the supplementary material:

- `SIR_simulation.py` produces joint samples of (X, Y, Z) , as well as conditional samples of (X, Y, Z) given Z .
- `figure_4.py` carries out Experiment 2 described in Section 8.2 of the main paper. It also generates Figure 4.
- `figure_5.py` generates Figure 5 of the main paper.