Optimal subgroup selection

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Abstract

In clinical trials and other applications, we often see regions of the feature space that appear to exhibit interesting behaviour, but it is unclear whether these observed phenomena are reflected at the population level. Focusing on a regression setting, we consider the subgroup selection challenge of identifying a region of the feature space on which the regression function exceeds a pre-determined threshold. We formulate the problem as one of constrained optimisation, where we seek a low-complexity, data-dependent selection set on which, with a guaranteed probability, the regression function is uniformly at least as large as the threshold; subject to this constraint, we would like the region to contain as much mass under the marginal feature distribution as possible. This leads to a natural notion of regret, and our main contribution is to determine the minimax optimal rate for this regret in both the sample size and the Type I error probability. The rate involves a delicate interplay between parameters that control the smoothness of the regression function, as well as exponents that quantify the extent to which the optimal selection set at the population level can be approximated by families of well-behaved subsets. Finally, we expand the scope of our previous results by illustrating how they may be generalised to a treatment and control setting, where interest lies in the heterogeneous treatment effect.

1 Introduction

Consider a clinical trial that assesses the effectiveness of a drug or vaccine. It will typically be the case that efficacy is heterogeneous across the population, in the sense that the probability of a successful outcome depends on several recorded covariates. As a consequence, we may be unable to recommend the treatment for all individuals; nevertheless, it may be too conservative to reject it entirely. It is very tempting to trawl through the data to identify a subset of the population for which the treatment appears to perform well, but statisticians are well-versed in the dangers of this type of data snooping (Senn and Harrell, 1997; Feinstein, 1998; Rothwell, 2005; Wang et al., 2007; Kaufman and MacLehose, 2013; Altman, 2015; Zhang et al., 2015; Gabler et al., 2016; Lipkovich et al., 2017).

The aim of this paper is to study a subgroup selection problem, where we seek to identify a subset of the population for which a regression function exceeds a pre-determined threshold. In the clinical trial example above, this threshold would represent the level at which the treatment is deemed effective. Subgroup selection forms an important component of the more general field of subgroup analysis (Wang et al., 2007; Herrera et al., 2011; Ting et al.,...
which refers to the problem of understanding the association between a response and subgroups of subjects under study, as defined by one or more subgrouping variables. The main challenge is to provide valid inference, given that the subgroup will be chosen after seeing the data (Lagakos, 2006).

Our first contribution is to formulate subgroup selection as a constrained optimisation problem. Given independent covariate-response pairs and a family \( \mathcal{A} \) of subsets of our feature space, we seek a data-dependent selection set \( \hat{A} \) taking values in \( \mathcal{A} \) with the Type I error control property that, with probability at least \( 1 - \alpha \), the regression function is uniformly no smaller than the level \( \tau \) on \( \hat{A} \); subject to this constraint, we would like the proportion of the population belonging to \( \hat{A} \) to be as large as possible. In practice, \( \mathcal{A} \) would typically be chosen to be of relatively low complexity, so as to lead to an interpretable decision rule.

After introducing this new framework, our first result (Proposition 1 in Section 2) reveals the extent of the challenge. We show that if our regression function belongs to a Hölder class, but the corresponding Hölder constant is unknown, then there is a sense in which no algorithm that respects the Type I error guarantee can do better in terms of power than one that ignores the data. We therefore work over Hölder classes of known smoothness \( \beta \), and with a known upper bound on the Hölder constant; see Definition 1. This enables us to define a data-dependent selection set that satisfies our Type I error guarantee. The idea is to construct, for each hyper-cube \( B \) in a suitable collection within our feature space \( \mathbb{R}^d \), a \( p \)-value for testing the null hypothesis that the regression function is not uniformly above the level \( \tau \) on \( B \). The \( p \)-values are then combined via Holm’s procedure (Holm, 1979) to identify a finite union of hyper-cubes that satisfy our Type I error control property. Our final selection set \( \hat{A}_{\text{OSS}} \) maximises the empirical measure among all elements of \( \mathcal{A} \) that lie within this finite union of hyper-cubes.

Next, we define a notion of regret \( R_{\tau}(\hat{A}) \) that quantifies the power discrepancy between a particular algorithm \( \hat{A} \) and an oracle choice. Our aim is to study the optimal regret that can be attained while maintaining Type I error control. We find that the minimax optimal regret is determined by a combination of the smoothness \( \beta \) (initially assumed to lie in \( (0, 1] \)) and two further exponents \( \kappa, \gamma > 0 \) that quantify the extent to which the oracle selection set can be approximated by families of well-behaved subsets in \( \mathcal{A} \). In particular, \( \kappa \) and \( \gamma \) control respectively the degree of concentration of the marginal measure, and the separation between the regression function and the critical level \( \tau \) on these well-behaved subsets. See Definition 2 for a formal description.

Our main contribution in Section 2 is to establish in Theorem 2, that, with a sample size of \( n \), the minimax optimal rate of convergence of the regret over these distributional classes and over all algorithms that respect the Type I error guarantee at significance level \( \alpha \in (0, 1/2) \) is of order\(^1\)

\[
\min \left\{ \left( \frac{\log_+(n/\alpha)}{n} \right)^{\frac{\beta\gamma \kappa}{(2\beta + d) + \beta \gamma}} + \frac{1}{n^{1/2}}, 1 \right\}. \tag{1}
\]

The second term in the sum reflects the parametric rate, which corresponds to the difficulty of uniformly estimating the population measure of sets in a Vapnik–Chervonenkis class \( \mathcal{A} \).

\(^{1}\)Here, \( \log_+ x := \log x \) when \( x \geq e \) and \( \log_+ x := 1 \) otherwise. To be fully precise, the upper bound holds when \( \mathcal{A} \) is a Vapnik–Chervonenkis class; the lower bound holds when \( \beta \gamma (\kappa - 1) > dk \) and the class \( \mathcal{A} \) consists of convex sets and contains all axis-aligned hyper-rectangles.
The primary interest, however, is in the first term in the sum, which reveals an intricate interplay between the distributional parameters, the sample size and the significance level.

A limitation of our construction for the upper bound that follows from Propositions 4 and 5 is that it is unable to take advantage of higher orders of smoothness beyond $\beta = 1$. To overcome this, in Section 3, we introduce a modified algorithm based on a local polynomial approximation of the regression function, and prove in Theorem 6 that this new construction both respects the Type I error at significance level $\alpha$ and has a regret of optimal order (1) for general smoothness $\beta \in (0, \infty)$. The price we pay for this is a stronger assumption on the marginal feature distribution: we now ask for it to have a well-behaved density with respect to Lebesgue measure (though we do not require this density to be bounded away from zero on its support).

The lower bound constructions for Theorems 2 and 6 are addressed in Section 4. They involve three different finite collections of distributions within our classes, each designed to highlight different aspects of the challenge. The first is a two-point construction, with both distributions having regression functions that are close to $\tau$ on disconnected regions, but with each such function only being uniformly above $\tau$ on one of these regions; this identifies the dependence of the lower bound on $\alpha$. The second extends this construction to many distributions, each having its own region where the regression function is uniformly above $\tau$, which underlines the necessity of the logarithmic factor in $n$ in (1). Finally, the third family, which identifies the parametric rate, is another two-point construction with a shared regression function, but whose marginal feature distributions assign slightly different masses to the different connected components of the $\tau$-super level set of this regression function.

Finally, in Section 5, we consider the more general setting where individuals may belong to either a treatment or control group, and where interest lies in the heterogeneous treatment effect. We show that this heterogeneous treatment effect plays a very similar role to that of the regression function in earlier sections, so that our results generalise almost immediately. Proofs of our results are given in Section 6, while auxiliary results are deferred to Section 7.

One of the interesting messages of our work from an applied perspective is that, when carefully formulated, it is possible to make formally-justified, post-hoc observations concerning subgroup analyses from clinical studies. When attempted without due care, such observations have been rightly criticised in the medical literature: for example:

Analyses must be predefined, carefully justified, and limited to a few clinically important questions, and post-hoc observations should be treated with scepticism irrespective of their statistical significance. \hspace{1cm} (Rothwell, 2005)

The statisticians are right in denouncing subgroups that are formed post hoc from exercises in pure data dredging. \hspace{1cm} (Feinstein, 1998)

A standard approach to handle subgroup analysis is via statistical tests of interaction (Brookes et al., 2001, 2004; Kehl and Ulm, 2006). Zhang et al. (2017) propose a procedure to select a subgroup defined by a halfspace that seeks to maximise the expected difference in treatment effect in the context of an adaptive signature design trial. Several other methods have been proposed for studying subgroups defined through heterogeneous treatment effects. For instance, Foster et al. (2011) propose an approach to identify subgroups having enhanced treatment effect via the construction of ‘virtual twins’, while Ballarini et al. (2018)
Given a set $S$ define its diameter by $diam(S) = \sup_{x,y \in S} \|x - y\|$. For $r > 0$, let $B_r(x)$ and $\overline{B}_r(x)$ denote the open and closed $\ell_\infty$ balls of radius $r$ about $x \in \mathbb{R}^d$ respectively. For a function $f : \mathbb{R}^d \to \mathbb{R}$, and for $\xi > 0$, we also let $\chi_\xi(f) := \{x \in \mathbb{R}^d : f(x) \geq \xi\}$ denote its super-level set at level $\xi$. Given a symmetric matrix $A \in \mathbb{R}^{d \times d}$, we let $A^+$ denote its Moore–Penrose pseudo-inverse and write $\lambda_{\min}(A)$ for its minimal eigenvalue.

For $p \in [0, 1]$, we let Bern$(p)$ denote the Bernoulli distribution on $\{0, 1\}$ with mean $p$. Given a Borel probability measure $\mu$ on $\mathbb{R}^d$, we write $supp(\mu)$ for its support, i.e. the intersection of all closed sets $C \subseteq \mathbb{R}^d$ with $\mu(C) = 1$. For probability measures $P, Q$ on a measurable space $(\Omega, \mathcal{F})$, we denote their total variation distance by $TV(P, Q) := \sup_{B \in \mathcal{F}} |P(B) - Q(B)|$. If these measures are absolutely continuous with respect to a $\sigma$-finite measure $\lambda$, with Radon–Nikodym derivatives $f$ and $g$ respectively, we write $H(P, Q) := \left\{ \int\! f^{1/2} - g^{1/2} \, d\lambda \right\}^{1/2}$ for their Hellinger distance, and $\chi^2(P, Q) := \int\! f^2 / g \, d\lambda - 1$ for their $\chi^2$-divergence. For $a \in [0, 1]$, $b \in (0, 1)$, we define $kl(a, b)$ to be the Kullback–Leibler divergence between the Bern$(a)$ and
Bern(b) distributions; i.e., for \( a \in (0, 1) \),
\[
\text{kl}(a, b) := a \log \left( \frac{a}{b} \right) + (1 - a) \log \left( \frac{1 - a}{1 - b} \right),
\]
with \( \text{kl}(0, b) := -\log(1 - b) \) and \( \text{kl}(1, b) := -\log b \).

## 2 Subset selection framework and minimax rates

Suppose that the covariate-response pair \((X, Y)\) has joint distribution \(P\) on \(\mathbb{R}^d \times [0, 1]\). Let \(\mu \equiv \mu_P\) denote the marginal distribution of \(X\). Further, let \(\eta \equiv \eta_P : \mathbb{R}^d \to [0, 1]\) denote the regression function, defined by \(\eta(x) := \mathbb{E}(Y|X = x)\) for \(x \in \mathbb{R}^d\). We shall assume throughout that \(\eta\) is continuous, so it is uniquely defined on \(\text{supp}(\mu)\). We let \(\mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d)\) denote our class of candidate selection sets, and assume that \(\emptyset \in \mathcal{A}\) independent for all \(\mu, b\) Bern(\(\cdot\)) still controlling the Type I error over our Lipschitz class.

In several places below, we abbreviate \(\hat{A}\) for \(\hat{A}(\mathcal{D})\) as \(\hat{A}\) where the argument is clear from context.

Our first result reveals that even Lipschitz restrictions on the regression function in our class do not suffice to obtain a data-dependent selection set \(\hat{A}\) that satisfies both (2) and \(\mathbb{P}_P(\mu(\hat{A}) > 0) > \alpha\) for some \(P \in \mathcal{P}\). The negative implication is that, regardless of smoothness properties of the true regression function, the regret of any \(\hat{A}\) satisfying (2) can be no smaller than the infimum of the regrets of all selection sets that ignore the data while still controlling the Type I error over our Lipschitz class.

Given a probability measure \(\mu\) on \(\mathbb{R}^d\), we let \(\mathcal{P}_{\text{Lip}}(\mu)\) denote the set of all Borel probability distributions on \(\mathbb{R}^d \times [0, 1]\) with marginal \(\mu\) on \(\mathbb{R}^d\), and for which the corresponding regression function \(\eta\) is Lipschitz. We say that \(\hat{A} \in \hat{\mathcal{A}}_n\) is data independent if \(1_{\{\hat{A}(\mathcal{D}) = A\}}\) and \(\mathcal{D}\) are independent for all \(A \in \mathcal{A}\), and write \(\hat{A}\) for the set of data-independent selection sets.
Proposition 1. Let $\mu$ be a distribution on $\mathbb{R}^d$ without atoms and take $\mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d)$ with $\text{dim}_{\text{VC}}(\mathcal{A}) < \infty$. Further, let $\hat{A} \in \hat{\mathcal{A}}_n(\tau, \alpha, \mathcal{P}_{\text{Lip}}(\mu))$. Then for all $P \in \mathcal{P}_{\text{Lip}}(\mu)$, we have

$$\mathbb{P}_P(\mu(\hat{A}) = 0 \mid \hat{A} \subseteq X_r(\eta)) \geq \mathbb{P}_P(\{\mu(\hat{A}) = 0\} \cap \{\hat{A} \subseteq X_r(\eta)\}) \geq 1 - \alpha.$$  

Hence

$$R_r(\hat{A}) \geq M_r \cdot (1 - \alpha) = \inf\{R_r(\hat{A}) : \hat{A} \in \hat{\mathcal{A}}_n(\tau, \alpha, \mathcal{P}_{\text{Lip}}(\mu))\}. \tag{4}$$

In the light of Proposition 1, we will assume that our regression function belongs to a Hölder class for which both the Hölder exponent and the associated constant are known. In this section, we will work with smoothness exponents that are at most 1.

Definition 1 (Hölder class). Given $(\beta, C_S) \in (0, 1] \times [1, \infty)$ we let $\mathcal{P}_{\text{Höld}}(\beta, C_S)$ denote the class of all distributions $P$ on $\mathbb{R}^d \times [0, 1]$ such that the associated regression function $\eta$ is $(\beta, C_S)$-Hölder in the sense that

$$|\eta(x') - \eta(x)| \leq C_S \cdot \|x' - x\|_{\infty}^\beta,$$

for all $x, x' \in \mathbb{R}^d$.

While our algorithms will control the Type I error over Hölder classes, we will see that the optimal regret for a data-dependent selection set depends on further aspects of the underlying data generating mechanism. To describe the relevant classes, we first define a function $\omega \equiv \omega_{\mu,d} : \mathbb{R}^d \to [0, 1]$ by

$$\omega(x) := \inf_{r \in (0,1)} \frac{\mu(B_r(x))}{r^d}.$$  

Borrowing the terminology of Reeve et al. (2021), we will refer to $\omega$ as a lower density, even though our definition is slightly different as we work with an $\ell_\infty$-ball instead of a Euclidean ball. A nice feature of this definition is that it allows us to avoid assuming that $\mu$ is absolutely continuous with respect to Lebesgue measure; see Reeve et al. (2021) for several basic properties of lower density functions.

We are now in a position to define what we refer to as an approximable class of distributions; these are ones for which we can approximate $M_\tau$ well by $\mu(A)$, where $A \in \mathcal{A}$ is both such that the lower density on $A$ is not too small and such that the regression function on $A$ is bounded away from the critical threshold $\tau$.

Definition 2 (Approximable class). Given $\mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d)$ and $(\kappa, \gamma, C_{\text{App}}) \in (0, \infty)^2 \times [1, \infty)$, let $\mathcal{P}_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, C_{\text{App}})$ denote the class of all distributions $P$ on $\mathbb{R}^d \times [0, 1]$ with marginal $\mu$ on $\mathbb{R}^d$ and regression function $\eta : \mathbb{R}^d \to [0, 1]$ such that

$$\sup \{\mu(A) : A \in \mathcal{A} \cap \text{Pow}(X_\xi(\omega) \cap X_{\tau+\Delta}(\eta))\} \geq M_\tau - C_{\text{App}} \cdot (\xi^\kappa + \Delta^\gamma),$$

for all $(\xi, \Delta) \in (0, \infty)^2$.

We now provide several examples of distributions belonging to appropriate approximable classes. The proofs of the claims in these examples are given in Section 6.2.
Example 3. Consider the family of distributions the form provided that \( \int_{\mathbb{R}} \in \mathcal{S}_r \), dependent selection set in \( \hat{\mathcal{S}}_r \). Now, for \( R \), where, again, the infimum in \( \kappa = \gamma = 1 \), for a suitably large choice of \( C_{\text{App}} \), depending only on \( \nu \) and \( \tau \).

Example 2. Let \( \mu \) denote the uniform distribution on \([0, 1]^d\). Suppose that \( \eta : \mathbb{R}^d \rightarrow [0, 1] \) is coordinate-wise increasing, that \( \mathcal{S}_r := \{ x \in [0, 1]^d : \eta(x) = \tau \} \neq \emptyset \), and that there exist \( \delta, \epsilon \in (0, 1) \) and \( \gamma > 0 \) such that \( \eta(x) - \tau \geq \epsilon \cdot \text{dist}_{\infty}(x, \mathcal{S}_r)^{1/\gamma} \), for every \( x \in \mathcal{X}_r(\eta) \cap [0, 1]^d \) with \( \text{dist}_{\infty}(x, \mathcal{S}_r) \leq \delta \). If \( P \) denotes a distribution on \( \mathbb{R}^d \times [0, 1] \) with marginal \( \mu \) on \( \mathbb{R}^d \) and regression function \( \eta \), then \( P \in \mathcal{P}_{\text{App}}(\mathcal{A}_{\text{rect}}, \tau, \kappa, \gamma, C_{\text{App}}) \) for arbitrarily large \( \kappa \in (0, \infty) \), provided that \( C_{\text{App}} \geq 2d/(\epsilon^2 \delta) \).

Example 3. Consider the family of distributions \( \{ \mu_\kappa : \kappa \in (0, \infty) \} \) on \( \mathbb{R}^d \) with densities of the form \( x \mapsto g_\kappa(||x||_\infty) \), where \( g_\kappa : [0, \infty) \rightarrow [0, \infty) \) is given by

\[
g_\kappa(y) := \begin{cases} (\kappa/2^d) \cdot \left(1 + (1 - \kappa)y^d\right)^{-1/(1 - \kappa)} & \text{if } \kappa \in (0, 1) \\ (1/2^d) \cdot e^{-y^d} & \text{if } \kappa = 1 \\ (\kappa/2^d) \cdot \left(1 - (\kappa - 1)y^d\right)^{(1/(\kappa - 1))} \mathbb{1}_{\{y \leq 1/(\kappa - 1)^{1/d}\}} & \text{if } \kappa \in (1, \infty). \end{cases}
\]

Now, for \( \gamma \in (0, \infty) \), define the regression function \( \eta_\gamma : \mathbb{R}^d \rightarrow [0, 1] \) by

\[
\eta_\gamma(x) := \emptyset \vee \{\tau + C_S \cdot \text{sgn}(x_1)||x_1||_\gamma^\gamma\} \land 1,
\]

Writing \( P_{\kappa, \gamma} \) for the distribution on \( \mathbb{R}^d \times [0, 1] \) with marginal \( \mu_\kappa \) on \( \mathbb{R}^d \) and regression function \( \eta_\gamma \), we have that \( P_{\kappa, \gamma} \in \mathcal{P}_{\text{App}}(\mathcal{A}_{\text{rect}}, \tau, \kappa, \gamma, C_{\text{App}}) \) for \( C_{\text{App}} \equiv C_{\text{App}}(d, \tau, \kappa, \gamma, C_S) > 0 \) sufficiently large.

We can now state the main theorem of this section, which reveals the minimax optimal rate of convergence for the regret over \( \mathcal{P}_{\text{H"o}}(\beta, C_S) \cap \mathcal{P}_{\text{App}}(\mathcal{A}, \kappa, \gamma, C_{\text{App}}) \) for \( \mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d) \) and \( \mathcal{A} \subseteq \mathcal{A}_{\text{conv}} \) each \( \mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d) \) satisfying \( \mathcal{A}_{\text{rect}} \subseteq \mathcal{A} \subseteq \mathcal{A}_{\text{conv}} \) and every \( \kappa, \gamma, \tau \in (0, \infty) \), such that for all \( n \in \mathbb{N} \) and \( \alpha \in (0, 1/2] \), we have

\[
\inf_{\mathcal{A}} \sup_P R_\tau(\hat{A}) \leq C \cdot \min \left\{ \left( \frac{\log_+ (n/\alpha)}{n} \right)^{\frac{\beta \kappa \gamma}{(2 \beta + 4) + \beta \gamma}} + \frac{1}{n^{1/2}}, 1 \right\},
\]

where the infimum in (5) is taken over \( \mathcal{A}_n(\tau, \alpha, \mathcal{P}_{\text{H"o}}(\beta, C_S)) \) and the supremum is taken over \( \mathcal{P}_{\text{H"o}}(\beta, C_S) \cap \mathcal{P}_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, C_{\text{App}}) \).

(ii) Lower bound: Now suppose that \( \beta \gamma (\kappa - 1) < d \kappa, \epsilon_0 \in (0, 1/2) \), \( \tau \in (\epsilon_0, 1 - \epsilon_0) \) and \( \alpha \in (0, 1/2 - \epsilon_0] \). Then there exists \( c > 0 \), depending only on \( d, \beta, C_S, \kappa, \gamma, C_{\text{App}} \) and \( \epsilon_0 \), such that for any \( \mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d) \) satisfying \( \mathcal{A}_{\text{rect}} \subseteq \mathcal{A} \subseteq \mathcal{A}_{\text{conv}} \) and every \( n \in \mathbb{N} \), we have

\[
\inf_{\mathcal{A}} \sup_P R_\tau(\hat{A}) \geq c \cdot \min \left\{ \left( \frac{\log_+ (n/\alpha)}{n} \right)^{\frac{\beta \kappa \gamma}{(2 \beta + 4) + \beta \gamma}} + \frac{1}{n^{1/2}}, 1 \right\},
\]

where, again, the infimum in (6) is taken over \( \mathcal{A}_n(\tau, \alpha, \mathcal{P}_{\text{H"o}}(\beta, C_S)) \) and the supremum is taken over \( \mathcal{P}_{\text{H"o}}(\beta, C_S) \cap \mathcal{P}_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, C_{\text{App}}) \).
Since dim\(_{VC}(A_{\text{rect}}) < \infty\) (e.g. Shalev-Shwartz and Ben-David, 2014, Exercise 5 in Section 6.8), the choice \(A = A_{\text{rect}}\) provides a natural example satisfying both the lower and upper bounds in Theorem 2.

In order to introduce the algorithm that achieves the upper bound, we define the empirical marginal distribution \(\hat{\mu}_n\) and empirical regression function \(\hat{\eta}_n\), for \(B \subseteq \mathbb{R}^d\), by

\[
\hat{\mu}_n(B) := \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{X_i \in B\}}
\]

\[
\hat{\eta}_n(B) := \frac{1}{n \cdot \hat{\mu}_n(B)} \sum_{i=1}^{n} Y_i \cdot \mathbb{1}_{\{X_i \in B\}}
\]

whenever \(\hat{\mu}_n(B) > 0\), and \(\hat{\eta}_n(B) := 1/2\) otherwise. The main idea is to associate, to each \(B \subseteq \mathbb{R}^d\), a \(p\)-value for a test of the hypothesis that the regression function is uniformly above the level \(\tau\) on \(B\). More precisely, for \(B \subseteq \mathbb{R}^d\), we define

\[
\hat{p}_n(B) \equiv \hat{p}_{n,\tau,\beta,C_S}(B) := \exp \left\{ -n \cdot \hat{\mu}_n(B) \cdot \text{kl}(\hat{\eta}_n(B), \tau + C_S \cdot \text{diam}_{\infty}(B)^\beta) \right\},
\]

whenever \(\hat{\eta}_n(B) > \tau + C_S \cdot \text{diam}_{\infty}(B)^\beta\), and \(\hat{p}_n(B) = 1\) otherwise. Lemma 3 below confirms that \(\hat{p}_n(B)\) is indeed a \(p\)-value (even conditionally on \(D_X \equiv (X_i)_{i \in [n]}\)).

**Lemma 3.** Fix \((\beta, C_S) \in (0, 1] \times [1, \infty)\) and let \(P \in \mathcal{P}_{\text{H"{o}l}}(\beta, C_S)\). Suppose that \(D = ((X_i, Y_i))_{i \in [n]} \sim P^\otimes n\) and let \(D_X = (X_i)_{i \in [n]}\). Then given any \(B \subseteq \mathbb{R}^d\) with \(\inf_{x \in B} \eta(x) \leq \tau\), and any \(\alpha \in (0, 1)\), we have

\[
P_P(\hat{p}_n(B) \leq \alpha \mid D_X) \leq \alpha.
\]

We now exploit these \(p\)-values to specify a data-dependent selection set \(\hat{A}\) that controls the Type I error over \(\mathcal{P}_{\text{H"{o}l}}(\beta, C_S)\). First, define a set of hyper-cubes

\[
\mathcal{H} := \left\{ 2^{-q} \prod_{j=1}^{d} [2a_j - 1, 2a_j + 3) : (a_1, \ldots, a_d) \in \mathbb{Z}^d, \ q \in \mathbb{N} \right\}.
\]

Now, given \(x_{1:n} = (x_i)_{i \in [n]} \in (\mathbb{R}^d)^n\), we define

\[
\mathcal{H}(x_{1:n}) := \{ B \in \mathcal{H} : \{x_1, \ldots, x_n\} \cap B \neq \emptyset \ \text{and} \ \text{diam}_{\infty}(B) \geq 1/n \},
\]

so that \(|\mathcal{H}(x_{1:n})| \leq 2^d n(2 + \log_2 n)\). The overall algorithm, which applies Holm’s procedure
(Holm, 1979) to the \( p \)-values in (9) and is denoted by \( \hat{A}_{\text{OSS}} \in \hat{A}_n \), is given in Algorithm 1.

**Algorithm 1:** The data-dependent selection set \( \hat{A}_{\text{OSS}} \)

**Input:** Data \( \mathcal{D} = ((X_1, Y_1), \ldots, (X_n, Y_n)) \in (\mathbb{R}^d \times [0, 1])^n \), an ordered set \( \mathcal{A} \) of subsets of \( \mathbb{R}^d \) with \( \emptyset \in \mathcal{A} \), \( \alpha \in (0, 1) \), Hölder parameters \( (\beta, C_S) \in (0, 1] \times [1, \infty) \);

Compute \( \hat{p}_n(B) \) for each \( B \in \mathcal{H}(\mathcal{D}_X) \) using (9) and let \( \hat{L} := |\mathcal{H}(\mathcal{D}_X)| \);

Enumerate \( \mathcal{H}(\mathcal{D}_X) \) as \( (B(\ell))_{\ell \in [\hat{L}]} \), in such a way that \( \hat{p}_n(B(\ell)) \leq \hat{p}_n(B(\ell')) \) for \( \ell \leq \ell' \);

**if** \( \hat{L} \cdot \hat{p}_n(B(1)) \leq \alpha \) **then**

**Compute** \( \ell_\alpha := \max \{ \ell \in [\hat{L}]: (\hat{L} + 1 - \ell) \cdot \hat{p}_n(B(\ell)) \leq \alpha \} \);

**Choose** \( \hat{A}_{\text{OSS}}(\mathcal{D}) := \text{sargmax} \{ \hat{\mu}_n(A) : A \in \mathcal{A} \cap \text{Pow}(\bigcup_{\ell \in [\ell_\alpha]} B(\ell)) \} \);

**else**

**Set** \( \hat{A}_{\text{OSS}}(\mathcal{D}) = \emptyset \);

**end**

**Result:** The selected set \( \hat{A}_{\text{OSS}}(\mathcal{D}) \).

Proposition 4 below provides part of the proof of the upper bound in Theorem 2.

**Proposition 4.** Let \( \alpha \in (0, 1) \) and \( (\beta, C_S) \in (0, 1] \times [1, \infty) \). Then the data-dependent selection set \( \hat{A}_{\text{OSS}} \) controls the Type I error at level \( \alpha \) over \( \mathcal{P}_{\text{Hol}}(\beta, C_S) \); in other words, \( \hat{A}_{\text{OSS}} \in \hat{A}_n(\tau, \alpha, \mathcal{P}_{\text{Hol}}(\beta, C_S)) \).

Proposition 5 complements Proposition 4 by bounding the regret \( R_\tau(\hat{A}_{\text{OSS}}) \), and together these results prove the upper bound in Theorem 2. In fact, we provide a high-probability bound as well as an expectation bound.

**Proposition 5.** Take \( (\tau, \alpha) \in (0, 1) \), \( (\beta, C_S) \in (0, 1] \times [1, \infty) \), \( (\kappa, \gamma, C_{\text{App}}) \in (0, \infty)^2 \times [1, \infty) \) and \( \mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d) \) with \( \text{dim}_{\text{VC}}(\mathcal{A}) < \infty \) and \( \emptyset \in \mathcal{A} \). There exists \( C \geq 1 \), depending only on \( d \), \( \beta, C_S, \kappa, \gamma, C_{\text{App}} \) and \( \text{dim}_{\text{VC}}(\mathcal{A}) \), such that for all \( P \in \mathcal{P}_{\text{Hol}}(\beta, C_S) \cap \mathcal{P}_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, C_{\text{App}}) \), \( n \in \mathbb{N} \) and \( \delta \in (0, 1) \), we have

\[
\mathbb{P}_P \left[ M_\tau - \mu(\hat{A}_{\text{OSS}}) > \tilde{C} \left\{ \left( \frac{\log_+ (n/(\alpha \land \delta))}{n} \right)^{\frac{\beta \kappa}{\kappa(2\beta + \delta) + \beta \gamma}} + \left( \frac{\log_+ (1/\delta)}{n} \right)^{\frac{1}{2}} \right\} \right] \leq \delta.
\]

As a consequence, for \( \alpha \in (0, 1/2) \),

\[
R_\tau(\hat{A}_{\text{OSS}}) \leq C \left\{ \left( \frac{\log_+ (n/\alpha)}{n} \right)^{\frac{\beta \kappa}{\kappa(2\beta + \delta) + \beta \gamma}} + \frac{1}{n^{1/2}} \right\},
\]

where \( C > 0 \) depends only on \( \tilde{C} \).

In the lower bound part of Theorem 2, we have the condition \( \beta \gamma (\kappa - 1) < d \kappa \). A constraint of this form is natural in light of the tension between \( \beta, \kappa \) and \( \gamma \). In particular, large values of \( \kappa \) and \( \gamma \) mean that little \( \mu \)-mass in \( \mathcal{X}_r(\eta) \) is lost by restricting to sets \( A \in \mathcal{A} \) for which the lower density of \( A \) is not too small, and the regression function on \( A \) is uniformly well above \( \tau \); but the smoothness of the regression function constrains the rate of change of \( \eta \), and therefore the extent to which this is possible. This intuition is formalised in Lemma 34, where we prove that \( \beta \gamma (\kappa - 1) \leq d \kappa \), provided there exists a distribution in our class for which the pre-image of \( \tau \) under \( \eta \) is non-empty, and \( \mu \) is sufficiently well-behaved.
Since the lower bound construction for the proof of Theorem 2(ii) is common to both the setting of this section and that of the upcoming Section 3 on higher-order smoothness, we will defer discussion of this construction until Section 4.

## 3 Higher-order smoothness

In this section, we explain how our previous procedure and analysis can be modified and extended to cover a general smoothness level $\beta > 0$ for the regression function. Given $\nu = (\nu_1, \ldots, \nu_d) \in \mathbb{N}_0^d$ and $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$, we define $\|s\|_1 := \sum_{j=1}^d \nu_j$, $s! := \prod_{j=1}^d \nu_j!$ and $x^\nu := \prod_{j=1}^d x_j^{\nu_j}$. For an $\|\nu\|_1$-times differentiable function $g : \mathbb{R}^d \to \mathbb{R}$, define $\partial_x^\nu (g) := \frac{\partial^{\|\nu\|_1} g}{\partial x_1^{\nu_1} \cdots \partial x_d^{\nu_d}}(x)$. Given $\beta \in (0, \infty)$ we let $\mathcal{V}(\beta) := \{\nu \in \mathbb{N}_0^d : \|\nu\|_1 \leq \lceil \beta \rceil - 1\}$, so that $|\mathcal{V}(\beta)| = \frac{\lceil \beta \rceil + d - 1}{d}$, and for a $(\lceil \beta \rceil - 1)$-times differentiable function $g : \mathbb{R}^d \to \mathbb{R}$, let $T_x^{\beta}(g) : \mathbb{R}^d \to \mathbb{R}$ denote the associated Taylor polynomial at $x \in \mathbb{R}^d$, defined by

$$T_x^{\beta}(g)(x') := \sum_{\nu \in \mathcal{V}(\beta)} \frac{(x' - x)^\nu}{\nu!} \cdot \partial_x^\nu (g),$$

for $x' \in \mathbb{R}^d$.

**Definition 3** (General Hölder class). Given $(\beta, C_S) \in (0, \infty) \times [1, \infty)$ we let $\mathcal{P}_{H\ddot{o}l}(\beta, C_S)$ denote the class of all distributions $P$ on $\mathbb{R}^d \times [0, 1]$ such that the associated regression function $\eta : \mathbb{R}^d \to [0, 1]$ is $(\lceil \beta \rceil - 1)$-differentiable and satisfies

$$|\eta(x') - T_x^{\beta}[\eta](x')| \leq C_S \cdot \|x' - x\|_\infty^\beta,$$

for all $x, x' \in \mathbb{R}^d$. Moreover, we let $\mathcal{P}_{H\ddot{o}l}(\beta, C_S) := \bigcap_{\beta' \in (0, \beta]} \mathcal{P}_{H\ddot{o}l}(\beta', C_S)$.

Throughout this section, and in contrast to Section 2, we will require that the marginal distribution $\mu$ is absolutely continuous with respect to Lebesgue measure, and write $f_\mu$ for its density. Given a probability measure $\mu$ on $\mathbb{R}^d$ and some $\nu \in (0, 1)$, we define

$$\mathcal{R}_\nu(\mu) := \bigcap_{r \in (0, 1)} \left\{ x \in \mathbb{R}^d : \mu(B_r(x)) \geq \nu \cdot r^d \cdot \sup_{x' \in B_{(1+r)}(x)} f_\mu(x') \right\}.$$  \hspace{1cm} (10)

To provide some intuition about $\mathcal{R}_\nu(\mu)$, we first note that if $S \subseteq \text{supp}(\mu)$ is a $(c_0, r_0)$-regular set (Audibert and Tsybakov, 2007, Equation (2.1)) and if $\mu$ is absolutely continuous with respect to $L_d$ with corresponding density $f_\mu$ satisfying $K_\mu := \sup_{x \in \text{supp}(\mu)} f_\mu(x)/\inf_{x \in S} f_\mu(x) < \infty$, then $S \subseteq \mathcal{R}_\nu(\mu)$ for $\nu \leq c_0 V_d(r_0 \wedge 1)^d K_\mu^{-1}$. Moreover, we can still have $\mathcal{R}_\nu(\mu) = \text{supp}(\mu)$ even when $\mu$ is not compactly supported and there is no uniform positive lower bound for $f_\mu$ on its support. For instance, the family of probability measures $\{\mu_\kappa : \kappa \in (0, 1)\}$ on $\mathbb{R}^d$ considered in Example 3 satisfies $\mathcal{R}_\nu(\mu_\kappa) = \mathbb{R}^d$ for $\nu \leq 2^d \cdot \{1 + 3^d (1 - \kappa)\}^{-1/(1-\kappa)}$.

We are now in a position to define an appropriate definition of approximable classes for regression functions with higher-order smoothness.
Definition 4 (Approximable classes for higher-order smoothness). Given \( \mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d) \) and \((\kappa, \gamma, v, C_{\text{App}}) \in (0, \infty)^2 \times (0, 1) \times [1, \infty)\), we let \( \mathcal{P}_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, v, C_{\text{App}}) \) denote the class of all distributions \( P \) on \( \mathbb{R}^d \times [0, 1] \) with marginal \( \mu \) on \( \mathbb{R}^d \) and regression function \( \eta \) such that
\[
\sup\{ \mu(A) : A \in \mathcal{A} \cap \text{Pow}(\mathcal{R}_\nu(\mu) \cap \mathcal{X}(f_\mu) \cap \mathcal{X}_\tau + \Delta(\eta)) \} \geq M_\tau - C_{\text{App}} \cdot (\xi^\kappa + \Delta^\gamma),
\]
for all \((\xi, \Delta) \in (0, \infty)^2\).

Finally, then, we can state the main theorem of this section.

Theorem 6. Take \((\tau, \alpha) \in (0, 1)^2, (\beta, C_S) \in (0, \infty) \times [1, \infty)\) and \((\kappa, \gamma, v, C_{\text{App}}) \in (0, \infty)^2 \times (0, 1) \times [1, \infty)\).

(i) Upper bound: Let \( \mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d) \) satisfy \( \dim_{\text{VC}}(\mathcal{A}) < \infty \) and \( \emptyset \in \mathcal{A} \). Then there exists \( C \geq 1 \), depending only on \( d, \beta, C_S, \kappa, \gamma, v, C_{\text{App}} \) and \( \dim_{\text{VC}}(\mathcal{A}) \), such that for all \( n \in \mathbb{N} \) and \( \alpha \in (0, 1/2) \), we have
\[
\inf \sup_{\hat{A}} R_{\tau}(\hat{A}) \leq C \cdot \min \left\{ \left( \frac{\log_+(n/\alpha)}{n} \right)^{\frac{\beta \kappa \gamma}{\kappa (2\beta \alpha + \beta \gamma)}} + \frac{1}{n^{1/2}}, 1 \right\},
\]
where the infimum in (12) is taken over \( \hat{A}_n(\tau, \alpha, \mathcal{P}_{\text{Hö}}(\beta, C_S)) \) and the supremum is taken over \( \mathcal{P}_{\text{Hö}}(\beta, C_S) \cap \mathcal{P}_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, v, C_{\text{App}}) \).

(ii) Lower bound: Now suppose that \( \beta \gamma (\kappa - 1) < d \kappa, \epsilon_0 \in (0, 1/2), \tau \in (\epsilon_0, 1 - \epsilon_0), \alpha \in (0, 1/2 - \epsilon_0) \) and \( v \in (0, (4d^{1/2})^{-d}] \). Then there exists \( c > 0 \), depending only on \( d, \beta, C_S, \kappa, \gamma, C_{\text{App}} \) and \( \epsilon_0 \), such that for any \( \mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d) \) satisfying \( \mathcal{A}_{\text{rect}} \subseteq \mathcal{A} \subseteq \mathcal{A}_{\text{conv}} \) and any \( n \in \mathbb{N} \), we have
\[
\inf \sup_{\hat{A}} R_{\tau}(\hat{A}) \geq c \cdot \min \left\{ \left( \frac{\log_+(n/\alpha)}{n} \right)^{\frac{\beta \kappa \gamma}{\kappa (2\beta \alpha + \beta \gamma)}} + \frac{1}{n^{1/2}}, 1 \right\},
\]
where, again, the infimum in (13) is taken over \( \hat{A}_n(\tau, \alpha, \mathcal{P}_{\text{Hö}}(\beta, C_S)) \) and the supremum is taken over \( \mathcal{P}_{\text{Hö}}(\beta, C_S) \cap \mathcal{P}_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, v, C_{\text{App}}) \).

In order to prove the upper bound in Theorem 6, we will introduce a modified algorithm. The key alteration is a different choice of \( p \)-values that now makes use of data points outside (as well as within) our hyper-cube of interest to test whether or not the regression function is uniformly above \( \tau \) on the hyper-cube. Given \( \beta \in (0, \infty), x, x' \in \mathbb{R}^d, h \in (0, 1] \) and \( \eta \in \mathcal{P}_{\text{Hö}}(\beta, C_S) \), we let
\[
\Phi_{x,h}(x') := \left( \frac{x' - x}{h} \right)_{\nu \in \nu(V)} \in \mathbb{R}^{V(\beta)} \quad \text{and} \quad w_{x,h}^{\beta} := \left( \frac{h_{|\nu|1}}{\nu_!} \cdot \partial_\nu(\eta) \right)_{\nu \in \nu(V)} \in \mathbb{R}^{V(\beta)},
\]
so that \( T_{x}^{\beta}[g](x') = \langle w_{x,h}^{\beta}, \Phi_{x,h}(x') \rangle \) for all \( x, x' \in \mathbb{R}^d \) and \( h \in (0, 1] \), where \( \langle \cdot, \cdot \rangle \) denotes the Euclidean inner product. Moreover, if we let \( e_0 := \left( 1_{\nu = (0, \ldots, 0)} \right)_{\nu \in \nu(V)} \in \mathbb{R}^{V(\beta)} \), then \( \eta_P(x) = \langle e_0, w_{x,h}^{\beta} \rangle \). A natural estimator of \( w_{x,h}^{\beta} \) is the local least squares estimator obtained by taking \( N_{x,h} := \{ i \in [n] : X_i \in \hat{B}_h(x) \} \) and letting
\[
\hat{w}_{x,h}^{\beta} \in \arg \min_{w \in \mathbb{R}^{S(\beta)}} \sum_{i \in N_{x,h}} (Y_i - \langle w, \Phi_{x,h}^{\beta}(X_i) \rangle)^2.
\]
In fact, it will be convenient to choose a particular element of this argmin: if we define
\[ V_{x,h}^\beta := \sum_{i \in N_{x,h}} Y_i \cdot \Phi_{x,h}^\beta(X_i) \in \mathbb{R}^{S(\beta)} \]
\[ Q_{x,h}^\beta := \sum_{i \in N_{x,h}} \Phi_{x,h}^\beta(X_i) \Phi_{x,h}^\beta(X_i)^\top \in \mathbb{R}^{S(\beta) \times S(\beta)}, \]
then we will take \( \hat{\nu}_{x,h}^\beta := (Q_{x,h}^\beta)^+ V_{x,h}^\beta \). Thus, \( \hat{\eta}(x) := 0 \vee \left( 1 \wedge \langle e_0, \hat{\nu}_{x,h}^\beta \rangle \right) \) is an estimator of \( \eta(x) \). Next we associate a \( p \)-value to closed hyper-cubes \( B \subseteq \mathbb{R}^d \) with \( \text{diam}_\infty(B) \leq 1 \) as follows. Let \( x \in \mathbb{R}^d \) and \( r \in [0,1/2] \) denote the centre and \( \ell_\infty \)-radius of \( B \), so that \( B = B_r(x) \). Let \( h := (2r)^{1+\frac{1}{\alpha}} \in [0,1] \), and define
\[ \hat{p}_n^+(B) \equiv \hat{p}_{n,r,\beta,C_S}(B) \]
\[ := \exp \left\{- \frac{2}{e_0^\top (Q_{x,h}^\beta)^{-1} e_0} \left( \hat{\eta}(x) - \tau - C_S \left( 1 + 2 \sqrt{e_0^\top (Q_{x,h}^\beta)^{-1} e_0 \cdot |N_{x,h}|} r^{\beta A_1} \right)^2 \right\}, \]
whenever \( Q_{x,h}^\beta \) is invertible and \( \hat{\eta}(x) \geq \tau + C_S \left( 1 + 2 \sqrt{e_0^\top (Q_{x,h}^\beta)^{-1} e_0 \cdot |N_{x,h}|} r^{\beta A_1} \right) \), and \( \hat{p}_n^+(B) := 1 \) otherwise. Lemma 18 in Section 6.4 shows that these are indeed \( p \)-values.

We will also make use of an alternative set of hyper-cubes
\[ \mathcal{H}^+ := \left\{ 2^{-q} \prod_{j=1}^d [a_j, a_j + 1] : (a_1, \ldots, a_d) \in \mathbb{Z}^d, q \in \mathbb{N} \right\}. \]
Now, given \( x_{1:n} = (x_i)_{i \in [n]} \in (\mathbb{R}^d)^n \), we define
\[ \mathcal{H}^+(x_{1:n}) := \{ B \in \mathcal{H}^+ : \{x_1, \ldots, x_n\} \cap B \neq \emptyset \text{ and } \text{diam}_\infty(B) \geq 1/n \}, \]
so that \( |\mathcal{H}^+(x_{1:n})| \leq 2^d n \log_2 n \), and \( |\mathcal{H}^+(D_X)| \leq n \log_2 n \) with probability 1 when \( \mu \) is absolutely continuous with respect to Lebesgue measure. We denote our modified procedure for general smoothness, obtained by applying Algorithm 1 with the \( p \)-values (14) and the hyper-cubes given by (15), as \( \hat{A}_{\text{OSS}} \).

Propositions 7 and 8 are the analogues of Propositions 4 and 5 for \( \hat{A}_{\text{OSS}}^+ \) and, in combination, prove the upper bound in Theorem 6.

**Proposition 7.** Let \( \tau \in (0,1) \), \( \alpha \in (0,1) \) and \( (\beta, C_S) \in (0,\infty) \times [1,\infty) \). Then \( \hat{A}_{\text{OSS}}^+ \in \hat{A}_n (\tau,\alpha,P_{\text{Hai}}(\beta,C_S)) \).

**Proposition 8.** Take \( \alpha \in (0,1) \), \( (\beta, C_S) \in (0,\infty) \times [1,\infty) \), \( (\kappa,\gamma,\nu,C_{\text{App}}) \in (0,\infty)^2 \times (0,1) \times [1,\infty) \) and \( A \subseteq B(\mathbb{R}^d) \) with \( \dim_{\text{VC}}(A) < \infty \) and \( \emptyset \in A \). There exists \( \tilde{C} \geq 1 \), depending only on \( d \), \( \beta \), \( C_S \), \( \kappa \), \( \gamma \), \( \nu \), \( C_{\text{App}} \) and \( \dim_{\text{VC}}(A) \), such that for all \( P \in P_{\text{Hai}}(\beta,C_S) \cap P_{\text{App}}^+(A,\tau,\kappa,\gamma,\nu,C_{\text{App}}) \), \( n \in \mathbb{N} \) and \( \delta \in (0,1) \), we have
\[ \mathbb{P}_P \left[ M_\tau - \mu(\hat{A}_{\text{OSS}}^+) > \tilde{C} \left\{ \left( \log_+ \frac{n/(\alpha \wedge \delta)}{n} \right)^{\frac{\beta_C}{(2+\delta)+\beta_C}} + \left( \log_+ \frac{1/\delta}{n} \right)^{\frac{\beta_C}{2}} \right\} \right] \leq \delta, \]
As a consequence, for \( \alpha \in (0,1/2) \),
\[ R_\tau(\hat{A}_{\text{OSS}}^+) \leq C \left\{ \left( \log_+ \frac{n/\alpha}{n} \right)^{\frac{\beta_C}{(2+\delta)+\beta_C}} + \frac{1}{n^{1/2}} \right\}, \]
where \( C > 0 \) depends only on \( \tilde{C} \).
4 Lower bound constructions

As mentioned at the end of Section 2, our lower bound constructions are common to both Theorem 2 and Theorem 6. In fact, both lower bounds will follow from Propositions 9 and 10 below. As shorthand, given \( \mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d) \), \( \tau \in (0, 1) \), \( (\beta, \kappa, \gamma) \in (0, \infty)^3 \), \( v \in (0, 1) \) and \( (C_S, C_{\text{App}}) \in [1, \infty)^2 \), we write

\[
\mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \kappa, \gamma, v, C_S, C_{\text{App}}) := \mathcal{P}_{\text{H\ae}}(\beta, C_S) \cap \mathcal{P}_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, C_{\text{App}}) \cap \mathcal{P}^+_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, v, C_{\text{App}}).
\]

**Proposition 9.** Take \( \epsilon_0 \in (0, 1/2) \), \( \tau \in (\epsilon_0, 1-\epsilon_0) \), \( (\beta, C_S) \in (0, \infty) \times [1, \infty) \), \( (\kappa, \gamma, v, C_{\text{App}}) \in (0, \infty)^2 \times (0, 1) \times [1, \infty) \) with \( \beta \gamma (\kappa - 1) < d \kappa \), and \( v \in (0, (4d^1/2)^{-d}) \). Suppose that \( \mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d) \) satisfies \( \mathcal{A}_{\text{rect}} \subseteq \mathcal{A} \subseteq \mathcal{A}_{\text{conv}} \).

(i) There exists \( c_0 > 0 \), depending only on \( d, \beta, \gamma, C_S, C_{\text{App}} \) and \( \epsilon_0 \), such that, for every \( \alpha \in (0, 1/8] \), \( n \in \mathbb{N} \) and \( \hat{A} \in \hat{\mathcal{A}}_n(\tau, \alpha, \mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \kappa, \gamma, v, C_S, C_{\text{App}})) \), we can find \( P \in \mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \kappa, \gamma, v, C_S, C_{\text{App}}) \) with regression function \( \eta: \mathbb{R}^d \to [\tau - \epsilon_0/2, \tau + \epsilon_0/2] \) and marginal distribution \( \mu \) on \( \mathbb{R}^d \), satisfying

\[
\mathbb{E}_P\left[\left\{ M_\tau(P, \mathcal{A}) - \mu(\hat{A}) \right\} \cdot 1_{\{\hat{A} \subseteq \mathcal{X}_r(\eta)\}} \right] \geq c_0 \cdot \left( \frac{\log(1/(4\alpha))}{n} \wedge 1 \right)^{\frac{\beta \gamma}{\kappa (2\beta + d) + \beta \gamma}}.
\]

(ii) There exists \( c_1 > 0 \), depending only on \( d, \beta, \gamma, C_S, C_{\text{App}} \) and \( \epsilon_0 \), such that, given \( \alpha \in (0, 1/2 - \epsilon_0] \), \( n \in \mathbb{N} \) and \( \hat{A} \in \hat{\mathcal{A}}_n(\tau, \alpha, \mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \kappa, \gamma, v, C_S, C_{\text{App}})) \), we can find \( P \in \mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \kappa, \gamma, v, C_S, C_{\text{App}}) \) with regression function \( \eta: \mathbb{R}^d \to [\tau - \epsilon_0/2, \tau + \epsilon_0/2] \) and marginal distribution \( \mu \) on \( \mathbb{R}^d \), satisfying

\[
\mathbb{E}_P\left[\left\{ M_\tau(P, \mathcal{A}) - \mu(\hat{A}) \right\} \cdot 1_{\{\hat{A} \subseteq \mathcal{X}_r(\eta)\}} \right] \geq c_1 \cdot \left( \frac{\log_+ n}{n} \right)^{\frac{\beta \gamma}{\kappa (2\beta + d) + \beta \gamma}}.
\]

Two remarks are in order. First, note that for any \( \hat{A} \in \hat{\mathcal{A}}_n \), we have

\[
R_\tau(\hat{A}) = \frac{\mathbb{E}_P\left[\left\{ M_\tau(P, \mathcal{A}) - \mu(\hat{A}) \right\} \cdot 1_{\{\hat{A} \subseteq \mathcal{X}_r(\eta)\}} \right]}{\mathbb{P}_P(\mathcal{A} \subseteq \mathcal{X}_r(\eta))} \geq \mathbb{E}_P\left[\left\{ M_\tau(P, \mathcal{A}) - \mu(\hat{A}) \right\} \cdot 1_{\{\hat{A} \subseteq \mathcal{X}_r(\eta)\}} \right],
\]

so Proposition 9 does indeed yield lower bounds on the worst-case regret. Second,

\[
\hat{\mathcal{A}}_n(\tau, \alpha, \mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \kappa, \gamma, v, C_S, C_{\text{App}})) \supseteq \hat{\mathcal{A}}_n(\tau, \alpha, \mathcal{P}_{\text{H\ae}}(\beta, C_S)),
\]

so it suffices to provide a lower bound for the regret when \( \hat{A} \) belongs to the larger set.

To lay the groundwork for the proof of Proposition 9, let \( L \in \mathbb{N} \), \( r \in (0, \infty) \), \( w \in (0, (2r)^{-d} \wedge 1) \), \( s \in (0, 1 \wedge (r/2)) \) and \( \theta \in (0, \epsilon_0/2) \). Our goal is to define a collection of probability distributions \( \{ \mathcal{P}^\dagger \equiv \mathcal{P}^\dagger_{L,r,u,w,s,\theta} : \ell \in [L] \} \) on \( \mathbb{R}^d \times [0, 1] \); we will show that these distributions belong to \( \mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \kappa, \gamma, v, C_S, C_{\text{App}}) \) for appropriate choices of \( L, r, u, s \) and \( \theta \), and are such that any data-dependent selection set \( \hat{A} \in \hat{\mathcal{A}}_n(\tau, \alpha, \mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \kappa, \gamma, v, C_S, C_{\text{App}})) \) must satisfy the lower bound in Proposition 9. To this end, let \( r_\gamma(w) := \frac{1}{2} \left( \left\{(4\sqrt{d})^d - 2^d \right\} r^d + w^{-1} \right)^{1/d} \) and choose \( \{z_1, \ldots, z_L\} \subseteq \mathbb{R}^d \) such that \( \|z_\ell - z_{\ell'}\|_\infty > 2 (r_\gamma(w) + 1) \) for all distinct \( \ell, \ell' \in [L] \). We introduce sets \( K^0_r(1), \ldots, K^0_r(L) \subseteq \mathbb{R}^d \), \( K^1_r(1), \ldots, K^1_r(L) \subseteq \mathbb{R}^d \) defined by \( K^0_r(\ell) := \hat{B}_r(z_\ell) \)
and $K_1^i(\ell) := \tilde{B}_{r^i(w)}(z_\ell) \setminus B_{2r^i(z_\ell)}(z_\ell)$ for $\ell \in [L]$. We also define the probability measure $\mu_{L,r,w}$ on $\mathbb{R}^d$ to be the uniform distribution on $J_{L,r,w} := \bigcup_{\ell \in [L]} K_1^i(\ell)$; since $L_d(K_0^i(\ell) \cup K_1^i(\ell)) = (2r^i)^d + (2r^i(w))^d - (4d/2r)^d = w^{-1}$ for all $\ell \in [L]$, it follows that the density of $\mu_{L,r,w}$ with respect to $L_d$ takes the constant value $w/L$ on $J_{L,r,w}$.

Now define a function $h : [0, 1] \to [0, 1]$ by $h(z) := e^{-z^2/(1-z^2)}$ for $z \in [0, 1)$ and $h(1) := 0$, so that $h(0) = 1$, max$_{k \in \mathbb{N}}$ max$_{z \in [0, 1)} |h(k)(z)| = 0$ and

$$A_m := \max_{k \in [m]} \sup_{z \in [0, 1]} |h(k)(z)| \in (0, \infty)$$

for each $m \in \mathbb{N}$. This allows us to define regression functions $\eta_{L,r,w,s,\theta}^\ell : \mathbb{R}^d \to [0, 1]$ for $\ell \in [L]$ by

$$\eta_{L,r,w,s,\theta}^\ell(x) := \begin{cases} 
\tau + \theta & \text{if } \|x - z_\ell\|_2 \leq d^{1/2}r \\
\tau - \theta & \text{if } \|x - z_\ell\|_2 \leq s \text{ for some } \ell' \in [L] \setminus \{\ell\} \\
\tau + \theta - 2\theta \cdot h\left(\frac{\|x - z_\ell\|_2}{s} - 1\right) & \text{if } s < \|x - z_\ell\|_2 \leq 2s \text{ for some } \ell' \in [L] \setminus \{\ell\} \\
\tau + \theta & \text{if } 2s < \|x - z_\ell\|_2 \leq d^{1/2}r \text{ for some } \ell' \in [L] \setminus \{\ell\} \\
\tau - \theta + 2\theta \cdot h\left(\frac{\|x - z_\ell\|_2}{dr^{1/2}} - 1\right) & \text{if } d^{1/2}r < \|x - z_\ell\|_2 < 2d^{1/2}r \text{ for some } \ell' \in [L] \\
\tau - \theta & \text{otherwise.}
\end{cases}$$

(17)

Thus, $\eta_{L,r,w,s,\theta}^\ell$ is infinitely differentiable and uniformly above the level $\tau$ on $K_0^i(\ell)$, but both takes a value below $\tau$ at the centre $z_\ell$ of each $K_0^i(\ell')$ with $\ell' \in [L] \setminus \{\ell\}$, and is uniformly below the level $\tau$ on each $K_1^i(\ell')$ with $\ell' \in [L]$. Finally, then, for $\ell \in [L]$, we can let $P_{L,r,w,s,\theta}^\ell$ denote the unique Borel probability distribution on $\mathbb{R}^d \times [0, 1]$ with marginal $\mu_{L,r,w}$ on $\mathbb{R}^d$ and regression function $\eta_{L,r,w,s,\theta}^\ell$. Figure 1 provides an illustration of the regression functions used in this construction.

Lemmas 29 and 31 verify that $\{P_{L,r,w,s,\theta}^\ell : \ell \in [L]\} \subseteq \mathcal{P}(\mathcal{A}, \tau, \beta, \kappa, \gamma, \nu, C_S, C_{\text{App}})$ for appropriate choices of $r$, $w$, $s$ and $\theta$. Moreover, Proposition 33 reveals both that the chi-squared divergences between pairs of distributions in our construction are small, and yet that the distributions are sufficiently different that any set $A \in \mathcal{A} \cap \text{Pow}(\mathcal{X}_r(\eta_0) \cap \mathcal{X}_r(\eta_{e_0}))$ for distinct $\ell, \ell' \in [L]$ must have much smaller $\mu$-measure than $M_r$. To conclude, we apply a constrained risk inequality due to Brown and Low (1996) in the proof of Proposition 9(i) and a version of Fano’s lemma in the proof of Proposition 9(ii).

Proposition 10 provides the final (parametric) part of the lower bounds in Theorems 2 and 6.

**Proposition 10.** Take $e_0 \in (0, 1/2]$, $\tau \in (\epsilon_0, 1 - \epsilon_0)$, $(\beta, C_\delta) \in (0, \infty) \times [1, \infty)$, $(\kappa, \gamma, \nu, C_{\text{App}}) \in (0, \infty)^2 \times (0, 1) \times [1, \infty)$ with $\beta\gamma(\kappa - 1) < d\kappa$ and $\nu \in (0, 4^{-d}]$. Suppose that $A \subseteq \mathcal{B}(\mathbb{R}^d)$ satisfies $\mathcal{A}_{\text{rect}} \subseteq A \subseteq \mathcal{A}_{\text{conv}}$. Then there exists $c_2 > 0$, depending only on $e_0$, $d$, $\beta$, $\kappa$, $\gamma$, $C_\delta$ and $C_{\text{App}}$, such that for any $n \in \mathbb{N}$, $\alpha \in (0, 1/2 - \epsilon_0]$ and $A \in \mathcal{A}_n(\tau, \alpha, \mathcal{P}(\mathcal{A}, \tau, \beta, \kappa, \gamma, \nu, C_S, C_{\text{App}}))$, we can find $P \in \mathcal{P}(\mathcal{A}, \tau, \beta, \kappa, \gamma, \nu, C_S, C_{\text{App}})$ with regression function $\eta : \mathbb{R}^d \to [\tau - \epsilon_0/2, \tau + \epsilon_0/2]$ and marginal distribution $\mu$ on $\mathbb{R}^d$ that satisfies

$$\mathbb{E}_P\left[\left\{M_r(P, A) - \mu(A)\right\} \cdot 1_{\{A \subseteq \mathcal{X}_r(\eta_0)\}}\right] \geq \frac{c_2}{\sqrt{n}}.$$
Figure 1: Illustration of the lower bound construction of $P_{L,r,w,s,\theta}^\ell$ in Proposition 9. Blue and red regions correspond to the regression function $\eta_{L,r,w,s,\theta}^\ell$ being above and below $\tau$ respectively. Note the different behaviour in the $\ell$th region $K_0^0(\ell)$ from the others. The marginal measure $\mu_{L,r,w,s,\theta}^\ell$ on $\mathbb{R}^d$ is uniformly distributed on $\bigcup_{\ell \in [L]}(K_0^0(\ell) \cup K_1^1(\ell))$; the boundaries of these regions are denoted with black lines.
The construction for the proof of Proposition 10 is somewhat different from those in the proof of Proposition 9: it hinges on the difficulty of estimating \( \mu(A) \) for \( A \in \mathcal{A} \). To formalise this idea, given \( t \in [1, \infty) \), \( \theta \in (0, \epsilon_0/2] \), \( s \in (0, 1] \) and \( \zeta \in \left[0, \frac{4d}{(2t)^d + 2s} \right] \), we first define a pair of distributions \( \{P_{t,\theta,s,\zeta}^{\ell}\}_{\ell \in \{-1,1\}} \) on \( \mathbb{R}^d \times [0, 1] \). Define \( \eta \equiv \eta_{t,\theta,s} : \mathbb{R}^d \to [0, 1] \) by

\[
\eta(x) \equiv \eta_{t,\theta,s}(x_1, \ldots, x_d) := \begin{cases} 
\tau + \theta & \text{for } x_1 \leq -t - s \\
\tau + \theta \{1 - 2h\left(\frac{x_1 - 1}{s}\right)\} & \text{for } -t - s < x_1 \leq -t \\
\tau - \theta & \text{for } -t < x_1 \leq t \\
\tau + \theta \{1 - 2h\left(\frac{x_1 - 1}{s}\right)\} & \text{for } t < x_1 \leq t + s \\
\tau + \theta & \text{for } x_1 \geq t + s.
\end{cases}
\]

Define \( A_0 := [-t, t]^d \), \( A_{-1} := [-t-2s, -t-s] \times [-\frac{s}{2}, \frac{s}{2}]^{d-1} \) and \( A_1 := [t+s, t+2s] \times [-\frac{s}{2}, \frac{s}{2}]^{d-1} \). For \( \ell \in \{-1,1\} \), let \( \mu_{\zeta}^{\ell} \equiv \mu_{t,\theta,s,\zeta}^{\ell} \) be the Lebesgue-absolutely continuous measure supported on \( A_{-1} \cup A_0 \cup A_1 \subseteq \mathbb{R}^d \) with piecewise constant density \( f_{\mu_{\zeta}^{\ell}} : \mathbb{R}^d \to [0, \infty) \) given by

\[
f_{\mu_{\zeta}^{\ell}}(x) := \begin{cases} 
\frac{1}{(2t)^d + 2s^d} + \frac{j d}{s^d} & \text{for } x \in A_j \text{ with } j \in \{-1, 0, 1\}, \\
0 & \text{for } x \notin A_{-1} \cup A_0 \cup A_1.
\end{cases}
\]

Now for \( \ell \in \{-1,1\} \), let \( P_{\zeta}^{\ell} \equiv P_{t,\theta,s,\zeta}^{\ell} \) denote the unique distribution on \( \mathbb{R}^d \times [0, 1] \) with marginal \( \mu_{\zeta}^{\ell} \) on \( \mathbb{R}^d \) and regression function \( \eta \). Figure 2 illustrates this construction.

![Figure 2: Illustration of the lower bound construction of \( P_{\zeta}^{1} \equiv P_{t,\theta,s,\zeta}^{1} \) in Proposition 10. Blue and red regions correspond to the regression function \( \eta_{t,\theta,s} \) being above and below \( \tau \) respectively.](image)

In the proof of Proposition 10, we will show that \( \{P_{t,\theta,s,\zeta}^{\ell} : \ell \in \{-1,1\}\} \subseteq \mathcal{P}(\mathcal{A}, \tau, \beta, \kappa, \gamma, v, C_S, C_{\text{App}}) \) for suitable \( t, \theta, s \) and \( \zeta \). Moreover, \( P_{t,\theta,s,\zeta}^{-1} \) and \( P_{t,\theta,s,\zeta}^{1} \) are close in chi-squared divergence, but nevertheless we cannot have both \( \mu_{\zeta}^{-1}(A) \) and \( \mu_{\zeta}^{1}(A) \) close to \( M_{\tau}(P_{\zeta}^{-1}, \mathcal{A}) = M_{\tau}(P_{\zeta}^{1}, \mathcal{A}) \) for \( A \in \mathcal{A} \cap \text{Pow}(\mathcal{X}_{\zeta}(\eta)) \). Hence, any data-dependent selection
set \( \hat{A} \) that satisfies our Type I error guarantee must incur large regret for at least one of these distributions.

5 Application to heterogeneous treatment effects

The aim of this section is to show how our previous results may be applied to the two-arm setting with a treatment and control, where we are interested in regions of substantial treatment effect. To this end, let \( \bar{P} \) denote the distribution of a random triple \((X, T, \bar{Y})\) taking values in \( \mathbb{R}^d \times \{0, 1\} \times [0, 1] \), where \( X \) represents covariates, \( T \) is a treatment indicator and \( \bar{Y} \) denotes the corresponding response. Assume that \( X \sim \mu \), and that the function \( \pi : \mathbb{R}^d \to [0, 1] \), given by \( \pi(x) := \mathbb{P}(T = 1|X = x) \), is known. For \( \ell \in \{0, 1\} \), let \( \bar{y}_\ell(x) := \mathbb{E}(\bar{Y}|X = x, T = \ell) \). The heterogeneous treatment effect is the function \( \varphi : \mathbb{R}^d \to [-1, 1] \) defined by \( \varphi(x) := \bar{y}_1(x) - \bar{y}_0(x) \) for \( x \in \mathbb{R}^d \). Given \( t \in [-1, 1] \) and a class of sets \( A \subseteq \mathcal{B}((\mathbb{R}^d), \mathcal{P}) \), our primary interest is in identifying subsets \( \hat{A} \subseteq A \) that are contained in \( \mathcal{X}_t(\varphi) := \{ x \in \mathbb{R}^d : \varphi(x) \geq t \} \) based on data \( \bar{D} := ((X_1, T_1, \bar{Y}_1), \ldots, (X_n, T_n, \bar{Y}_n)) \sim \bar{P}^n \).

Given a family \( \mathcal{P} \) of distributions on \( \mathbb{R}^d \times \{0, 1\} \times [0, 1] \) and a significance level \( \alpha \in (0, 1) \), we let \( \hat{A} \in \mathcal{HTE}(t, \alpha, \varphi, \mathcal{P}) \) denote the set of functions \( \hat{A} : \mathbb{R}^d \times \{0, 1\} \times [0, 1] \to A \) such that \((x, \bar{D}) \mapsto 1_{\hat{A} \in \mathcal{P}}(x) \) is a Borel measurable function on \( \mathbb{R}^d \times \{0, 1\} \times [0, 1] \) and we have the Type I error guarantee that

\[
\inf_{\bar{P} \in \mathcal{P}} \mathbb{P}(\hat{A}(\bar{D}) \subseteq \mathcal{X}_t(\varphi)) \geq 1 - \alpha.
\]

Similarly to our formulation in Section 2, we seek \( \hat{A} \in \mathcal{HTE}(t, \alpha, \varphi, \mathcal{P}) \) with low regret

\[
R_t^\alpha(\hat{A}) := \sup \{ \mu(A) : A \in A \cap \mathcal{P} \} - \mathbb{E}_{\bar{P}} \{ \mu(\hat{A}(\bar{D})) \mid \hat{A}(\bar{D}) \subseteq \mathcal{X}_t(\varphi) \}.
\]

Given \((\beta, C_{S}) \in (0, \infty) \times [1, \infty) \) and a Borel measurable function \( \pi : \mathbb{R}^d \to [0, 1] \) we let \( \mathcal{P}^H(\beta, C_{S}, \pi) \) denote the class of distributions \( \bar{P} \) on \( \mathbb{R}^d \times \{0, 1\} \times [0, 1] \) such that \( \varphi \) is \((\beta, C_{S})\)-Hölder (see Definition 3), and such that \( \pi(x) = \mathbb{P}_{\bar{P}}(T = 1|X = x) \) for all \( x \in \mathbb{R}^d \). Similarly, given \((\kappa, \gamma, v, C_{App}) \in (0, \infty)^2 \times (0, 1) \times [1, \infty) \), we let \( \mathcal{P}^H(\beta, C_{S}, \pi) \cap \mathcal{P}^H(\kappa, \gamma, v, C_{App}) \) denote the class of all distributions \( \bar{P} \) such that \( \mu \) is absolutely continuous, with Lebesgue density \( f_{\mu} \), and such that (11) holds with \( \varphi \) in place of \( \eta \), with \( t \) in place of \( \tau \), and with \( \sup \{ \mu(A) : A \in A \cap \mathcal{P} \} \) in place of \( M_\tau \).

The following result on the minimax rate of regret in this heterogeneous treatment effect context is an almost immediate corollary of Theorem 6.

**Corollary 11.** Take \( \zeta_0 \in (0, 1/2), t \in [-1 - \zeta_0, 1 - \zeta_0], (\beta, C_{S}) \in (0, \infty) \times [1, \infty), (\kappa, \gamma, v, C_{App}) \in (0, \infty)^2 \times (0, 1) \times [1, \infty) \) with \( \beta \gamma (\kappa - 1) < d \kappa \) and \( v \in (0, (4d^{1/2})^{-d}] \), and let \( \pi : \mathbb{R}^d \to [0, 1 - \zeta_0] \) be Borel measurable. Let \( A \subseteq \mathcal{B}(\mathbb{R}^d) \) satisfy \( A_{\text{rect}} \subseteq A \subseteq A_{\text{conv}}, \dim_{VC}(A) < \infty \) and \( \emptyset \in A \). Given \( n \in \mathbb{N} \) and \( \alpha \in (0, 1/2 - \zeta_0) \), we have

\[
\inf_{\bar{P}} \sup_{\hat{A} \in \mathcal{HTE}(t, \alpha, \mathcal{P}^H(\beta, C_{S}, \pi))} R_t^\alpha(\hat{A}) \asymp \min \left\{ \left( \frac{\log_2(n/\alpha)}{n} \right)^{\frac{\beta\kappa\gamma}{\kappa(2\beta d + \beta \gamma)}} + \frac{1}{n^{1/2}}, 1 \right\},
\]

where the infimum in (18) is taken over \( \mathcal{HTE}(t, \alpha, \mathcal{P}^H(\beta, C_{S}, \pi)) \), the supremum is taken over \( \mathcal{HTE}(\beta, C_{S}, \pi) \cap \mathcal{HTE}(\kappa, \gamma, v, C_{App}) \). In (18), \( \asymp \) indicates that the ratio of the left- and right-hand sides is bounded above and below by positive quantities depending only on \( d, \beta, C_{S}, \kappa, \gamma, v, C_{App}, \zeta_0 \) and \( \dim_{VC}(A) \).
To establish the upper bound in Corollary 11, we reduce the problem to the setting of Section 3 by letting \( \rho_{\min} := \min \{ \inf_{x \in \mathbb{R}^d} \pi(x), 1 - \sup_{x \in \mathbb{R}^d} \pi(x) \} \geq \zeta_0 \) and introducing proxy labels

\[
Y := \frac{1}{2} \left\{ 1 + \frac{\rho_{\min}}{\pi(X)(1 - \pi(X))} \cdot (T - \pi(X)) \cdot Y \right\},
\]

so that \( Y \) takes values in \([0, 1]\) and satisfies both \( \eta(x) := \mathbb{E}(Y | X = x) = \frac{1}{2}(1 + \rho_{\min} \cdot \varphi(x)) \) and \( \mathcal{X}_t(\varphi) = \mathcal{X}_t(\eta) \) with \( t := \frac{1}{2}(1 + \rho_{\min} \cdot t) \). The upper bound then follows from Theorem 6(i).

To deduce the lower bound, we convert distributions \( P \) of random pairs \((X, Y)\) into distributions \( \tilde{P} \) of random triples \((X, T, Y)\) for which \( \mathbb{P}_{\tilde{P}}(T = 1 | X = x, Y = y) = \pi(x) \) and \( \tilde{Y} := T \cdot Y + (1 - T) \cdot (1 - Y) \), so that the corresponding heterogeneous treatment effect satisfies \( \varphi(x) = 2\eta(x) - 1 \). We may therefore deduce the lower bound in Corollary 11 from Theorem 6(ii), applied with \( t := (1 + t)/2 \).

### 6 Proofs

#### 6.1 Proof of the hardness result

**Proof of Proposition 1.** Fix \( \epsilon \in (0, 1) \), and let \((P_x)_{x \in \mathbb{R}^d}\) be a disintegration of \( P \) into conditional probability measures on \([0, 1]\); see Section 7.1 and Lemma 35. Since \( \mathcal{A} \) has finite VC dimension, it follows from the Vapnik–Chervonenkis concentration inequality (Lemma 36) that there exists a finite set \( \mathbb{T} \subset \mathbb{R}^d \) for which

\[
\sup_{A \in \mathcal{A}} \left| \frac{1}{|\mathbb{T}|} \sum_{t \in \mathbb{T}} 1\{t \in A\} - \mu(A) \right| \leq \epsilon. \tag{19}
\]

Since \( \mathbb{T} \) is finite and \( \mu \) has no atoms, we may choose a radius \( r > 0 \) sufficiently small that \( \mu(\bigcup_{t \in \mathbb{T}} B_r(t)) \leq \epsilon \). Now define a function \( \rho : \mathbb{R}^d \to [0, 1] \) by \( \rho(x) := 1 \wedge \bigwedge_{t \in \mathbb{T}} \{(2/r) \cdot \|x - t\|_{\infty}\} \), noting that \( \rho \) is Lipschitz. Further, define a family of probability distributions \((Q_x)_{x \in \mathbb{R}^d}\) on \([0, 1]\) by

\[
\int_{[0,1]} h(y) \, dQ_x(y) = \int_{[0,1]} h(\rho(x) \cdot y) \, dP_x(y),
\]

for all Borel functions \( h : [0, 1] \to [0, 1] \), and define a probability distribution \( Q \) on \( \mathbb{R}^d \times [0, 1] \) by \( Q(A \times B) = \int_A Q_x(B) \, d\mu(x) \). It follows that \((Q_x)_{x \in \mathbb{R}^d}\) is a disintegration of \( Q \) into conditional probability measures on \([0, 1]\). In addition, taking a random pair \((X^Q, Y^Q) \sim Q\) we see by (49) that for \( \mu \)-almost every \( x \in \mathbb{R}^d \),

\[
\eta_Q(x) = \mathbb{E}(Y^Q \mid X^Q = x) = \int_{[0,1]} y \, dQ_x(y) = \rho(x) \cdot \int_{[0,1]} y \, dP_x(y) = \rho(x) \cdot \eta_P(x).
\]

Hence, we may extend the definition of \( \eta_Q \) to \( \mathbb{R}^d \) in such a way that \( \eta_Q(\cdot) = \rho(\cdot) \eta_P(\cdot) \), which is a product of Lipschitz functions, so is itself Lipschitz; thus, \( Q \in \mathcal{P}_{\text{Lip}}(\mu) \). Note also that for every \( t \in \mathbb{T} \), we have \( \eta_Q(t) = \rho(t) \eta_P(t) = 0 < \tau \), so \( \mathbb{T} \cap \mathcal{X}_t(\eta_Q) = \emptyset \). Moreover, \( \eta_Q(x) \leq \eta_P(x) \)
for all $x \in \mathbb{R}^d$, so $X_r(\eta_Q) \subseteq X_r(\eta_P)$. Hence, since $\hat{A}$ controls the Type I error at the level $\alpha$ over $\mathcal{P}_{\text{Lip}}(\mu)$, we have

$$\mathbb{P}_Q\{\hat{A} \subseteq (\mathbb{R}^d \setminus T) \cap X_r(\eta_P)\} \geq \mathbb{P}_Q\{\hat{A} \subseteq (\mathbb{R}^d \setminus T) \cap X_r(\eta_Q)\} = \mathbb{P}_Q\{\hat{A} \subseteq X_r(\eta_Q)\} \geq 1 - \alpha. \quad (20)$$

Now $Q_x = P_x$ for $x \notin \bigcup_{t \in T} B_r(t)$. Hence

$$H^2(P, Q) \leq 2\text{TV}(P, Q) \leq 2\mu\left(\bigcup_{t \in T} B_r(t)\right) \leq 2\epsilon,$$

so

$$\text{TV}^2(P^\otimes n, Q^\otimes n) \leq H^2(P^\otimes n, Q^\otimes n) = 2\left\{1 - \prod_{i=1}^n \left(1 - \frac{H^2(P, Q)}{2}\right)\right\} \leq 2(1 - (1 - \epsilon)^n). \quad (21)$$

Note that by (19) if $A \in \mathcal{A}$ satisfies $A \cap T = \emptyset$, then $\mu(A) \leq \epsilon$. Hence, by (20) and (21), we have

$$\mathbb{P}_P\{\{\mu(\hat{A}) \leq \epsilon\} \cap \{\hat{A} \subseteq \mathcal{X}_r(\eta)\}\} \geq \mathbb{P}_P\{\hat{A} \subseteq (\mathbb{R}^d \setminus T) \cap \mathcal{X}_r(\eta_P)\} \geq 1 - \alpha - \sqrt{2(1 - (1 - \epsilon)^n)}.$$

Letting $\epsilon \downarrow 0$ gives (3). Thus,

$$R_r(\hat{A}) = M_r - \mathbb{E}_P(\mu(\hat{A}) | \hat{A} \subseteq \mathcal{X}_r(\eta)) \geq (1 - \alpha) \cdot M_r.$$

Finally, note that for any $\xi > 0$, we may take $A_\xi \in \mathcal{A}$ with $\mu(A_\xi) > M_r - \xi$ and $A_\xi \subseteq \mathcal{X}_r(\eta)$. Hence, we may define $\hat{A} \in \mathcal{A}$ that takes the value $A_\xi$ with probability $\alpha$ and $\emptyset$ otherwise; it has regret $R_r(\hat{A}) < (1 - \alpha) \cdot M_r + \alpha \cdot \xi$. Letting $\xi \downarrow 0$ yields the final equality in (4). \qed

### 6.2 Proofs of claims in Examples 1, 2 and 3

**Example 1:** The marginal density of $X$ is convex on $(-\infty, -\nu - 2]$ and on $[\nu + 2, \infty)$, so writing $\phi$ for the standard normal density, we have $\omega(x) = \phi(x - \nu) + \phi(x + \nu)$ for $|x| \geq \nu + 2$. Hence there exists $\xi_0 \in (0,1/\sqrt{2\pi}]$, depending only on $\nu$, such that for $\xi \in (0, \xi_0]$ we have $\mathcal{X}_\xi(\omega) = [-x_\xi, x_\xi]$, where $x_\xi \in \left[\nu + \sqrt{2\log\left(\frac{1}{(2\pi)^{1/2}}\right)}, \nu + \sqrt{2\log\left(\frac{2^{1/2}}{\pi^{1/2}}\right)}\right]$ satisfies $\phi(x_\xi - \nu) + \phi(x_\xi + \nu) = \xi$. In fact, when $\nu \geq 2$, we may take $\xi_0 = 2\phi(\nu)$. Moreover, $\eta(x) = \frac{\phi(x - \nu)}{\phi(x - \nu) + \phi(x + \nu)} = \frac{1}{1 + e^{-2\nu}}$, so $\mathcal{X}_{\nu + \Delta}(\eta) = [x_{\nu, \tau, \Delta}, \infty)$, where $x_{\nu, \tau, \Delta} := \frac{1}{2\nu} \log\left(\frac{\tau + \Delta}{\tau - \Delta}\right)$. By reducing $\xi_0 > 0$, depending only on $\nu$ and $\tau$, if necessary, we may assume that $-x_\xi \leq x_{\nu, \tau, \Delta} \leq x_\xi$ for $\xi \in (0, \xi_0]$ and $\Delta \in (0, (1 - \tau)/2)$. Writing $\Phi$ for the standard normal distribution function, we deduce that for $\xi \in (0, \xi_0]$,

$$\sup\{\mu(A) : A \in \mathcal{A}_{\text{int}} \cap \text{Pow}(\mathcal{X}_\xi(\omega) \cap \mathcal{X}_{\nu + \Delta}(\eta))\} = \mu([x_{\nu, \tau, \Delta}, x_\xi]) = \frac{1}{2} \Phi(x_\xi - \nu) - \frac{1}{2} \Phi(x_{\nu, \tau, \Delta} - \nu) + \frac{1}{2} \Phi(x_\xi + \nu) - \frac{1}{2} \Phi(x_{\nu, \tau, \Delta} + \nu).$$
Using the Mills ratio and the mean value inequality, it follows that for $\xi \in (0, \xi_0]$, 

$$M_\tau - \sup \{ \mu(A) : A \in \mathcal{A}_{\text{int}} \cap \text{Pow} (\mathcal{X}_\xi(\omega) \cap \mathcal{X}_{\tau+\Delta}(\eta)) \}$$

$$= 1 - \frac{1}{2}\Phi(x_\xi - \nu) - \frac{1}{2}\Phi(x_\xi + \nu) - \frac{1}{2}\Phi(x_{\nu,\tau,0} - \nu) - \frac{1}{2}\Phi(x_{\nu,\tau,0} + \nu)$$

$$+ \frac{1}{2}\Phi(x_{\nu,\Delta} - \nu) + \frac{1}{2}\Phi(x_{\nu,\Delta} + \nu)$$

$$\leq \frac{\phi(x_\xi - \nu)}{2(x_\xi - \nu)} + \frac{\phi(x_\xi + \nu)}{2(x_\xi + \nu)} + \frac{\Delta}{\sqrt{2\pi \nu \tau(1 - \tau)}}$$

$$\leq \frac{\xi}{2\sqrt{2\log((2\pi)^{1/2}\xi_0)}} + \frac{\Delta}{\sqrt{2\pi \nu \tau(1 - \tau)}}.$$ 

On the other hand, when $\xi > \xi_0$, we have 

$$M_\tau - \sup \{ \mu(A) : A \in \mathcal{A}_{\text{int}} \cap \text{Pow} (\mathcal{X}_\xi(\omega) \cap \mathcal{X}_{\tau+\Delta}(\eta)) \} \leq 1 \leq \frac{\xi}{\xi_0}.$$ 

We conclude that $P \in \mathcal{P}_{\text{App}}(\mathcal{A}_{\text{int}}, \tau, \kappa, \gamma, C_{\text{App}})$ with $\kappa = \gamma = 1$ when we take 

$$C_{\text{App}}^{-1} = \min \left\{ 2\sqrt{2\log((2\pi)^{1/2}\xi_0)}, \sqrt{2\pi \nu \tau(1 - \tau)}, \xi_0 \right\}.$$ 

**Example 2:** Given $\epsilon_0 > 0$, choose $A_0 \in \mathcal{A}_{\text{rect}} \cap \text{Pow} (\mathcal{X}_\tau(\eta) \cap [0, 1]^d)$ such that $\mu(A_0) \geq M_\tau - \epsilon_0$. Let $\partial A_0$ and $r = (r_1, \ldots, r_d) \in [0, 1]^d$ denote the boundary and vector of side-lengths of $A_0$ respectively. Observe that for $\Delta \leq \epsilon \cdot \delta^{1/\gamma}$, 

$$\mathcal{X}_{\tau+\Delta}(\eta) \supseteq \left\{ x \in \mathcal{X}_\tau(\eta) \cap [0, 1]^d : \text{dist}_\infty(x, \mathcal{S}_\tau) \geq (\Delta/\epsilon)^\gamma \right\}$$

$$\supseteq \left\{ x \in A_0 : \text{dist}_\infty(x, \partial A_0) \geq (\Delta/\epsilon)^\gamma \right\}.$$ 

Moreover, $\mathcal{X}_\xi(\omega) = [0, 1]^d$ for $\xi \leq 1$. For $s > 0$, let $A_{0,s} := \left\{ x \in A_0 : \text{dist}_\infty(x, \partial A_0) \geq s \right\}$. Note that for $s \leq \min_j r_j/2$, 

$$\mu(A_0) - \mu(A_{0,s}) \leq \prod_{j=1}^d r_j - \prod_{j=1}^d (r_j - 2s) \leq 1 - (1 - 2s)^d \leq 2ds.$$ 

On the other hand, if $s > \min_{j \in [d]} r_j/2$, then 

$$\mu(A_0) - \mu(A_{0,s}) \leq \prod_{j=1}^d r_j \leq \min_{j \in [d]} r_j < 2s.$$ 

Then, for $\xi \in [0, 1]$ and any $\Delta \in (0, \epsilon \cdot \delta^{1/\gamma}]$, 

$$M_\tau - \sup \{ \mu(A) : A \in \mathcal{A}_{\text{rect}} \cap \text{Pow} (\mathcal{X}_\xi(\omega) \cap \mathcal{X}_{\tau+\Delta}(\eta)) \} \leq M_\tau - \mu(A_{0,(\Delta/\epsilon)^\gamma})$$

$$\leq M_\tau - \mu(A_0) + 2d \left( \frac{\Delta}{\epsilon} \right)^\gamma$$

$$\leq \epsilon_0 + 2d \left( \frac{\Delta}{\epsilon} \right)^\gamma.$$
On the other hand, if $\xi > 1$ or $\Delta > \epsilon \cdot \delta^{1/\gamma}$, then for any $\kappa \in (0, \infty)$ and $C_{\text{App}} \geq 1/(\epsilon^\gamma \delta)$, we have

$$M_\tau - \sup \{ \mu(A) : A \in A_{\text{rect}} \cap \text{Pow}(X_\xi(\omega) \cap X_{\tau+\Delta}(\eta)) \} \leq 1 \leq C_{\text{App}} \cdot (\xi^\kappa + \Delta^\gamma).$$

Since $\epsilon_0 > 0$ was arbitrary, the conclusion follows.

**Example 3:** Writing $\omega_\kappa := \omega_{\mu_\kappa, d}$ for the lower-density of $\mu_\kappa$, we have for $x \in \mathbb{R}^d$ that

$$\omega_\kappa(x) \geq \sup_{t \in \|x\|_\infty, \infty} g_\kappa(t) \left\{ \mathcal{L}_d(B_{1\wedge t}(x) \cap B_t(0)) \wedge \inf_{r \in (0,1/t)} \frac{\mathcal{L}_d(B_r(x) \cap B_t(0))}{r^d} \right\} \geq \sup_{t \in \|x\|_\infty, \infty} (1 \wedge t^d) g_\kappa(t) \geq \begin{cases} g_\kappa(\|x\|_\infty) \wedge g_\kappa(1) & \text{if } \kappa \in (0, 2) \\ \left( \frac{1}{2^{2(\kappa-1)}} \cdot g_\kappa(\|x\|_\infty) \right) \wedge g_\kappa\left( \frac{1}{2^{(\kappa-1)/d}} \right) & \text{if } \kappa \in [2, \infty). \end{cases}$$

Now, writing $a_{d,\kappa} := \frac{1}{2^{(\kappa-1)/d}} \cdot 1_{\{\kappa \geq 2\}} + 1_{\{\kappa < 2\}}$ and $\xi_{d,\kappa} := g_\kappa(a_{d,\kappa})$, we have for $\xi \leq \xi_{d,\kappa}$ that $X_\xi(\omega_\kappa) \supseteq \{ x \in \mathbb{R}^d : \|x\|_\infty \leq R_{\xi, d, \kappa} \}$, where

$$R_{\xi, d, \kappa} := \begin{cases} \left( \frac{(\kappa/(2^2\xi))^{3-\kappa}-1}{1-\kappa} \right)^{1/d} & \text{if } \kappa \in (0, 1) \\ \log^{1/d} \left( \frac{1}{2\xi} \right) & \text{if } \kappa = 1 \\ \left( \frac{1-(2^2\xi/(\kappa a_{d,\kappa})^{\kappa-1})}{\kappa-1} \right)^{1/d} & \text{if } \kappa \in (1, \infty). \end{cases}$$

We now calculate that

$$M_\tau \equiv M_\tau(P_{\kappa, \gamma}, A_{\text{rect}}) = \mu_\kappa([0, \infty) \times \mathbb{R}^{d-1}) = 1/2. \quad (22)$$

Observe that $X_{\tau+\Delta}(\eta_\tau) = \{ x = (x_1, \ldots, x_d)^T \in \mathbb{R}^d : x_1 \geq (\Delta/C_S)^\gamma \}$ for $\Delta \in (0, 1 - \tau]$. Hence, for $\Delta \in (0, 1 - \tau]$ and $\xi \leq \xi_{d, \kappa}$, we have

$$\sup \{ \mu_\kappa(A) : A \in A_{\text{rect}} \cap \text{Pow}(X_\xi(\omega_\kappa) \cap X_{\tau+\Delta}(\eta_\tau)) \} \geq \sup \{ \mu_\kappa(A) : A \in A_{\text{rect}} \cap \text{Pow}(B_{R_{\xi, d, \kappa}}(0) \cap ([\Delta/C_S]^{\gamma}, \infty) \times \mathbb{R}^{d-1}) \} = \mu_\kappa(B_{R_{\xi, d, \kappa}}(0) \cap ([\Delta/C_S]^{\gamma}, \infty) \times \mathbb{R}^{d-1})) \geq \frac{1}{2}\mu_\kappa(B_{R_{\xi, d, \kappa}}(0)) - \mu_\kappa([0, (\Delta/C_S)^\gamma] \times \mathbb{R}^{d-1}). \quad (23)$$

For $x = (x_1, \ldots, x_d)^T \in \mathbb{R}^d$, let $x_{-1} := (x_2, \ldots, x_d)^T \in \mathbb{R}^{d-1}$. Then

$$\mu_\kappa([0, (\Delta/C_S)^\gamma] \times \mathbb{R}^{d-1}) = \int_{[0, (\Delta/C_S)^\gamma] \times \mathbb{R}^{d-1}} g_\kappa(\|x\|_\infty) \, dx \leq \int_{[0, (\Delta/C_S)^\gamma] \times \mathbb{R}^{d-1}} g_\kappa(\|x_{-1}\|_\infty) \, dx = b_{d,\kappa} \cdot \left( \frac{\Delta}{C_S} \right)^\gamma, \quad (24)$$
where
\[ b_{d,\kappa} := \int_{\mathbb{R}^{d-1}} g_\kappa(\|x-1\|_\infty) \, dx - 1 = (d-1) \cdot 2^{d-1} \int_0^\infty y^{d-2} g_\kappa(y) \, dy \]
\[
= \begin{cases} 
\frac{(1-\kappa)^{1/d} \Gamma(2-1/d) \Gamma(\frac{\kappa}{\kappa/(1-\kappa)})}{2 \Gamma(\kappa/(1-\kappa))} & \text{if } \kappa \in (0, 1), \\
\frac{\Gamma(2-1/d)}{2} & \text{if } \kappa = 1, \\
\frac{(\kappa-1)^{1/d} \Gamma(2-1/d) \Gamma(2+\frac{1-\kappa}{d})}{2 \Gamma(2-\frac{1}{d}+\frac{1}{\kappa})} & \text{if } \kappa \in (1, \infty).
\end{cases}
\]

Moreover, for \( \xi \leq \xi_{d,\kappa} \leq \kappa/2^d \),
\[
1 - \mu_\kappa(\tilde{B}_{R_{\xi_{d,\kappa}}}(0)) = d \cdot 2^d \int_{R_{\xi_{d,\kappa}}} y^{d-1} g_\kappa(y) \, dy = \left( \frac{2^d \xi}{a_{d,\kappa}^d} \right)^\kappa.
\]

But for \( \Delta > 1 - \tau \) or \( \xi > \xi_{d,\kappa} \), we have
\[
\sup \{ \mu_\kappa(A) : A \in \mathcal{A}_{\text{rect}} \cap \text{Pow}(X_\xi(\omega_\kappa) \cap X_{\tau+\Delta}(\eta_\gamma)) \} \geq 0 \geq \frac{1}{2} - \left( \frac{\Delta}{1-\tau} \right)^\gamma - \left( \frac{\xi}{\xi_{d,\kappa}} \right)^\kappa.
\]

We deduce from (22), (23), (24) and (25) that \( P_{\kappa,\gamma} \in \mathcal{P}_\text{App}(\mathcal{A}_{\text{rect}}, \tau, \kappa, \gamma, C_\text{App}) \), with
\[
C_\text{App} = \left( \frac{b_{d,\kappa}^{1/\gamma}}{C_S} \vee \frac{1}{1-\tau} \right)^\gamma \vee \left( \frac{2^d}{a_{d,\kappa}^d} \right)^\kappa \vee \left( \frac{1}{\xi_{d,\kappa}} \right)^\kappa.
\]

### 6.3 Proof of the upper bound in Theorem 2

Recall that Theorem 2(i) will follow from Lemma 3, together with Propositions 4 and 5.

**Proof of Lemma 3.** Let \( m := n \cdot \hat{\mu}_n(B) = \sum_{i \in [n]} 1_{\{X_i \in B\}}. \) If \( m = 0 \), then \( \hat{\mu}_n(B) = 1 \), so we may assume without loss of generality that \( m \geq 1 \). Let \( (i_j)_{j \in [m]} \) denote a strictly increasing sequence such that \( X_{i_j} \in B \) for all \( j \in [m] \), and define \( t := \tau + C_S \cdot \text{diam}_\infty(B)^\beta. \) For each \( j \in [m] \) let \( Z_j := Y_{i_j} \) so that
\[
\mathbb{E}(Z_j \mid \mathcal{D}_X) = \mathbb{E}(Y_{i_j} \mid \mathcal{D}_X) = \eta(X_{i_j}) \leq \inf_{x \in B} \eta(x) + C_S \cdot \text{diam}_\infty(B)^\beta \leq t,
\]
where we used the fact that \( P \in \mathcal{P}_\text{Hil}(\beta, C_S) \). Moreover, \( (Z_j)_{j \in [m]} \) are conditionally independent given \( \mathcal{D}_X \). Writing \( \bar{Z} := m^{-1} \sum_{j \in [m]} Z_j \), we have by construction of \( \hat{\mu}_n(B) \) that
\[
\mathbb{P}(\hat{\mu}_n(B) \leq \alpha \mid \mathcal{D}_X) = \mathbb{P}\left[ \exp\left\{ -n \cdot \hat{\mu}_n(B) \cdot \text{kl}(\hat{\eta}_n(B), t) \right\} \leq \alpha \right. \left. \text{and } \hat{\eta}_n(B) > t \mid \mathcal{D}_X \right] = \mathbb{P}\left[ \text{kl}(\bar{Z}, t) \geq m^{-1} \cdot \log(1/\alpha) \text{ and } \bar{Z} > t \mid \mathcal{D}_X \right] \leq \alpha,
\]
where the final inequality follows from a Chernoff bound, stated for convenience as Lemma 38. \( \square \)

The proof of Proposition 4 will rely on the following lemma.
Lemma 12. Fix $\alpha \in (0,1)$, $(\beta,C_S) \in (0,1] \times [1,\infty)$ and let $P \in \mathcal{P}_{H\ddot{o}}(\beta,C_S)$. Suppose that $\mathcal{D} = ((X_i,Y_i))_{i \in [n]} \sim P^{\otimes n}$ and let $\mathcal{D}_X = (X_i)_{i \in [n]}$. Then, with $(B(\ell))_{\ell \in [\ell]}$ and $\ell$ as in Algorithm 1 (and setting $\ell_\alpha := 0$ when $\tilde{L} \cdot \hat{p}_n(B(1)) > \alpha$), we have

$$\mathbb{P}\left(\inf_{x \in \bigcup_{\ell \in [\ell]} B(\ell)} \eta(x) \leq \tau \mid \mathcal{D}_X \right) \leq \alpha.$$  

Proof. Let $\mathcal{N}(\mathcal{D}_X) := \{B \in \mathcal{H}(\mathcal{D}_X) : \inf_{x \in B} \eta(x) \leq \tau \}$ and $m := |\mathcal{N}(\mathcal{D}_X)|$. Note that

$$\left\{ \inf_{x \in \bigcup_{\ell \in [\ell]} B(\ell)} \eta(x) \leq \tau \right\} \cap \{m = 0\} \subseteq \left\{ \inf_{x \in \bigcup_{\ell \in [\ell]} B(\ell)} \eta(x) \leq \tau \right\} \cap \{m = 0\} = \emptyset.$$

On the other hand, when $m \geq 1$, we may write

$$\ell := \min\{\ell \in [\ell] : B(\ell) \in \mathcal{N}(\mathcal{D}_X)\},$$

so that when $\tilde{L} \cdot \hat{p}_n(B(1)) \leq \alpha$, we have $\min_{\ell \in [\ell]} \inf_{x \in B(\ell)} \eta(x) \leq \tau$ if and only if $\ell \leq \ell_\alpha$. When $m \geq 1$, we have by the minimality of $\ell$ that $\ell \leq \tilde{L} + 1 - m$, so

$$\mathbb{P}\left(\inf_{x \in \bigcup_{\ell \in [\ell]} B(\ell)} \eta(x) \leq \tau \mid \mathcal{D}_X \right) = \mathbb{P}\left(\left\{ \inf_{x \in \bigcup_{\ell \in [\ell]} B(\ell)} \eta(x) \leq \tau \right\} \cap \{\tilde{L} \cdot \hat{p}_n(B(1)) \leq \alpha\} \cap \{m \geq 1\} \mid \mathcal{D}_X \right) \leq \sum_{B \in \mathcal{N}(\mathcal{D}_X)} \mathbb{P}\left(\hat{p}_n(B) \leq \frac{\alpha}{m} \mid \mathcal{D}_X \right) \leq \alpha,$$

where we applied Lemma 3 for the final inequality. \hfill $\square$

Proof of Proposition 4. By construction in Algorithm 1, we have $\hat{A}_{OSS}(\mathcal{D}) \subseteq \bigcup_{\ell \in [\ell]} B(\ell)$. Hence the result follows from Lemma 12. \hfill $\square$

We now turn to the proof of Proposition 5. A key component of this result is the following proposition, which states that if a set $A \in \mathcal{A}$ may be covered with a finite collection of hyper-cubes $\{B_1,\ldots,B_L\} \subseteq \mathcal{H}$, each with sufficiently large diameter and $\mu$-measure, in such a way that $\eta$ is well above the level $\tau$ on each $B_\ell$, then $\hat{A}_{OSS}$ will return a set of $\mu$-measure comparable with $\mu(A)$.

Proposition 13. Take $\alpha \in (0,1)$, $n \in \mathbb{N}$, $\delta \in (0,1)$, $(\beta,C_S) \in (0,1] \times [1,\infty)$, $P \in \mathcal{P}_{H\ddot{o}}(\beta,C_S)$ and $\mathcal{A} \subseteq \mathcal{B}(\mathbb{R}^d)$ with $\dim_{VC}(\mathcal{A}) < \infty$ and $\emptyset \in \mathcal{A}$. Given $L \in \mathbb{N}$, suppose that there exists hyper-cubes $\{B_1,\ldots,B_L\} \subseteq \mathcal{H}$ such that $\min_{q \in [L]} \mu(B_q) \geq 8 \log(4L/\delta)/n$, $\min_{q \in [L]} \text{diam}_\infty(B_q) \geq 1/n$ and

$$\min_{q \in [L]} \left\{ \sup_{x \in B_q} \eta(x) - 2C_S \cdot \text{diam}_\infty(B_q) \beta - \sqrt{\frac{2 \log(2^{d+1}L \cdot n(2 + \log_n 2)/(\alpha \cdot \delta))}{n \cdot \mu(B_q)}} \right\} \geq \tau. \quad (26)$$

23
Let $S^\dagger := \bigcup_{q \in [L]} B_q$, and taking the universal constant $C_{\text{VC}} > 0$ from Lemma 36, let

$$J_{n,\delta}(S^\dagger) := \sup \{ \mu(A) : A \in A \cap \text{Pow}(S^\dagger) \} - 2C_{\text{VC}} \sqrt{\frac{\dim_{\text{VC}}(A)}{n}} - \sqrt{\frac{2 \log(2/\delta)}{n}}.$$ 

Then

$$\mathbb{P}\{ \mu(\hat{\text{Aoss}}(D)) < J_{n,\delta}(S^\dagger) \} \leq \delta.$$ 

Proposition 13 will be proved through a series of lemmas below.

**Lemma 14.** Let $P$ be a distribution on $\mathbb{R}^d \times [0,1]$ having marginal $\mu$ on $\mathbb{R}^d$, and let $\delta \in (0,1)$, $n \in \mathbb{N}$ and $L \in \mathbb{N}$. Suppose further that $\{B_1, \ldots, B_L\} \subseteq \mathcal{H}$ with $\min_{q \in [L]} \mu(B_q) \geq 8 \log(4L/\delta)/n$, and define the event

$$\mathcal{E}_{1,\delta} := \left\{ \min_{q \in [L]} \left( \hat{\mu}_n(B_q) - \frac{\mu(B_q)}{2} \right) > 0 \right\},$$

where the empirical distribution $\hat{\mu}_n$ is defined in (7). Then $\mathbb{P}(\mathcal{E}_{1,\delta}) \leq \delta/4$.

**Proof.** By the multiplicative Chernoff bound (Lemma 39), for each $q \in [L]$,

$$\mathbb{P}\left( \hat{\mu}_n(B_q) \leq \frac{\mu(B_q)}{2} \right) = \mathbb{P}\left( \sum_{i=1}^n \mathbb{1}_{\{X_i \in B_q\}} \leq \frac{n}{2} \cdot \mu(B_q) \right) \leq \exp\left( -\frac{n}{8} \cdot \mu(B_q) \right) \leq \frac{\delta}{4L}.$$ 

The result therefore follows by a union bound. $\square$

**Lemma 15.** Let $P$ be a distribution on $\mathbb{R}^d \times [0,1]$ having regression function $\eta : \mathbb{R}^d \rightarrow [0,1]$, and let $\delta \in (0,1)$, $n \in \mathbb{N}$ and $L \in \mathbb{N}$. Suppose that $\{B_1, \ldots, B_L\} \subseteq \mathcal{H}$ and define the event

$$\mathcal{E}_{2,\delta} := \left\{ \max_{q \in [L]} \left( \inf_{x \in B_q} \eta(x) - \hat{\eta}_n(B_q) - \sqrt{\frac{\log(4L/\delta)}{2n \cdot \hat{\mu}_n(B_q)}} \right) < 0 \right\},$$

where the empirical distribution $\hat{\mu}_n$ and empirical regression function $\hat{\eta}_n$ are defined in (7) and (8) respectively. Then $\mathbb{P}(\mathcal{E}_{2,\delta}) \leq \delta/4$.

**Proof.** By Hoeffding’s inequality (Lemma 38), for every $q \in [L]$, we have

$$\text{esssup} \mathbb{P}\left( \hat{\eta}_n(B_q) \leq \inf_{x \in B_q} \eta(x) - \sqrt{\frac{\log(4L/\delta)}{2n \cdot \hat{\mu}_n(B_q)}} \bigg| \mathcal{D}_X \right) \leq \frac{\delta}{4L}.$$ 

The result now follows by the law of total expectation, combined with a union bound. $\square$

**Lemma 16.** Let $(\beta, C_S) \in (0,1] \times [1,\infty)$, $P \in \mathcal{P}_{\text{Hil}}(\beta, C_S)$, $\delta \in (0,1)$, $n \in \mathbb{N}$, $L \in \mathbb{N}$ and $\xi \in (0,1)$. Suppose that for some $\{B_1, \ldots, B_L\} \subseteq \mathcal{H}$ we have $\min_{q \in [L]} \mu(B_q) \geq 8 \log(4L/\delta)/n$ and

$$\min_{q \in [L]} \left\{ \sup_{x \in B_q} \eta(x) - 2C_S \cdot \text{diam}_\infty(B_q)^{\beta} - \sqrt{\frac{2 \log(4L/(\xi \cdot \delta))}{n \cdot \mu(B_q)}} \right\} \geq \tau.$$  \tag{27}

Then, recalling the definition of the p-values $\hat{p}_n$ from (9), we have

$$\mathbb{P}\left( \max_{q \in [L]} \hat{p}_n(B_q) \geq \xi \right) \leq \delta/2.$$ 

24
Proof. By Lemmas 14 and 15, we have \( \mathbb{P}(E_{1,\delta}^c \cup E_{2,\delta}^c) \leq \delta/2 \). On \( E_{1,\delta} \cap E_{2,\delta} \), we have for each \( q \in [L] \) that
\[
\hat{\eta}_n(B_q) > \inf_{x \in B_q} \eta(x) - \frac{\log(4L/\delta)}{n \cdot \mu(B_q)} \sqrt{n \cdot \mu(B_q)}
\]
\[
\geq \sup_{x \in B_q} \eta(x) - C_S \cdot \text{diam}_\infty(B_q)^3 - \frac{\log(4L/\delta)}{n \cdot \mu(B_q)} \sqrt{n \cdot \mu(B_q)}
\]
\[
\geq \tau + C_S \cdot \text{diam}_\infty(B_q)^3 + \sqrt{\frac{\log(1/\xi)}{n \cdot \mu(B_q)}},
\]
where we used the fact that \( P \in \mathcal{P}_{\text{Hö}}(\beta, C_S) \), (27) and the fact that \( \sqrt{2(a+b)} \geq \sqrt{a} + \sqrt{b} \) for all \( a, b \geq 0 \). Thus, on \( E_{1,\delta} \cap E_{2,\delta} \), we have for every \( q \in [L] \) that
\[
\hat{\mu}_n(B_q) \leq \exp\left(-\frac{n \cdot \mu(B_q)}{2} \cdot \text{kl}\{\hat{\eta}_n(B_q), \tau + C_S \cdot \text{diam}_\infty(B_q)^3\}\right) < \xi,
\]
as required, where the final bound uses Pinsker’s inequality. \( \square \)

We can now complete the proof of Proposition 13 before returning to complete the proof of Proposition 5.

Proof of Proposition 13. We begin by defining events
\[
E_{PV} := \left\{ \max_{q \in [L]} \hat{\mu}_n(B_q) \leq \frac{\alpha}{2^4n(2 + \log_2 n)} \right\},
\]
\[
E_{VC} := \left\{ \sup_{A \in \mathcal{A}} |\hat{\mu}_n(A) - \mu(A)| \leq C_{VC} \sqrt{\frac{\text{dim}_\mathcal{A}(A)}{n}} + \sqrt{\frac{\log(2/\delta)}{2n}} \right\}.
\]
By Lemma 16, with \( \xi = \alpha/(2^4n(2 + \log_2 n)) \), and Lemma 36, we have \( \mathbb{P}(E_{PV} \cup E_{VC}) \leq \delta \). On \( E_{PV} \), we have for each \( q \in [L] \) that \( \hat{\mu}_n(B_q) < 1 \), so \( \mu_n(B_q) > 0 \), and we deduce that \( B_q \in \mathcal{H}(\mathcal{D}_X) \). Now \( \hat{L} = |\mathcal{H}(\mathcal{D}_X)| = 2^4n(2 + \log_2 n) \), so on the event \( E_{PV} \) we also have \( \hat{L} \cdot \hat{\mu}_n(B_q) \leq \alpha \) for all \( q \in [L] \). Consequently, on the event \( E_{PV} \), we have for each \( q \in [L] \) that \( B_q = B_{l(q)} \) for some \( l(q) \leq l_\alpha \), so \( S^\dagger \subseteq \bigcup_{\ell \in [l_\alpha]} B_{(\ell)} \). Now take \( \zeta > 0 \) and choose \( A^*_{\dagger} \in \mathcal{A} \cap \text{Pow}(S^\dagger) \) with \( \mu(A^*_{\dagger}) > \sup \{ \mu(A) : A \in \mathcal{A} \cap \text{Pow}(S^\dagger) \} - \zeta \). It follows that \( A^*_{\dagger} \in \mathcal{A} \cap \text{Pow}(\bigcup_{\ell \in [l_\alpha]} B_{(\ell)}) \) and hence on the event \( E_{PV} \cap E_{VC} \) that
\[
\mu(A^*_{\dagger}) \geq \hat{\mu}_n(A^*_{\dagger}) - C_{VC} \sqrt{\frac{\text{dim}_\mathcal{A}(A)}{n}} - \sqrt{\frac{\log(2/\delta)}{2n}}
\]
\[
\geq \mu(A^*_{\dagger}) - C_{VC} \sqrt{\frac{\text{dim}_\mathcal{A}(A)}{n}} - \sqrt{\frac{2 \log(2/\delta)}{n}} \geq J_{n,\delta}(S^\dagger) - \zeta.
\]
Letting \( \zeta \downarrow 0 \), we conclude that \( \mu(A^*_{\dagger}) \geq J_{n,\delta}(S^\dagger) \), as required. \( \square \)
Proof of Proposition 5. We define \( \rho := \kappa(2\beta + d) + \beta \gamma, \theta := 8\log(3^{d+1} \cdot n/(\alpha \land \delta))/n, \)
\( r := (C_S^{-}(\gamma + 2\kappa) \cdot \theta^\kappa)^{1/r}, \xi := (C_S^d \theta^{\beta})^{\gamma/r} \) and \( \Delta := 2^5(C_S^d \theta^{\beta})^{\kappa/r}. \) We initially assume that \( \Delta \leq 1, \)
so that \( 1/n \leq \theta \leq r \leq 2^{-5}. \) Now choose a maximal subset \( \{x_1, \ldots, x_L\} \subseteq X_\zeta(\omega) \cap X_{r+\Delta}(\eta) \)
with the property that \( \|x_q \cdot x_q\|_\infty > r \) for distinct \( q, q' \in [L]. \) Then \( X_\zeta(\omega) \cap X_{r+\Delta}(\eta) \subseteq \bigcup_{q \in [L]} \bar{B}_r(x_q) \) and \( \bar{B}_{r/3}(x_q) \cap \bar{B}_{r/3}(x_{q'}) = \emptyset \) for distinct \( q, q' \in [L]. \) Now, since \( \xi \leq 1, \)
we can find \( C_S \leq \theta^{-\beta/d} \) and so
\[
L \leq \sum_{q=1}^{L} \frac{\mu(\bar{B}_{r/3}(x_q))}{\xi \cdot (r/3)^d} \leq \frac{1}{\xi \cdot (r/3)^d} \cdot \mu\left( \bigcup_{q=1}^{L} \bar{B}_{r/3}(x_q) \right) \leq \frac{3^d}{\theta} \leq 3^d n.
\]
For each \( q \in [L] \) we can find \( B_q \in \mathcal{H} \) such that \( \bar{B}_r(x_q) \subseteq B_q \) and such that \( r \leq \text{diam}_\infty(B_q) \leq 2^{-\left[\log_2(\frac{1}{n})\right]+1} \leq 4r, \) which is possible since \( r \leq 1/32. \) We then have that for every \( q \in [L], \)
\[
\mu(B_q) \geq \mu(\bar{B}_r(x_q)) \geq \xi \cdot r^d \geq \theta \geq 8\log(4L/\delta)/n.
\]
Hence
\[
\min_{q \in [L]} \left\{ \sup_{x \in B_q} \eta(x) - 2C_S \cdot \text{diam}_\infty(B_q)^\beta - \frac{2\log(2^{2+d} L \cdot n(2 + \log_2 n)/(\alpha \cdot \delta))}{n \cdot \mu(B_q)} \right\} \\
\geq \min_{q \in [L]} \left\{ \eta(x_q) - 2^{1+2\beta} \cdot C_S \cdot r^\beta - \frac{2\log(2^{4+d} 3^d n^2 \log_2(n)/(\alpha \cdot \delta))}{n \cdot \xi \cdot r^d} \right\} \\
\geq \tau + \Delta - 2^3 C_S r^\beta - \sqrt{\frac{\theta}{\xi \cdot r^d}} \geq \tau,
\]
so (26) holds. Thus, taking \( S^\dagger := \bigcup_{q \in [L]} B_q \supseteq X_\zeta(\omega) \cap X_{r+\Delta}(\eta), \) when \( \Delta \leq 1 \) we may apply Proposition 13 to see that with probability at least \( 1 - \delta, \) we have
\[
\mu(\hat{A}_{\text{OSS}}) \geq \mu(A : A \in A \cap \text{Pow}(S^\dagger)) - 2C_{\text{VC}} \sqrt{\frac{\text{dim}_{\text{VC}}(A)}{n}} \geq \mu(A : A \in A \cap \text{Pow}(X_\zeta(\omega) \cap X_{r+\Delta}(\eta))) - 2C_{\text{VC}} \sqrt{\frac{\text{dim}_{\text{VC}}(A)}{n}} \geq M_r - C_{\text{App}} \cdot (\xi^\kappa + \Delta \gamma) - 2C_{\text{VC}} \sqrt{\frac{\text{dim}_{\text{VC}}(A)}{n}} - \sqrt{\frac{2\log(2/\delta)}{n}} \geq M_r - C_{\text{App}} \cdot (1 + 2^5 \gamma) \cdot (C_S^d \cdot \theta^\beta)^{\gamma/r} - 2C_{\text{VC}} \sqrt{\frac{\text{dim}_{\text{VC}}(A)}{n}} - \sqrt{\frac{2\log(2/\delta)}{n}} \geq M_r - C \left\{ \left( \frac{\log_+ (n/(\alpha \land \delta))}{n} \right)^{\frac{\alpha \land \delta}{(2\beta + d) + \beta \gamma}} + \left( \frac{\log_+ (1/\delta)}{n} \right)^{1/2} \right\},
\]
where \( C \geq 1 \) depends only on \( d, \beta, C_S, \kappa, \gamma, C_{\text{App}} \) and \( \text{dim}_{\text{VC}}(A). \) Finally, if \( \Delta > 1, \) then (28) holds because \( \mu(\hat{A}_{\text{OSS}}) \geq 0, \)
\( M_r \leq 1 \) and \( C_{\text{App}} \geq 1, \) so (29) holds too. This completes the proof of the first claim of the proposition.
For the second claim, observe by Proposition 4 that for $\alpha \in (0, 1/2]$, 

$$ R_r(\hat{A}_{OSS}) \leq \frac{M_r - \mathbb{E} \mu(\hat{A}_{OSS})}{\mathbb{P}(\hat{A}_{OSS} \subseteq \mathcal{X}_r(\eta))} \leq \frac{M_r - \mathbb{E} \mu(\hat{A}_{OSS})}{1 - \alpha} \leq \tilde{C} \left\{ \left( \frac{\log(n/\alpha)}{n} \right)^{\frac{\beta \gamma}{\alpha(\beta + d) + \beta \gamma}} + \frac{1}{n^{1/2}} \right\}, $$

where the final bound follows by integrating the tail bound in the first part of the proposition.

\[ \square \]

### 6.4 Proof of the upper bound in Theorem 6

First we state the following consequence of Hoeffding’s inequality.

**Lemma 17.** Fix $(\beta, C_S) \in (0, \infty) \times [1, \infty)$ and let $P \in \mathcal{P}_{H\ddot{o}f}(\beta, C_S)$. Suppose that $\mathcal{D} = (\mathcal{X}_i, Y_i)_{i \in [n]} \sim P^\otimes n$ and let $\mathcal{D}_X = (X_i)_{i \in [n]}$. Given $x \in \mathbb{R}^d$, $h \in [0, 1]$, and $\alpha \in (0, 1)$ define

$$ \hat{\Delta}_{x,h}(\alpha) := \begin{cases} \sqrt{e_0^\top (Q_{x,h}^\beta)}^{-1} e_0 \cdot \left( C_S \cdot h^\beta \cdot |N_{x,h}|^{1/2} + \sqrt{\frac{\log(1/\alpha)}{2}} \right) & \text{when } Q_{x,h}^\beta \text{ is invertible}, \\ 1 & \text{otherwise}. \end{cases} $$

Then

$$ \max\{ \mathbb{P}(\hat{\eta}(x) - \eta(x) \geq \hat{\Delta}_{x,h}(\alpha) \mid \mathcal{D}_X), \mathbb{P}(\eta(x) - \hat{\eta}(x) \geq \hat{\Delta}_{x,h}(\alpha) \mid \mathcal{D}_X) \} \leq \alpha. $$

**Proof.** Fix a realisation of $\mathcal{D}_X = (X_i)_{i \in [n]}$. It suffices to restrict our attention to the case where $Q_{x,h}^\beta$ is invertible. Writing $u_i := \langle e_0, (Q_{x,h}^\beta)^{-1} \Phi_{x,h}(X_i) \rangle$ for $i \in [n]$, we have

$$ \sum_{i \in N_{x,h}} e_i \cdot \langle w_{x,h}^\beta, \Phi_{x,h}^\beta(X_i) \rangle = e_0^\top (Q_{x,h}^\beta)^{-1} \sum_{i \in N_{x,h}} \Phi_{x,h}^\beta(X_i) (w_{x,h}^\beta) \Phi_{x,h}^\beta(X_i) = e_0^\top w_{x,h}^\beta = \eta(x). $$

Hence,

$$ \langle e_0, \hat{w}_{x,h}^\beta \rangle = e_0^\top (Q_{x,h}^\beta)^{-1} V_{x,h} = \sum_{i \in N_{x,h}} Y_i \cdot e_0^\top (Q_{x,h}^\beta)^{-1} \Phi_{x,h}^\beta(X_i) $$

$$ = \sum_{i \in N_{x,h}} u_i \cdot \left( \{ Y_i - \eta(X_i) \} + \{ \eta(X_i) - T_x^\beta[\eta](X_i) \} + \{ w_{x,h}^\beta, \Phi_{x,h}^\beta(X_i) \} \right) $$

$$ = \sum_{i \in N_{x,h}} u_i \cdot \left( \{ Y_i - \eta(X_i) \} + \{ \eta(X_i) - T_x^\beta[\eta](X_i) \} \right) + \eta(x). \tag{30} $$

Note also that

$$ \sum_{i \in N_{x,h}} u_i^2 = \sum_{i \in N_{x,h}} e_0^\top (Q_{x,h}^\beta)^{-1} \Phi_{x,h}^\beta(X_i) \Phi_{x,h}^\beta(X_i)^\top (Q_{x,h}^\beta)^{-1} e_0 = e_0^\top (Q_{x,h}^\beta)^{-1} e_0. \tag{31} $$

In addition, since $P \in \mathcal{P}_{H\ddot{o}f}(\beta, C_S)$, for each $i \in N_{x,h}$, we have

$$ |\eta(X_i) - T_x^\beta[\eta](X_i)| \leq C_S \cdot \|X_i - x\|_\infty^\beta \leq C_S \cdot h^\beta, \tag{32} $$

27
and so by (32), the Cauchy–Schwarz inequality and (31), we have
\[
\left| \sum_{i \in N_{x,h}} u_i \cdot \{\eta(X_i) - T_x^\beta[\eta](X_i)\} \right| \leq C_S \cdot h^\beta \cdot \sum_{i \in N_{x,h}} |u_i| \\
\leq C_S \cdot h^\beta \cdot \sqrt{|N_{x,h}|} \cdot e_0^\tau (Q_{x,h}^\beta)^{-1} e_0.
\]
(33)
We conclude, by the definition of \(\tilde{\eta}(x)\), (30), (31), (33) and Hoeffding’s inequality, that
\[
\mathbb{P}\left( \tilde{\eta}(x) - \eta(x) \geq \tilde{\Delta}_{x,h}(\alpha) \right) = \mathbb{P}\left( \sum_{i \in N_{x,h}} u_i \cdot \{Y_i - \eta(X_i)\} \geq \sqrt{\frac{\log(1/\alpha)}{2}} \sum_{i \in N_{x,h}} u_i^2 \right) \leq \alpha.
\]
The other inequality follows similarly.

Lemma 18. Fix \((\beta, C_S) \in (0, \infty) \times [1, \infty)\) and let \(P \in \mathcal{P}_{\text{Hö}}(\beta, C_S)\). Suppose that \(\mathcal{D} = ((X_i, Y_i))_{i \in [n]} \sim P^{\otimes n}\) and let \(\mathcal{D}_X = (X_i)_{i \in [n]}\). Then for any closed hyper-cube \(B \subseteq \mathbb{R}^d\) with \(\text{diam}_\infty(B) \leq 1\) and \(\inf_{x' \in B} \eta(x') \leq \tau\), and any \(\alpha \in (0,1)\), we have
\[
\mathbb{P}(\tilde{p}_\beta^+(B) \leq \alpha \mid \mathcal{D}_X) \leq \alpha.
\]
Proof. Recall that \(x \in \mathbb{R}^d\) and \(r \in [0, 1/2]\) denote the centre and \(\ell_\infty\)-radius of \(B\), and that \(h = (2r)^{\lceil 1/2 \rceil} \in [0, 1]\). Again, it restricts our attention to the case where \(Q_{x,h}^\beta\) is invertible. Since \(\inf_{x' \in B} \eta(x') \leq \tau\) and \(P \in \mathcal{P}_{\text{Hö}}(\beta, C_S)\), we have \(\eta(x) \leq \tau + C_S \cdot r^\beta \cdot 1\), and hence the lemma follows from Lemma 17.

Proof of Proposition 7. This follows from Lemma 18 in the same way as Proposition 4 followed from Lemma 3.

We now turn to the proof of Proposition 13, which will rely on several lemmas. For \(a > 0\), let \(\mathcal{K}(a)\) denote the set of measurable sets \(K \subseteq B_1(0)\) with \(L_d(K) \geq a\).

Lemma 19. Given \(d \in \mathbb{N}, \beta \in (0, \infty)\) and \(a \in (0,1)\), we have
\[
c_{\min}(d, \beta, a) := 1 \wedge \inf_{K \in \mathcal{K}(a)} \left\{ \lambda_{\min}\left( \int_K \Phi_{0,1}^\beta(z) \Phi_{0,1}^\beta(z)^\top \, d\mu_d(z) \right) \right\} > 0.
\]
Proof. Suppose, for a contradiction, that \(c_{\min}(d, \beta, a) = 0\). Then we can find a sequence \(K(t)\) in \(\mathcal{K}(a)\), along with a sequence \((w(t))_{t \in \mathbb{N}}\) with \(w(t) \in \mathbb{R}^{V(\beta)}\) with \(\|w(t)\|_2 = 1\) and
\[
\lim_{t \to \infty} \int_{K(t)} \langle w(t), \Phi_{0,1}^\beta(z) \rangle^2 \, d\nu_d(z) = \lim_{t \to \infty} \left( \int_{K(t)} \Phi_{0,1}^\beta(z) \Phi_{0,1}^\beta(z)^\top \, d\mu_d(z) \right) w(t) = 0.
\]
(34)
By moving to a subsequence if necessary, we may assume that \(\lim_{t \to \infty} w(t) = w^*\) for some \(w^* \in \mathbb{R}^{V(\beta)}\) with \(\|w^*\|_2 = 1\). Now since \(z \mapsto \langle w^*, \Phi_{0,1}^\beta(z) \rangle\) is a non-zero polynomial, the zero-set \(Z_{w^*} := \{ z \in B_1(0) : \langle w^*, \Phi_{0,1}^\beta(z) \rangle = 0 \}\) satisfies \(\mu_d|Z_{w^*} = 0\) (e.g. Okamoto, 1973, Lemma 1). In addition, by the continuity of \(z \mapsto \langle w^*, \Phi_{0,1}^\beta(z) \rangle\), the set \(Z_{w^*}\) is closed. By countable additivity of the finite measure \(\mu_d|_{B_1(0)}\), there exists \(\varepsilon_a > 0\) such
that $\mathcal{L}_d(Z^{e}_w) \leq a/2$ where $Z^{e}_w := \bigcup_{z \in Z^{e}_w} B_r(z) = Z_w + B_{e_a}(z)$. By continuity again, 
\[
\delta_a := \inf_{z \in B_1(0) \setminus Z^{e}_w} \left| \langle w^*, \Phi_{0,1}^\beta(z) \rangle \right| > 0.
\]
Now choose $\ell_0 \in \mathbb{N}$ sufficiently large that
\[
\sup_{\ell \geq \ell_0} \| w^{(\ell)} - w^* \|_2 \leq \frac{\delta_a}{2\sqrt{|\mathcal{V}(\beta)|}},
\]
so that, by Cauchy–Schwarz,
\[
\left| \langle w^{(\ell)}, \Phi_{0,1}^\beta(z) \rangle \right| \geq \left| \langle w^*, \Phi_{0,1}^\beta(z) \rangle \right| - \left| \langle w^{(\ell)} - w^*, \Phi_{0,1}^\beta(z) \rangle \right| \geq \delta_a - \frac{\delta_a}{2\sqrt{|\mathcal{V}(\beta)|}} \cdot \| \Phi_{0,1}^\beta(z) \|_2 \geq \frac{\delta_a}{2}
\]
for all $\ell \geq \ell_0$ and $z \in B_1(0) \setminus Z^{e}_w$. Hence, for all $\ell \geq \ell_0$,
\[
\int_{K^{(\ell)}} \langle w^{(\ell)}, \Phi_{0,1}^\beta(z) \rangle^2 \mathcal{L}_d(z) \geq \int_{K^{(\ell)} \setminus Z^{e}_w} \langle w^{(\ell)}, \Phi_{0,1}^\beta(z) \rangle^2 \mathcal{L}_d(z) \geq \frac{a \cdot \delta_a^2}{8} > 0,
\]
which contradicts (34), and completes the proof of the lemma. 

**Lemma 20.** Suppose that $v \in (0, 1)$, $\xi \in (0, \infty)$, $\beta \in (0, \infty)$, $x \in \mathbb{R}^d$ and $r \in (0, 1/2]$ satisfy $B_r(x) \cap \mathcal{R}_v(\mu) \cap \mathcal{X}_\xi(f_\mu) \neq \emptyset$. Given any $h \in [2r, 1]$, we have $\mu(B_h(x)) \geq v \cdot \xi \cdot (h/2)^d$. In addition, if either $\beta \in (0, 1]$ or $3r \leq vh$, then
\[
\lambda_{\min} \left( \int_{B_h(x)} \Phi_{x,h}^\beta(z) \Phi_{x,h}^\beta(z)^\top d\mu(z) \right) \geq 2^{-(3d+1)} \cdot v \cdot c_{\min}^0 \cdot \mu(B_h(x)),
\]
where $c_{\min}^0 \equiv c_{\min}(d, \beta, 2^{-(d+1)} v) \in (0, 1]$ is taken from Lemma 19.

**Proof.** First choose $x_0 \in B_r(x) \cap \mathcal{R}_v(\mu) \cap \mathcal{X}_\xi(f_\mu)$ and note that $B_{h/2}(x_0) \subset B_{h-r}(x) \subset B_h(x)$. Hence, since $x_0 \in \mathcal{R}_v(\mu) \cap \mathcal{X}_\xi(f_\mu)$, we deduce
\[
\mu(B_h(x)) \geq \mu(B_{h-r}(x_0)) \geq \mu(B_{h/2}(x_0)) \geq v \cdot \left( \frac{h}{2} \right)^d \cdot \xi.
\]
For $\beta \in (0, 1]$, we have $\Phi_{x,h}^\beta(\cdot) \equiv 1$, so (35) is immediate. Suppose now that $3r \leq vh$, so that $B_{(1+v)(h-r)}(x_0) \supseteq B_{h+r}(x_0) \subseteq B_h(x)$. Thus, since $x_0 \in \mathcal{R}_v(\mu)$, we infer that with $M_{x,h} := \sup_{x' \in B_h(x)} f_\mu(x')$,
\[
\mu(B_h(x)) \geq \mu(B_{h-r}(x_0)) \geq v(h-r)^d \cdot \sup_{x' \in B_{(1+v)(h-r)}(x_0)} f_\mu(x') \geq v \cdot \left( \frac{h}{2} \right)^d \cdot M_{x,h}.
\]
Moreover, if we take $J_{x,h} := \{ x' \in B_h(x) : f_\mu(x') \geq 2^{-(2d+1)} \cdot v \cdot M_{x,h} \}$, then
\[
\mu(B_h(x)) \leq \mathcal{L}_d(J_{x,h}) \cdot M_{x,h} + \mathcal{L}_d(B_h(x) \setminus J_{x,h}) \cdot 2^{-(2d+1)} \cdot v \cdot M_{x,h}
\]
\[
\leq \mathcal{L}_d(J_{x,h}) \cdot M_{x,h} + \frac{v}{2} \cdot \left( \frac{h}{2} \right)^d \cdot M_{x,h},
\]

29
so by (36) we have \( \mathcal{L}_d(J_{x,h}) \geq 2^{-(d+1)} \cdot v \cdot h^d \). Taking \( K_{x,h} := h^{-1} \cdot (J_{x,h} - x) \subseteq \bar{B}_1(0) \), we have \( \mathcal{L}_d(K_{x,h}) \geq 2^{-(d+1)} \cdot v \). Given any \( w \in \mathbb{R}^{\mathcal{V}(\beta)} \) with \( \|w\|_2 = 1 \), it follows from Lemma 19 that

\[
\int_{B_h(x)} \langle w, \Phi_{x,h}^\beta(z) \rangle^2 d\mu(z) \geq 2^{-(2d+1)} \cdot v \cdot M_{x,h} \cdot \int_{J_{x,h}} \langle w, \Phi_{x,h}^\beta(z) \rangle^2 d\mathcal{L}_d(z) 
\geq 2^{-(2d+1)} \cdot v \cdot M_{x,h} \cdot h^d \cdot \int_{K_{x,h}} \langle w, \Phi_{0,1}^\beta(z') \rangle^2 d\mathcal{L}_d(z') 
\geq 2^{-(3d+1)} \cdot v \cdot c_{\min}^0 \cdot \mu(\bar{B}_h(x)).
\]

The result follows.

**Lemma 21.** Suppose that \( v \in (0, 1) \), \( \xi \in (0, \infty) \), \( \beta \in (0, \infty) \), \( x \in \mathbb{R}^d \), \( r \in (0, 1/2] \) and \( h \in [2r, 1] \) satisfy \( B_r(x) \cap \mathcal{R}_v(\mu) \cap \mathcal{X}(f_\mu) \neq \emptyset \), and choose \( \delta \in (0, 1) \). Suppose also that

\[
h \geq \left\{ \frac{2^{3(d+1)} \cdot |\mathcal{V}(\beta)|}{c_{\min}^0 \cdot v^2 \cdot \xi \cdot n} \cdot \log\left( \frac{2|\mathcal{V}(\beta)|}{\delta} \right) \right\}^{1/d}, \tag{37}
\]

and that either \( \beta \in (0, 1] \) or \( 3r \leq vh \). Then

\[
\mathbb{P}\left( \{ |\mathcal{N}_{x,h}| \leq 2n \cdot \mu(\bar{B}_h(x)) \} \cap \{ \lambda_{\min}(Q_{x,h}^\beta) \geq 2^{-(3d+2)} \cdot n \cdot c_{\min}^0 \cdot v \cdot \mu(\bar{B}_h(x)) \} \right) \geq 1 - \delta.
\]

**Proof.** By Lemma 20 and (37), we have that \( \mu(\bar{B}_h(x)) \geq v \cdot \xi \cdot (h/2)^d \geq (8/3) \log(2/\delta)/n \). Hence, by the multiplicative Chernoff bound (Lemma 39),

\[
\mathbb{P}\{ |\mathcal{N}_{x,h}| > 2n \cdot \mu(\bar{B}_h(x)) \} \leq \frac{\delta}{2}. \tag{38}
\]

In addition, if either \( \beta \in (0, 1] \) or \( 3r \leq vh \), then by Lemma 20 again,

\[
\lambda_{\min}\left( \int_{B_h(x)} \Phi_{x,h}^\beta(z)\Phi_{x,h}^\beta(z)^\top d\mu(z) \right) \geq 2^{-(3d+1)} \cdot v \cdot c_{\min}^0 \cdot \mu(\bar{B}_h(x)) 
\geq 2^{-(4d+1)} \cdot v^2 \cdot c_{\min}^0 \cdot \xi \cdot h^d 
\geq \frac{8|\mathcal{V}(\beta)|}{n} \cdot \log\left( \frac{2|\mathcal{V}(\beta)|}{\delta} \right).
\]

Note also that \( \lambda_{\max}(\Phi_{x,h}(X_i)\Phi_{x,h}(X_i)^\top \cdot 1_{\{X_i \in \bar{B}_h(x)\}}) \leq |\mathcal{V}(\beta)| \). Hence, by a matrix multiplicative Chernoff bound (Lemma 40) applied with \( m = n \), \( Z_i = \Phi_{x,h}(X_i)\Phi_{x,h}(X_i)^\top \cdot 1_{\{X_i \in \bar{B}_h(x)\}} \) and \( q = |\mathcal{V}(\beta)| \), we have

\[
\mathbb{P}\left\{ \lambda_{\min}(Q_{x,h}^\beta) < 2^{-(3d+2)} \cdot n \cdot c_{\min}^0 \cdot v \cdot \mu(\bar{B}_h(x)) \right\} 
\leq \mathbb{P}\left\{ \lambda_{\min}(Q_{x,h}^\beta) < \frac{n}{2} \cdot \lambda_{\min}\left( \int_{B_h(x)} \Phi_{x,h}^\beta(z)\Phi_{x,h}^\beta(z)^\top d\mu(z) \right) \right\} \leq \frac{\delta}{2}. \tag{39}
\]

The result now follows by combining (38) and (39) with a union bound. \( \square \)
Lemma 22. Suppose that $\alpha \in (0, 1)$, $(\beta, C_S) \in (0, \infty) \times [1, \infty)$, $(\kappa, \gamma, v, C_{\text{App}}) \in (0, \infty)^2 \times (0, 1) \times [1, \infty)$, take $P \in \mathcal{P}_{\text{HGl}}(\beta, C_S) \cap \mathcal{P}^{+}_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, v, C_{\text{App}})$ and let $C_{pv} := 2^{2d+5} \cdot C_S \cdot \left( \frac{1}{\sqrt{\delta}} \right)^{-1}$. Suppose further that $\xi, \Delta \in (0, \infty)$, $x \in \mathbb{R}^d$ and $r \in (0, 1/2]$ satisfy $\bar{B}_r(x) \cap \mathcal{R}_v(\mu) \cap \mathcal{X}_\xi(f_\mu) \cap \mathcal{X}_{\tau+\Delta}(\eta) \neq \emptyset$, where $\mu$ is the marginal distribution of $P$ on $\mathbb{R}^d$, and $\eta : \mathbb{R}^d \rightarrow [0, 1]$ is the regression function. Given any $\delta \in (0, 1)$ with

$$r \geq \frac{1}{2} \cdot \frac{C_{pv}^2 \cdot |\mathcal{Y}(\beta)|}{\xi \cdot n} \cdot \log \left( \frac{4|\mathcal{Y}(\beta)|}{\delta} \right)$$

and $\Delta \geq C_{pv} \cdot \left( r^{\beta \lambda_1} + \sqrt{\frac{\log(2/(\alpha \wedge \delta))}{\xi \cdot n \cdot r^{d(\beta \lambda_1)/\beta}}} \right)$,

and either $\beta \in (0, 1]$ or $r \leq \left(2(v/3)^\beta \right)^{1/\nu}$, we have $\mathbb{P}\{ \hat{p}^+_n(B_r(x)) \leq \alpha \} \geq 1 - \delta$.

Proof. First recall that in the construction of our $p$-values $\hat{p}^+_n(\cdot)$ in (14) we take $h = (2r)^{1\wedge \frac{1}{\beta}}$.

To prove the lemma we define events

$$\mathcal{E}_\delta^\eta := \left\{ \hat{\eta}(x) > \eta(x) - \sqrt{\frac{e_0^\top (Q_x^\beta)^{-1} e_0}{\delta}} \right\},$$

and

$$\mathcal{E}_\delta^\mu := \left\{ \lambda_{\min}(Q_x^\beta) \geq 2^{-(3d+2)} \cdot e_0^0 \cdot v^2 \cdot \max \left\{ \xi \cdot n \cdot \left( \frac{h}{2} \right)^d, \frac{|\mathcal{N}_{x,h}|}{2v} \right\} \right\}.$$

Note that since $P \in \mathcal{P}_{\text{HGl}}(\beta, C_S)$ and $\bar{B}_r(x) \cap \mathcal{X}_{\tau+\Delta}(\eta) \neq \emptyset$, we have $\eta(x) \geq \tau + \Delta - C_S \cdot r^{\beta \lambda_1}$.

Hence, on the event $\mathcal{E}_\delta^\eta \cap \mathcal{E}_\delta^\mu$ we have

$$\hat{\eta}(x) - \tau - C_S \left( 1 + 2\sqrt{\frac{e_0^\top (Q_x^\beta)^{-1} e_0}{\delta} \cdot |\mathcal{N}_{x,h}|} \right) r^{\beta \lambda_1} \geq \eta(x) - \tau - C_S \left( 1 + 4\sqrt{\frac{e_0^\top (Q_x^\beta)^{-1} e_0}{\delta} \cdot |\mathcal{N}_{x,h}|} \right) r^{\beta \lambda_1} - \frac{1}{2} \cdot e_0^\top (Q_x^\beta)^{-1} e_0 \cdot \log(2/\delta)$$

and

$$\geq \frac{1}{2} \cdot e_0^\top (Q_x^\beta)^{-1} e_0 \cdot \log(2/\alpha) \geq \frac{1}{2} \cdot e_0^\top (Q_x^\beta)^{-1} e_0 \cdot \log(2/\alpha).$$

Hence, on the event $\mathcal{E}_\delta^\eta \cap \mathcal{E}_\delta^\mu$ we have $\hat{p}^+_n(B_r(x)) \leq \alpha$. Now by Lemma 17 we have $\mathbb{P}(\mathcal{E}_\delta^\mu^c \cap \mathcal{E}_\delta^\eta^c) \leq \delta/2$. Moreover, by Lemma 20 we have $\mu(\bar{B}_r(x)) \geq v \cdot \xi \cdot (h/2)^d$. Hence, by Lemma 21 we have $\mathbb{P}(\mathcal{E}_\delta^\mu^c) \leq \delta/2$. Thus $\mathbb{P}(\mathcal{E}_\delta^\eta^c \cup (\mathcal{E}_\delta^\mu^c) \leq \delta$, and the conclusion follows.

Given any $v \in (0, 1)$, $\xi, \Delta \in (0, \infty)$, $r \in (0, 1/2]$, we let

$$\mathcal{H}_v(\xi, \Delta, r) := \left\{ B \in \mathcal{H}^+ : \text{diam}_\infty(B) = 2r \text{ and } B \cap \mathcal{R}_v(\mu) \cap \mathcal{X}_\xi(f_\mu) \cap \mathcal{X}_{\tau+\Delta}(\eta) \neq \emptyset \right\}.$$

Lemma 23. We have $|\mathcal{H}_v(\xi, \Delta, r)| \leq (2r)^d \cdot (v \cdot \xi)^{-1}$ for every $v \in (0, 1)$, $\xi, \Delta \in (0, \infty)$ and $r \in (0, 1/2]$.
Proof. Given \( B = 2r \prod_{j \in [d]} [a_j, a_j + 1] \in \mathcal{H}_v'(\xi, \Delta, r) \), for some \((a_j)_{j \in [d]} \in \mathbb{Z}^d\), we write \( \phi(B) := (a_j \mod 2)_{j \in [d]} \in \{0, 1\}^d \) and \( \psi(B) := r \prod_{j \in [d]} [2a_j - 1, 2a_j + 3] \). Note that if \( \phi(B_0) = \phi(B_1) \) for distinct \( B_0, B_1 \in \mathcal{H}_v'(\xi, \Delta, r) \) then \( \mu(\psi(B_0) \cap \psi(B_1)) = 0 \), since \( \mu \) is absolutely continuous with respect to Lebesgue measure on \( \mathbb{R}^d \). Moreover, by Lemma 20 we have \( \mu(\psi(B)) \geq v \cdot \xi \cdot r^d \), so

\[
|\mathcal{H}_v'(\xi, \Delta, r)| \cdot v \cdot \xi \cdot r^d \leq \sum_{B \in \mathcal{H}_v'(\xi, \Delta, r)} \mu(\psi(B)) = \sum_{z \in \{0, 1\}^d} \sum_{B \in \mathcal{H}_v'(\xi, \Delta, r) \cap \phi^{-1}\{z\}} \mu(\psi(B)) \leq 2^d,
\]

as required. \( \square \)

Proof of Proposition 8. Let

\[
\rho := \kappa(2\beta + d) + \beta \gamma, \quad \theta := \frac{1}{n} \log_* \left( \frac{8n^{\delta \beta \gamma} |\mathcal{V}(\beta)| \log_2 n}{\alpha \wedge \delta} \right),
\]

\[
\xi := \theta^{\beta \gamma / \rho}, \quad r := 2^{-\left[\frac{\delta \beta \gamma}{n \log_2 (1/\theta)}\right]},
\]

and define

\[
A_0 := \left\{ \begin{array}{ll}
2v \lor C_{pv} |\mathcal{V}(\beta)|^{1/2} \lor 2^{\frac{\beta - 2}{\rho - 1}} (3v) \theta^{d \beta / \rho - 1} & \text{if } \beta > 1 \\
2^{\beta} \lor C_{pv} |\mathcal{V}(\beta)|^{1/2} & \text{if } \beta \leq 1.
\end{array} \right.
\]

Then, for \( \theta \leq A_0^{-\frac{\beta}{\rho}} \) we have

\[
\left( \frac{C_{pv}^2 \cdot |\mathcal{V}(\beta)|}{\xi} \cdot \theta \right)^{\frac{\beta}{\rho - 1}} \leq r \leq \frac{1}{2},
\]

and \( r \leq \{2(v/3)^{\beta}\}^{\frac{1}{\rho - 1}} \) if \( \beta > 1 \). Now let

\[
\Delta := C_{pv} \cdot \left( r^{\beta \wedge 1} + \sqrt{\frac{\theta}{\xi \cdot r^{d(\beta \wedge 1) / \beta}}} \right),
\]

so that \( \Delta \leq 3 \cdot C_{pv} \cdot \theta^{\frac{\beta}{\rho}} \) when \( \theta \leq A_0^{-\frac{\beta}{\rho}} \). By Lemma 23, we have \( |\mathcal{H}_v'(\xi, \Delta, r)| \leq (2/r)^d \cdot (v \cdot \xi)^{-1} \leq \theta^{-\frac{\beta}{\rho - 1}} \leq n^{\delta \beta / \rho} \) when \( \theta \leq A_0^{-\frac{\beta}{\rho}} \). Hence we may apply a union bound and Lemma 22 with \( \delta / (2n^{\delta \beta / \rho}) \) in place of \( \delta \) and \( \alpha / (n \log_2 n) \) in place of \( \alpha \) to deduce that whenever \( \theta \leq A_0^{-\frac{\beta}{\rho}} \), we have

\[
\mathbb{P}\left( \bigcup_{B \in \mathcal{H}_v'(\xi, \Delta, r)} \left\{ \bar{\hat{p}}_n^+(B) > \frac{\alpha}{|\mathcal{H}^+(D_X)|} \right\} \right) \leq \sum_{B \in \mathcal{H}_v'(\xi, \Delta, r)} \mathbb{P}\left( \bar{\hat{p}}_n^+(B) > \frac{\alpha}{n \log_2 n} \right) \leq \frac{\delta}{2}.
\]

Hence, whenever \( \theta \leq A_0^{-\frac{\beta}{\rho}} \), we have

\[
\mathcal{R}_v(\mu) \cap \mathcal{X}_v(f_\mu) \cap \mathcal{X}_{v+\Delta}(\eta) \subseteq \bigcup_{B \in \mathcal{H}_v'(\xi, \Delta, r)} B \subseteq \bigcup_{\ell \in [\nu]} B(\ell),
\]

32
with probability at least $1 - \delta/2$. Thus, with probability at least $1 - \delta/2$, when $\theta \leq A_0^{\frac{e}{\pi}}$,

$$M_\tau - \sup\left\{ \mu(A) : A \in \mathcal{A} \cap \text{Pow}\left( \bigcup_{\ell \in [L]} B(\ell) \right) \right\}$$

$$\leq M_\tau - \sup\left\{ \mu(A) : A \in \mathcal{A} \cap \text{Pow}(\mathcal{R}_\nu(\mu) \cap \mathcal{X}_\nu(f_\mu) \cap \mathcal{X}_{\tau+\Delta}(\eta)) \right\}$$

$$\leq C_{\text{App}} \cdot \left[ 1 + \left\{ (3 \cdot C_{pw}) \vee A_0 \right\}^\gamma \right] \cdot \theta^\frac{\delta\alpha_\gamma}{\tau}.$$  \hspace{1cm} (40)

Moreover, the same final bound on the left-hand side of (40) holds trivially when $\theta > A_0^{\frac{e}{\pi}}$ because in that case the right-hand side is at least 1. Finally, since $\hat{A}^+_{\text{OSS}}$ is chosen from $\mathcal{A} \cap \text{Pow}(\bigcup_{\ell \in [L]} B(\ell))$ with maximal empirical measure, it follows from Lemma 36 that with probability at least $1 - \delta$,

$$M_\tau - \mu(\hat{A}^+_{\text{OSS}}) \leq C_{\text{App}} \cdot \left[ 1 + \left\{ (3 \cdot C_{pw}) \vee A_0 \right\}^\gamma \right] \cdot \theta^\frac{\delta\alpha_\gamma}{\tau} + 2C_{\text{VC}} \sqrt{\frac{\dim_{\text{VC}}(\mathcal{A})}{n}} + \sqrt{\frac{2\log(2/\delta)}{n}}.$$

The second part of Proposition 8 follows integrating the tail bound and applying Proposition 7, as at the end of the proof of Theorem 5. \hfill \Box

### 6.5 Proofs of lower bounds in Theorems 2 and 6

Recall the construction of the probability distributions $\{P_{L,r,w,s,\theta}^\ell : \ell \in [L]\}$ on $\mathbb{R}^d \times \{0, 1\}$ from Section 4, with corresponding regression functions $\{\eta_{L,r,w,s,\theta}^\ell : \ell \in [L]\}$ and common marginal distribution $\mu_{L,r,w}$ on $\mathbb{R}^d$. Recall also the definition of $\mathcal{R}_\nu(\cdot)$ from (10). Our initial goal is to prove that $\{P_{L,r,w,s,\theta}^\ell : \ell \in [L]\}$ is a subset of $\mathcal{P}_{\text{Hö}}(\beta, C_{\text{S}})$ (see Lemma 29) and $\mathcal{P}_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, C_{\text{App}}) \cap \mathcal{P}_{\text{App}}(A, \tau, \kappa, \gamma, \nu, C_{\text{App}})$ (see Lemma 31) for suitable $L$, $r$, $w$, $s$ and $\theta$.

The first of these lemmas will rely on several auxiliary results.

Given two multi-indices $\nu = (\nu_1, \ldots, \nu_d)^\top$, $\nu' = (\nu_1', \ldots, \nu_d')^\top \in \mathbb{N}_0^d$, we write $\nu \prec \nu'$ if either $\|\nu\|_1 < \|\nu'\|_1$ or both $\|\nu\|_1 = \|\nu'\|_1$ and there exists $j \in \{0, 1, \ldots, d-1\}$ such that $\nu_j = \nu_j'$ and $\nu_{j+1} < \nu_{j+1}'$. Now, given $m \in \mathbb{N}$ and $j \in [m]$, we write

$$Q_j(\nu, m) := \left\{ (k_1, \ldots, k_j, \ell_1, \ldots, \ell_j) \in \mathbb{N}_0^j \times (\mathbb{N}_0^j)^j : 0 < \ell_1 < \ldots < \ell_j, \sum_{q=1}^j k_q = m, \sum_{q=1}^j k_q\ell_q = \nu \right\}.$$

In addition, for multi-indices $\nu = (\nu_1, \ldots, \nu_d)^\top \in \mathbb{N}_0^d$, we let $\nu! := \prod_{m=1}^{\|\nu\|_1} \nu_j!$. The following lemma is a version of the Faà di Bruno formula.

**Lemma 24** (Corollary 2.10 of Constantine and Savits (1996)). Let $x \in \mathbb{R}^d$ and $\nu = (\nu_1, \ldots, \nu_d)^\top \in \mathbb{N}_0^d$. Suppose that all partial derivative of order $\|\nu\|_1$ of $f : \mathbb{R}^d \to \mathbb{R}$ exist and are continuous in a neighbourhood of $x$, and that $g : \mathbb{R} \to \mathbb{R}$ is $\|\nu\|_1$-times continuously differentiable in a neighbourhood of $f(x)$. Then

$$\partial_\nu^\nu(g \circ f) = \nu! \cdot \sum_{m=1}^{\|\nu\|_1} g^{(m)}(f(x)) \prod_{j=1}^{\|\nu\|_1} \sum_{(k_1, \ldots, k_j, \ell_1, \ldots, \ell_j) \in Q_j(\nu, m)} \prod_{q=1}^j \frac{\partial_{k_q}^j(f)}{k_q!} \cdot \ell_q! \cdot (\ell_q!)^{k_q}.$$
Lemma 25. Given $\nu = (\nu_1, \ldots, \nu_d)^T \in \mathbb{N}_0^d$, we have $\sup_{\|x\|_2 \geq 1} |\partial^\nu_x(\| \cdot \|_2)| < \infty$.

Proof. For $t \in [d]$, write $e_t = (0, \ldots, 0, 1, 0, \ldots, 0)^T \in \mathbb{R}^d$ for the $t^{th}$ standard basis vector in $\mathbb{R}^d$. By Lemma 24 with $f(x) = \|x\|_2$ and $g(z) = \sqrt{z}$, we have for $x = (x_1, \ldots, x_d)^T \in \mathbb{R}^d$ that

$$\partial^\nu_x(\| \cdot \|_2) = \nu! \sum_{m=1}^{\|\nu\|_1} \frac{(-1)^{m+1}(2m-3)!!}{2^m\|x\|_2^{2m-1}} \sum_{j=1}^{\|\nu\|_1} \sum_{(k_1, \ldots, k_j, \ldots, j_j) \in \mathcal{Q}_j(\nu,m)} \prod_{q=1}^j 2^{k_q} \{ \sum_{t=1}^d (x_t \mathbb{1}(\ell_t = e_t) + (\ell_t = 2e_t)) \}^{k_q} \cdot (\ell_q)!^{k_q}.$$

It follows that for all $x \in \mathbb{R}^d$ with $\|x\|_2 \geq 1$ we have

$$|\partial^\nu_x(\| \cdot \|_2)| \leq \nu! \sum_{m=1}^{\|\nu\|_1} \frac{(2m-3)!!}{\|x\|_2^{2m-1}} \sum_{j=1}^{\|\nu\|_1} \sum_{(k_1, \ldots, k_j, \ldots, j_j) \in \mathcal{Q}_j(\nu,m)} \prod_{q=1}^j \frac{\|x\|_2^{k_q}}{(\ell_q)!^{k_q}} \leq \nu! \sum_{m=1}^{\|\nu\|_1} \frac{(2m-3)!!}{\|x\|_2^{2m-1}} \sum_{j=1}^{\|\nu\|_1} \sum_{(k_1, \ldots, k_j, \ldots, j_j) \in \mathcal{Q}_j(\nu,m)} \prod_{q=1}^j \frac{1}{(\ell_q)!^{k_q}} < \infty,$$

as required. \hfill \Box

Lemma 26. For each $m, d \in \mathbb{N}$, there exists $C_{m,d} > 0$, depending only on $m$ and $d$, such that for any infinitely differentiable function $g : [0, \infty) \to [0, \infty)$ with $g'(z) = 0$ for all $z \in [0, 1]$, and any $\nu = (\nu_1, \ldots, \nu_d)^T \in \mathbb{N}_0^d$ with $\|\nu\|_1 = m$, we have

$$|\partial^\nu_x(g \circ \| \cdot \|_2)| \leq C_{m,d} \cdot \max_{k \in [m]} \sup_{z \in [0, \infty)} |g^{(k)}(z)|$$

for all $x \in \mathbb{R}^d$.

Proof. The lemma follows from combining Lemmas 24 and 25, and by considering the cases $\|x\|_2 < 1$ and $\|x\|_2 \geq 1$ separately. \hfill \Box

Lemma 27. Let $L, d \in \mathbb{N}$, $r \in (0, \infty)$, $s \in (0, 1 \wedge (r/2)]$, $w \in (0, (2r)^{-d} \wedge 1)$ and $\theta \in (0, \epsilon_0/2]$. Then for $\ell \in [L]$, $\nu = (\nu_1, \ldots, \nu_d)^T \in \mathbb{N}_0^d$ with $\|\nu\|_1 = m$ and $x \in \mathbb{R}^d$, we have

$$|\partial^\nu_x(\eta^\ell_{L,r,w,s,\theta})| \leq 2A_m C_{m,d} \cdot \frac{\theta}{s^m}, \quad (41)$$

where $A_m$ is taken from (16) and $C_{m,d}$ is taken from Lemma 26. Hence, given any $\xi \in [0, 1]$ and $x, x' \in \mathbb{R}^d$, we have

$$|\partial^\nu_x(\eta^\ell_{L,r,w,s,\theta}) - \partial^\nu_{x'}(\eta^\ell_{L,r,w,s,\theta})| \leq 2A_m+1 (2C_{m,d} \lor dC_{m+1,d}) \cdot \frac{\theta}{s^{m+1}} \cdot \|x - x'\|_\infty. \quad (42)$$

Proof. To prove (41), we construct an open cover of $\mathbb{R}^d$ by $\{U_1, \ldots, U_{L+1}\}$ where $U_{\ell'} := B_{\nu_{\ell'}^d}(z_{\ell'})$ for $\ell' \in [L]$ and $U_{L+1} := \mathbb{R}^d \setminus \bigcup_{\ell' \in [L]} B_{2\nu_{\ell'}^d/2r}(z_{\ell'})$. First suppose that $\ell' \in [L] \setminus \{\ell\}$
and consider the function $g_0 : [0, \infty) \to [0, \infty)$ defined by

$$g_0(t) := \begin{cases} 
\tau - \theta & \text{if } t \leq 1 \\
\tau + \theta - 2\theta \cdot h(t-1) & \text{if } 1 < t \leq 2 \\
\tau + \theta & \text{if } 2 < t < \frac{d^{1/2}r}{\theta} \\
\tau - \theta + 2\theta \cdot h \left( \frac{s t}{d^{1/2}r} - 1 \right) & \text{if } \frac{d^{1/2}r}{\theta} < t < \frac{2d^{1/2}r}{\theta} \\
\tau - \theta & \text{otherwise.}
\end{cases}$$

By Lemma 26, together with $s \leq r/2 \leq d^{1/2}r$, we have

$$\sup_{x \in \mathbb{R}^d} \left| \partial^\nu_x (g_0 \circ \| \cdot \|_2) \right| \leq C_{m,d} \cdot \max_{k \in [m]} \sup_{z \in [0,\infty)} \left| g_0^{(k)}(z) \right| \leq 2A_m C_{m,d} \theta.$$

Moreover, for all $x \in U_\ell$ we have $\eta_{L,r,w,s,\theta}^\ell(x) = g_0(\|s^{-1} \cdot (x - z_\ell)\|_2)$. Hence, for all $x \in U_\ell$ we have $|\partial^\nu_x(\eta_{L,r,w,s,\theta}^\ell)| \leq 2A_m C_{m,d} \theta s^{-m}$. Since $\|\nu\|_1 = m$. Next, consider the open set $U_\ell$ and define a function $g_1 : [0, \infty) \to [0, \infty)$ by

$$g_1(t) := \begin{cases} 
\tau + \theta & \text{if } t \leq 1 \\
\tau - \theta + 2\theta \cdot h(t-1) & \text{if } 1 < t < 2 \\
\tau - \theta & \text{otherwise.}
\end{cases}$$

By applying Lemma 26 again, we have $|\partial^\nu_x(g_1 \circ \| \cdot \|_2)| \leq 2A_m C_{m,d} \theta$ for all $x \in \mathbb{R}^d$. Moreover, for $x \in U_\ell$ we have $\eta_{L,r,w,s,\theta}^\ell(x) = g_1(\| (d^{1/2}r)^{-1} \cdot (x - z_\ell)\|_2)$. Hence, for all $x \in U_\ell$, we have $|\partial^\nu_x(\eta_{L,r,w,s,\theta}^\ell)| \leq 2A_m C_{m,d} \theta (d^{1/2}r)^{-m} \leq 2A_m C_{m,d} \theta s^{-m}$. Finally we note that $\eta_{L,r,w,s,\theta}^\ell|_{U_{\ell+1}} \equiv \tau - \theta$, so $\sup_{x \in U_{\ell+1}} |\partial^\nu_x(\eta_{L,r,w,s,\theta}^\ell)| = 0 \leq 2A_m C_{m,d} \theta s^{-m}$. The claim (41) follows.

To prove (42), we first consider the case where $\|x - x'\|_\infty \leq s$, in which case, we may apply the mean value theorem combined with (41) and Hölder’s inequality to obtain

$$|\partial^\nu_x(\eta_{L,r,w,s,\theta}) - \partial^\nu_x(\eta_{L,r,w,s,\theta})| \leq dA_{m+1} C_{m+1,d} \cdot \frac{\theta}{\| x - x' \|_\infty^{m+1}} \cdot \| x - x' \|_\infty^\xi.$$

Moreover, when $\|x - x'\|_\infty > s$, (42) follows immediately from (41) and the triangle inequality.

\[
\square
\]

**Lemma 28.** Take $\beta > 0$, $C_f > 0$ and let $f : \mathbb{R}^d \to \mathbb{R}$ be a $[\beta]$-times differentiable function such that for all $\nu = (\nu_1, \ldots, \nu_d) \in \mathbb{N}^d_0$ with $\|\nu\|_1 = [\beta] - 1 =: m$, and $x, x' \in \mathbb{R}^d$, we have

$$|\partial^\nu_x(f) - \partial^\nu_x(f)| \leq C_f \cdot \| x' - x \|^\beta_{\infty}.$$ 

Then for all $x, x' \in \mathbb{R}^d$ we have

$$|f(x') - T_x^\beta[f](x')| \leq C_f \cdot \left( \frac{m + d - 1}{d - 1} \right) \cdot \| x' - x \|^\beta_{\infty}.$$ 

35
Proof. By Taylor’s theorem, there exists $t \in (0, 1)$ such that
\[
 f(x') = \sum_{\nu \in \mathbb{N}_0^d: \|\nu\|_1 < m} \frac{(x' - x)^\nu}{\nu!} \cdot \partial_x^\nu(f) + \sum_{\nu \in \mathbb{N}_0^d: \|\nu\|_1 = m} \frac{(x' - x)^\nu}{\nu!} \cdot \partial_{x+t(x' - x)}^\nu(f).
\]

Hence,
\[
 |f(x') - T_x^\beta[f](x')| = \left| \sum_{\nu \in \mathbb{N}_0^d: \|\nu\|_1 = m} \frac{(x' - x)^\nu}{\nu!} \cdot (\partial_{x+t(x' - x)}^\nu(f) - \partial_x^\nu(f)) \right|
\leq C_f \cdot \left( \frac{m + d - 1}{d - 1} \right) \cdot \|x' - x\|_\infty^\beta,
\]
as required. 

\[\Box\]

Lemma 29. Let $\beta > 0$, $C_S > 1$, $L, d \in \mathbb{N}$, $r \in (0, \infty)$, $s \in (0, 1 \wedge (r/2)]$, $w \in (0, (2r)^{-d} \wedge 1)$ and $\theta \in (0, \epsilon_0/2)$. There exists $c_{\beta, d} > 0$, depending only on $\beta$ and $d$, such that whenever $\theta \leq c_{\beta, d} \cdot C_S \cdot s^3$, we have that for each $\ell \in [L]$, the function $\eta^\ell_{L,r,w,s,\theta} = (\beta, C_S)$-Hölder on $\mathbb{R}^d$; i.e. $P_{L,r,w,s,\theta} \in \mathcal{P}_{\mathcal{H}}(\beta, C_S)$.

Proof. By taking
\[
c_{\beta, d} := \min_{q \in \mathbb{N}_0^d: \|q\| \leq \|\beta\| - 1} \left\{ 2A_{q+1}(2C_{q,d} \vee dC_{q+1,d}) \cdot \left( \frac{q + d - 1}{d - 1} \right) \right\}^{-1},
\]
the result follows from Lemmas 27 and 28. 

\[\Box\]

Lemma 31 also requires one auxiliary lemma.

Lemma 30. Given $L, d \in \mathbb{N}$, $r > 0$ and $w \in (0, (2r)^{-d} \wedge 1)$, we have $\omega_{\mu_{L,r,w}}(x) \geq \frac{w}{L \cdot (4d/2)^d} \cdot \tilde{r}^d$ for all $x \in \bigcup_{\ell \in [L]} K^\ell_{\tilde{r}}$. Moreover, $\bigcup_{\ell \in [L]} K^\ell_{\tilde{r}} \subseteq \mathcal{R}_w(\mu_{L,r,w})$ for every $w \leq (4d/2)^{-d}$.

Proof. Let $\ell \in [L]$, let $x \in K^\ell_{\tilde{r}} = \tilde{B}_r(z_\ell)$ and let $\tilde{r} \in (0, 1)$. If $\tilde{r} \in (0, 2r)$, then $\tilde{B}_r(x) \cap K^\ell_{\tilde{r}}$ contains a hyper-cube of radius $\tilde{r}/2$, so $\mu_{L,r,w}(\tilde{B}_r(x)) \geq w \cdot L^{-1} \cdot \tilde{r}^d$. Consequently, when $\tilde{r} \in (0, 8d/2^d]$, we have
\[
 \mu_{L,r,w}(\tilde{B}_r(x)) \geq \mu_{L,r,w}(\tilde{B}_{\tilde{r}/(4d/2)}(x)) \geq \frac{w}{L \cdot (4d/2)^d} \cdot \tilde{r}^d.
\]

Note also that since $x \in K^\ell_{\tilde{r}} \subseteq \tilde{B}_{2d/\tilde{r}}(z_\ell)$ there exists $\sigma_x \in \{-1, 1\}^d$ and $\tilde{x} = z_\ell + \sigma_x \cdot 2d/\tilde{r} \in \mathbb{R}^d$ with $\|\tilde{x} - x\|_\infty \leq 2d/\tilde{r}$. Hence, if $\tilde{r} \in (4d/\tilde{r}, r_{\tilde{r}}(w))$, then $\tilde{B}_{\tilde{r}/4}(z_\ell + \sigma_x \cdot (2d/\tilde{r} + \tilde{r}/4)) \subseteq \tilde{B}_r(x) \cap K^\ell_{\tilde{r}/4}(\tilde{r}/4)$. Thus, we have $\mu_{L,r,w}(\tilde{B}_{\tilde{r}}(x)) \geq \mu_{L,r,w}(\tilde{B}_r(\tilde{r}/4)) \geq \mu_{L,r,w}(\tilde{B}_{\tilde{r}/4}) \geq (w/L) \cdot (\tilde{r}/4)^d$ for $\tilde{r} \in (4d/\tilde{r}, r_{\tilde{r}}(w))$, and consequently, $\mu_{L,r,w}(\tilde{B}_r(x)) \geq (w/L) \cdot (\tilde{r}/4)^d$ for $\tilde{r} \in (8d/2^d, 2r_{\tilde{r}}(w))$. Finally, if $\tilde{r} \in (2r_{\tilde{r}}(w), 1)$, then $K^\ell_{\tilde{r}/2} \subseteq \tilde{B}_{2r_{\tilde{r}}(w)}(z_\ell) \subseteq \tilde{B}_r(x)$ so $\mu_{L,r,w}(\tilde{B}_r(x)) \geq 1/L > (w/L) \cdot \tilde{r}^d$. The first conclusion of the lemma therefore follows. The second part then follows from the fact that the Lebesgue density of $\mu_{L,r,w}$ is at most $w/L$ on $\mathbb{R}^d$. 

\[\Box\]

36
Lemma 31. Let $\beta > 0$, $C_S > 1$, $L, d \in \mathbb{N}$, $r \in (0, \infty)$, $s \in (0, 1 \wedge (r/2)]$, $w \in (0, (2r)^{-d} \wedge 1)$ and $\theta \in (0, \epsilon_0/2]$, $\ell \in [L]$, $v \leq (4d^{1/2})^{-d}$ and let $\eta = \eta^\ell_{L,r,w,s,\theta}$, $\mu = \mu_{L,r,w}$ and $P = P^\ell_{L,r,w,s,\theta}$. Suppose also that $A_{\text{rect}} \subseteq A \subseteq A_{\text{conv}}$. Given any $A \in \mathcal{A} \cap \text{Pow}(\mathcal{X}_r(\eta))$ and $\ell' \in [L]$ with $A \cap K^\ell_r(\eta) \neq \emptyset$ and $z_{\ell'} \notin A$. For some $\ell' \in [L]$, we have $\mu(A) \leq (w/L) \cdot (2r)^d/2$. In particular, $\mu(A) \leq (w/L) \cdot (2r)^d/2$ whenever $A \cap K^\ell_r(\eta) \neq \emptyset$ for some $A \in \mathcal{A} \cap \text{Pow}(\mathcal{X}_r(\eta))$ and $\ell' \in [L] \setminus \{\ell\}$. Moreover, $M_r(P, A) = \mu(K^\ell_r(\eta)) = (w/L) \cdot (2r)^d$. Finally, if $(w/L) \cdot (2r)^d \leq C_{\text{App}} \cdot \min\{(w/\{4d^{1/2}\cdot L\})^\kappa, \theta^\gamma\}$, then $P \in \mathcal{P}_\text{App}(A, \tau, \kappa, \gamma, C_{\text{App}}) \cap \mathcal{P}_{\text{App}}^+(A, \tau, \kappa, \gamma, v, C_{\text{App}})$.

Proof. First take $A \in \mathcal{A} \cap \text{Pow}(\mathcal{X}_r(\eta))$ and $\ell' \in [L]$ with $A \cap K^\ell_r(\eta) \neq \emptyset$ and $z_{\ell'} \notin A$. Since $\eta(x) = \tau - \theta$ for all $x \in K^\ell_r(\eta)$, we must have $A \cap (K^\ell_r(\eta) \cup \{z_{\ell'}\}) = \emptyset$. Moreover, $A$ is convex with $A \cap K^\ell_r(\eta) \neq \emptyset$, and it follows that $A \subseteq \{x \in \mathbb{R}^d : ||x - z_{\ell'}||_{\infty} < 2d^{1/2}r\}$. Thus $A \cap \text{supp}(\mu) = A \cap \{x \in \mathbb{R}^d : ||x - z_{\ell'}||_{\infty} < 2d^{1/2}r\} \cap \text{supp}(\mu) = A \cap K^\ell_r(\eta)$ is the intersection of two axis-aligned hyper-rectangles, so it is itself an axis-aligned hyper-rectangle. Since $A \cap \text{supp}(\mu) \subseteq K^\ell_r(\eta)$, we deduce that $\mu(A) \leq (w/L) \cdot (2r)^d/2$. In particular, if $\ell' \in [L] \setminus \{\ell\}$, then $\eta(z_{\ell'}) = \tau - \theta$, so $z_{\ell'} \notin \mathcal{X}_r(\eta)$ and the conclusion $\mu(A) \leq (w/L) \cdot (2r)^d/2$ holds.

For the next part, note that $K^\ell_r(\eta) = \mathcal{B}_r(z_{\ell'}) \cap \mathcal{X}_r(\eta)$ since $\eta(x) = \tau + \theta$ for all $x \in K^\ell_r(\eta)$. Hence, $M_r(P, A) \geq \mu(K^\ell_r(\eta)) = (w/L) \cdot (2r)^d$. On the other hand, given $A \in \mathcal{A} \cap \text{Pow}(\mathcal{X}_r(\eta))$, we have either $A \cap \text{supp}(\mu) \subseteq K^\ell_r(\eta)$, in which case $\mu(A) \leq \mu(K^\ell_r(\eta)) = (w/L) \cdot (2r)^d$, or $A \cap \text{supp}(\mu) \cap K^\ell_r(\eta) \neq \emptyset$ for some $\ell' \in [L] \setminus \{\ell\}$, since $\text{supp}(\mu) \cap \mathcal{X}_r(\eta) \subseteq \bigcup_{\ell \in [L]} K^\ell_r(\eta)$, in which case $\mu(A) \leq (w/L) \cdot (2r)^d/2$. Hence $M_r(P, A) = (w/L) \cdot (2r)^d$.

For the final part, assume that $(w/L) \cdot (2r)^d \leq C_{\text{App}} \cdot \min\{(w/\{4d^{1/2}\cdot L\})^\kappa, \theta^\gamma\}$, and fix $(\xi, \Delta) \in (0, \infty)^2$. We consider two cases: first suppose that $\xi \leq w/\{L \cdot (4d^{1/2})^d\}$ and $\Delta \leq \theta$. By Lemma 30, we have $K^\ell_r(\eta) \subseteq \mathcal{X}_r(\omega_{\mu, d})$. Moreover, it follows from the construction of $\eta$ that $K^\ell_r(\eta) \subseteq \mathcal{X}_{r+\theta}(\eta) \subseteq \mathcal{X}_{r+\Delta}(\eta)$. Thus, with $A_{\xi, \Delta} = K^\ell_r(\eta) \cap \mathcal{X}_{\xi, \Delta}(\eta)$, we have

$$
\mu(A_{\xi, \Delta}) = \frac{w}{L} \cdot (2r)^d \geq \frac{w}{L} \cdot (2r)^d - C_{\text{App}} \cdot (\xi^\kappa + \Delta^\gamma) = M_r - C_{\text{App}} \cdot (\xi^\kappa + \Delta^\gamma).
$$

On the other hand, if $\xi > w/\{L \cdot (4d^{1/2})^d\}$ or $\Delta > \theta$, then with $A_{\xi, \Delta} = \emptyset \in \mathcal{A} \cap \text{Pow}(\mathcal{X}_r(\omega_{\mu, d}) \cap \mathcal{X}_{r+\Delta}(\eta))$, we have

$$
\mu(A_{\xi, \Delta}) = 0 \geq \frac{w}{L} \cdot (2r)^d - C_{\text{App}} \cdot \min\left\{\left(\frac{w}{(4d^{1/2})^d \cdot L}\right)^\kappa, \theta^\gamma\right\} \geq M_r - C_{\text{App}} \cdot (\xi^\kappa + \Delta^\gamma).
$$

We conclude that $P \in \mathcal{P}_\text{App}(A, \tau, \kappa, \gamma, C_{\text{App}})$. To prove $P \in \mathcal{P}_{\text{App}}^+(A, \tau, \kappa, \gamma, v, C_{\text{App}})$, we proceed similarly using the facts that $K^\ell_r(\eta) \subseteq \mathcal{R}_v(\mu)$ by Lemma 30 and that $\mu$ has Lebesgue density at least $w/L$ on $K^\ell_r(\eta)$.

Lemma 32 below bounds the $\chi^2$-divergence between pairs of distributions in our class $\{P^\ell_{L,r,w,s,\theta} : \ell \in [L]\}$.

Lemma 32. Suppose that $\epsilon_0 \in (0, 1/2)$, $\tau \in [\epsilon_0, 1-\epsilon_0)$, $L, d \in \mathbb{N}$, $r \in (0, \infty)$, $s \in (0, 1 \wedge (r/2)]$, $w \in (0, (2r)^{-d} \wedge 1)$ and $\theta \in (0, \epsilon_0/2]$. Then

$$
\chi^2(P^\ell_{L,r,w,s,\theta}, P^{\ell'}_{L,r,w,s,\theta}) \leq \frac{25 + 2d \cdot w \cdot \theta^2 \cdot s^d}{\epsilon_0 \cdot L}
$$

for all $\ell, \ell' \in [L]$.
Proof. Let $Q_{L,r,w} := \mu_{L,r,w} \times m_c$ where $m_c$ denotes the counting measure on $\{0,1\}$. Note that $P^\ell_{L,r,w,s,\theta}$ is absolutely continuous with respect to $Q_{L,r,w}$, for all $\ell \in [L]$. Given $\ell \in [L]$, define $p^\ell : \mathbb{R}^d \times \{0,1\} \to \mathbb{R}$ by

$$p^\ell(x,y) := \frac{dP^\ell_{L,r,w,s,\theta}}{dQ_{L,r,w}}(x,y) = (1 - y) \cdot (1 - \eta^\ell_{L,r,\theta}(x)) + y \cdot \eta^\ell_{L,r,\theta}(x).$$

Take $\ell, \ell' \in [L]$ with $\ell \neq \ell'$ and observe that $\eta^\ell_{L,r,w,s,\theta}(x) = \eta^{\ell'}_{L,r,w,s,\theta}(x)$ for all $x \in J_{L,r,w} \setminus (\bar{B}_{2s}(z_\ell) \cup \bar{B}_{2s}(z_{\ell'}))$. Note also that $\mu_{L,r,w}(\bar{B}_{2s}(z_\ell) \cup \bar{B}_{2s}(z_{\ell'})) = (2w/L) \cdot (4s)^d$; moreover, $\eta^\ell_{L,r,\theta}(x) \in [\tau - \theta, \tau + \theta] \subseteq [\epsilon_0/2, 1 - \epsilon_0/2]$ for all $x \in J_{L,r,w}$ and $\ell \in [L]$. Hence,

$$\chi^2(P^\ell_{L,r,w,s,\theta}, P^{\ell'}_{L,r,w,s,\theta}) = \int_{\mathbb{R}^d \times \{0,1\}} \left( \frac{dP^\ell_{L,r,w,s,\theta}}{dP^{\ell'}_{L,r,w}} - 1 \right)^2 dP^{\ell'}_{L,r,w}$$

$$= \int_{\mathbb{R}^d \times \{0,1\}} \frac{(p^\ell(x,y) - p^{\ell'}(x,y))^2}{p^{\ell'}(x,y)} dQ_{L,r,w}(x,y)$$

$$= \int_{\mathbb{R}^d \times \{0,1\}} \left( \frac{\eta^\ell_{L,r,w,s,\theta}(x) - \eta^{\ell'}_{L,r,w,s,\theta}(x)}{1 - \eta^\ell_{L,r,w,s,\theta}(x)} + \frac{\eta^{\ell'}_{L,r,w,s,\theta}(x) - \eta^\ell_{L,r,w,s,\theta}(x)}{\eta^\ell_{L,r,w,s,\theta}(x)} \right) d\mu_{L,r,w}(x)$$

$$\leq \frac{4}{\epsilon_0} \int_{B_{2s}(z_\ell) \cup B_{2s}(z_{\ell'})} \left( \eta^\ell_{L,r,w,s,\theta}(x) - \eta^{\ell'}_{L,r,w,s,\theta}(x) \right)^2 d\mu_{L,r,w}(x)$$

$$\leq \frac{4}{\epsilon_0} \cdot (2\theta)^2 \cdot \mu_{L,r,w}(\bar{B}_{2s}(z_\ell) \cup \bar{B}_{2s}(z_{\ell'})) = \frac{2^{5+2d} \cdot w \cdot \theta^2 \cdot s^d}{\epsilon_0 \cdot L},$$

as required. \hfill \square

We are now in a position to state the crucial proposition for the proof of Proposition 9.

**Proposition 33.** Suppose that $A_{\text{rect}} \subseteq A \subseteq A_{\text{conv}}$. Take $(\beta, \gamma, \kappa, C_S, C_{\text{App}}) \in (0, \infty)^3 \times [1, \infty)^2$ with $\beta \gamma(\kappa - 1) < d\kappa, \epsilon_0 \in (0, 1/2), \tau \in [\epsilon_0, 1 - \epsilon_0], \nu \leq (4d^{1/2})^{-d}$ and $\zeta > 0$. There exist $C_0 \geq 1, c_0, c_1 > 0$, depending only on $d, \beta, \gamma, \kappa, C_S, C_{\text{App}}$ and $\epsilon_0$, such that for any $n \geq C_0 \log(1 + \zeta)$ there exists a family of $L \geq \left\{ c_0 \left( n / \log(1 + \zeta) \right) \right\}^{\frac{\beta \gamma(\kappa - 1)}{\nu(2^{3+d}) + \nu \gamma}} \cup 4$ distributions

$$\{P_1, \ldots, P_L\} \subseteq \mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \gamma, \nu, C_S, C_{\text{App}})$$

with regression functions $\eta_1, \ldots, \eta_L$ and common marginal distribution $\mu$ on $\mathbb{R}^d$, such that

(a) $\chi^2(P^\otimes n_\ell, P^\otimes n_{\ell'}) \leq \zeta$ for all $\ell, \ell' \in [L]$;

(b) if $A \in \mathcal{A} \cap \text{Pow}(\mathcal{X}_\tau(\eta_\ell) \cap \mathcal{X}_\tau(\eta_{\ell'}))$ for some $\ell, \ell' \in [L]$ with $\ell \neq \ell'$, then

$$M_{\tau}(P_\ell, A) - \mu(A) \geq c_1 \cdot \left( \frac{\log(1 + \zeta)}{n} \right)^{\frac{\beta \gamma(\kappa - 1)}{\nu(2^{3+d}) + \nu \gamma}}. \quad (43)$$
Proof. We begin by defining some quantities for our construction. Let \( \rho := \kappa(2\beta + d) + \beta \gamma \),

\[
\xi_{n, \zeta} := \frac{\epsilon_0 \cdot (c^\rho_{\beta,d} \cdot C_S)^{d/\beta}}{2^{5+4d} d/2} \cdot \log(1 + \zeta), \quad \theta := \xi_{n, \zeta}^{\rho/\rho}, \quad \tau := C_{App}^{1/d} \cdot (8d/2)^{-1} \cdot \theta^{-\rho(\kappa - 1)/\kappa},
\]

\[
L := \left[(8d/2)^{-1} \cdot \theta^{-\gamma/\kappa} \cdot \{(2r)^{-d} \land 1\}\right], \quad w := (4d/2)^d \cdot L \cdot \theta^{\gamma/\kappa} \quad \text{and} \quad s := \left(\frac{\theta}{c^\rho_{\beta,d} \cdot C_S}\right)^{1/\beta}.
\]

Finally, let \( C_0 := C_0^0 \cdot \left(C_1^0 \lor C_2^0 \lor C_3^0 \lor C_4^0 \lor C_5^0\right) \), where

\[
C_0^0 := \frac{\epsilon_0 c_{\beta,d} \cdot C_S^{d/\beta}}{2^{5+4d} d/2}, \quad C_1^0 := \left(\frac{16d/2}{c_{\beta,d} \cdot C_S^1 \cdot C_{App}}\right)^{d/2} \cdot \theta^{-d/(\kappa - 1)} \cdot \xi_{n, \zeta}^{\rho/\rho}, \quad C_2^0 := \frac{1}{c^\rho_{\beta,d} \cdot C_S^\rho/(\beta \gamma)},
\]

\[
C_3^0 := \left(\frac{2}{\epsilon_0}\right)^{\frac{d}{\rho}}, \quad C_4^0 := \left(\frac{C_{App}}{2^{d-5} (d-1)/2}\right)^{\frac{d}{\rho}} \quad \text{and} \quad C_5^0 := (32d/2)^{d/5}.
\]

Observe that when \( n \geq C_0 \log(1 + \zeta) \), we have \( \xi_{n, \zeta} \leq 1/(C_1^0 \lor C_2^0 \lor C_3^0 \lor C_4^0 \lor C_5^0) \). Hence, the choice of \( C_0^3 \) ensures that \( s \leq r/2 \), the choice of \( C_0^4 \) guarantees that \( s \leq 1 \), the choice of \( C_0^3 \) ensures that \( \theta \leq \epsilon_0/2 \), and \( C_0^4 \) and \( C_0^5 \) are chosen to guarantee that

\[
L = \left[4 \cdot \min\left\{\frac{n}{C_0^0 C_0^3 \log(1 + \zeta)}, \frac{n}{(C_0^0 C_0^5 \log(1 + \zeta))^{d_{\rho}}}, \frac{n}{C_0^1 C_0^4 \log(1 + \zeta)}\right\}\right]^{\rho/\rho} \cdot \left(\frac{n}{C_0^1 C_0^4 \log(1 + \zeta)}\right)^{d_{\rho}} \cdot \left(\frac{n}{C_0^1 C_0^4 \log(1 + \zeta)}\right)^{d_{\rho}}.
\]

where \( c_0 := 2 \cdot \min\left\{(C_0^1 C_0^4)^{\beta_{\rho}}/\rho, (C_0^1 C_0^4)^{\beta_{\rho}}/\rho\right\} \). Note also that \( w \leq \frac{1}{2^{d \land (2r)^{-d} \land 1}}\). We may therefore apply the construction following (17) to define distributions \( P_{\ell} := P^\ell_{L,r,w,s,\theta} \) for \( \ell \in [L] \) when \( n \geq C_0 \log(1 + \zeta) \). We write \( \mu = \mu_{L, r, w} \) and \( \eta_{\ell} = \eta^\ell_{L, r, w, s, \theta} \) in this construction.

Our choice of \( s \) ensures that \( \theta = c_{\beta,d} \cdot C_S \cdot s^\beta \), so we may apply Lemma 29 to deduce that \( P_{\ell} \in \mathcal{P}_{\text{Hö}r}(\beta, C_S) \) for all \( \ell \in [L] \). Moreover, our choice of \( w \) and \( r \) guarantee that \( \langle w \rangle/(2r)^{d} \leq C_{App} \cdot \min\{w/(4d/2)^{d-1} \cdot L\}^{\rho} \), so we may apply Lemma 31 to conclude that \( P_{\ell} \in \mathcal{P}_{App}(\mathcal{A}, \tau, \kappa, \gamma, C_{App}) \cap \mathcal{P}_{App}^+(\mathcal{A}, \tau, \kappa, \gamma, v, C_{App}) \) for all \( \ell \in [L] \). Next, by Lemma 32, for each \( \ell, \ell' \in [L] \),

\[
\chi^2(P_{\ell}, P_{\ell'}) \leq \frac{2^{d+2d} \cdot w \cdot \theta^2 \cdot s^d}{\epsilon_0 \cdot L} = \frac{\log(1 + \zeta)}{n},
\]

by our choice of \( w, \theta \) and \( s \), so

\[
\chi^2(P_{\ell}^{\wedge n}, P_{\ell'}^{\wedge n}) \leq \left\{1 + \chi^2(P_{\ell}, P_{\ell'})\right\}^{n} - 1 \leq \left(1 + \frac{\log(1 + \zeta)}{n}\right)^{n} - 1 \leq \zeta.
\]

This proves (a). To prove (b), we take \( \ell, \ell' \in [L] \) with \( \ell \neq \ell' \) and \( A \in \mathcal{A} \cap \text{Pow}(\mathcal{X}_r(\eta) \cap \mathcal{X}_r(\eta_{\ell})). \) By Lemma 31, we have \( M_r(P_{\ell}, \mathcal{A}) = \mu(K^0_r(\ell)) = \langle w \rangle/(2r)^{d} \). On the other hand, if \( \mu(A) > 0 \), then since \( \text{supp}(\mu) = \bigcup_{\ell_0 \in [L]} K^0_r(\ell_0) \) and \( \bigcup_{\ell_0 \in [L]} K^0_r(\ell_0) \subseteq \mathbb{R}^d \setminus \mathcal{X}_r(\eta_{\ell_0}) \), we must have \( A \cap K^0_r(\ell_0) \neq \emptyset \) for some \( \ell_0 \in [L] \). Since at least one of \( \ell \neq \ell' \) or \( \ell \neq \ell' \) must hold, it follows from Lemma 31 that \( \mu(A) \leq \langle w \rangle/(2r)^{d}/2 \). Hence

\[
M_r(P_{\ell}, \mathcal{A}) - \mu(A) \geq \frac{w}{L} \cdot 2^{d-1} \cdot r^d \cdot C_{App} = \frac{C_{App}}{2} \cdot \theta^\gamma = \frac{C_{App}}{2} \cdot \left(\frac{C_0^0 \cdot \log(1 + \zeta)}{n}\right)^{\beta_{\rho}/\rho},
\]

so (43) holds with \( c_1 := \frac{C_{App}}{2} \cdot (C_0^0)^{\beta_{\rho}/\rho} \). \( \square \)
Proof of Proposition 9. Part (i): We initially assume that \( n \geq C_0 \log(1/(4\alpha)) \). By Proposition 33, with \( \zeta = 1/(4\alpha) - 1 > 0 \), there exists a pair of distributions \( P_1, P_2 \in \mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \kappa, \gamma, v, C_S, C_{\text{App}}) \) with common marginal distribution \( \mu \) on \( \mathbb{R}^d \) and corresponding regression functions \( \eta_1, \eta_2 \) such that \( \chi^2(P_2 \otimes n, P_1 \otimes n) + 1 \leq 1/(4\alpha) \) and if \( A \in \mathcal{A} \cap \text{Pow}(\mathcal{X}_\tau(\eta_1) \cap \mathcal{X}_\tau(\eta_2)) \), then

\[
M_\tau(P_2, \mathcal{A}) - \mu(A) \geq c_1 \cdot \left( \frac{\log(1/(4\alpha))}{n} \right)^{\frac{\beta\gamma}{\kappa(2\beta + d) + \beta\gamma}}.
\] (44)

We now define a test \( \varphi : (\mathbb{R}^d \times [0, 1])^n \to \{1, 2\} \) by

\[
\varphi(D) := \begin{cases} 1 & \text{if } \hat{A}(D) \subseteq \mathcal{X}_\tau(\eta_1) \\
2 & \text{otherwise.} \end{cases}
\]

Since \( \hat{A} \) controls the Type I error at level \( \alpha \) over \( \mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \kappa, \gamma, v, C_S, C_{\text{App}}) \), we have

\[
P_2^\otimes n(\{D \in (\mathbb{R}^d \times [0, 1])^n : \varphi(D) = 2\}) = \mathbb{P}_{P_1}(\hat{A}(D) \notin \mathcal{X}_\tau(\eta_1)) \leq \alpha.
\]

Hence, by an immediate consequence of Brown and Low (1996, Theorem 1), which we restate as Lemma 41 for convenience, with \( \epsilon = \sqrt{\alpha} \) we have

\[
\mathbb{P}_{P_2}(\hat{A}(D) \subseteq \mathcal{X}_\tau(\eta_1)) = P_2^\otimes n(\{D \in (\mathbb{R}^d \times [0, 1])^n : \varphi(D) = 1\}) \geq \left\{ 1 - \epsilon, \chi^2(P_2^\otimes n, P_1^\otimes n) + 1 \right\}^2 \geq \frac{1}{4}.
\]

Thus, by (44) we have

\[
\mathbb{E}_{P_2} \left[ \{M_\tau(P, \mathcal{A}) - \mu(\hat{A})\} \cdot 1_{\{\hat{A} \subseteq \mathcal{X}_\tau(\eta_2)\}} \right] \\
\geq \mathbb{P}_{P_2}(\{\hat{A}(D) \subseteq \mathcal{X}_\tau(\eta_1)\} \cap \{\hat{A}(D) \subseteq \mathcal{X}_\tau(\eta_2)\}) \cdot c_1 \cdot \left( \frac{\log(1/(4\alpha))}{n} \right)^{\frac{\beta\gamma}{\kappa(2\beta + d) + \beta\gamma}} \\
\geq \left\{ \mathbb{P}_{P_2}(\hat{A}(D) \subseteq \mathcal{X}_\tau(\eta_1)) - \mathbb{P}_{P_2}(\hat{A}(D) \notin \mathcal{X}_\tau(\eta_2)) \right\} \cdot c_1 \cdot \left( \frac{\log(1/(4\alpha))}{n} \right)^{\frac{\beta\gamma}{\kappa(2\beta + d) + \beta\gamma}} \\
\geq \left( \frac{1}{4} - \alpha \right) \cdot c_1 \cdot \left( \frac{\log(1/(4\alpha))}{n} \right)^{\frac{\beta\gamma}{\kappa(2\beta + d) + \beta\gamma}} \geq \frac{c_1}{8} \cdot \left( \frac{\log(1/(4\alpha))}{n} \right)^{\frac{\beta\gamma}{\kappa(2\beta + d) + \beta\gamma}},
\] (45)

as required. Moreover, if \( 1 \leq n < C_0 \log(1/(4\alpha)) \), then by (45) with \( n = \lceil C_0 \log(1/(4\alpha)) \rceil \), we have

\[
\mathbb{E}_{P_2} \left[ \{M_\tau(P, \mathcal{A}) - \mu(\hat{A})\} \cdot 1_{\{\hat{A} \subseteq \mathcal{X}_\tau(\eta_2)\}} \right] \geq \frac{c_1}{8} \cdot C_0^{-\frac{\beta\gamma}{\kappa(2\beta + d) + \beta\gamma}},
\]

again. This completes the proof of Part (i).

Part (ii): Fix \( \rho := \kappa(2\beta + d) + \beta\gamma \) and let \( C_1 \equiv C_1(1, \beta, \gamma, \kappa, C_S, C_{\text{App}}, \epsilon_0) \geq e^{\frac{2\rho}{\beta\gamma}} - 1 \) be large enough that for all \( n \geq C_1 \), we have both \( n \geq C_0 \log(1 + n^{\frac{\beta\gamma}{\kappa(\alpha + 1)}}) \) and \( c_0 \epsilon_0^3 (n/\log(1 + n^{\frac{\beta\gamma}{\kappa(\alpha + 1)}}))^\frac{\beta\gamma}{\kappa(\alpha + 1)} - 2\rho n^{\frac{\beta\gamma}{\kappa(\alpha + 1)}} \geq 2\rho n^{\frac{\beta\gamma}{\kappa(\alpha + 1)}} \).

Next, for \( n \geq C_1 \), we apply Proposition 33 with \( \zeta = n^{\frac{\beta\gamma}{\kappa(\alpha + 1)}} \) to obtain a family of \( L \geq c_0 (n/\log(1 + n^{\frac{\beta\gamma}{\kappa(\alpha + 1)}}))^\frac{\beta\gamma}{\kappa(\alpha + 1)} \) \( \geq 2\rho n^{\frac{\beta\gamma}{\kappa(\alpha + 1)}} / \epsilon_0^3 \) distributions \( \{P_1, \ldots, P_L\} \subseteq \mathcal{P}_{\text{Hil}}(\beta, C_S) \cap \mathcal{P}_{\text{App}}(\mathcal{A}, \tau, \kappa, \gamma, C_{\text{App}}) \cap \mathcal{P}_{\text{App}}^+(\mathcal{A}, \tau, \kappa, \gamma, v, C_{\text{App}}) \) with common marginal distribution \( \mu \) on \( \mathbb{R}^d \) and corresponding regression functions \( \eta_1, \ldots, \eta_L \), such that
(a) $\chi^2(P_{\ell}^{\otimes n}, P_{\ell'}^{\otimes n}) \leq n \frac{\beta(\kappa \wedge 1)}{2^\rho} \leq (\epsilon_0/4)^2 \cdot (L - 1)$ for all $\ell, \ell' \in [L]$;

(b) if $A \in \mathcal{A} \cap \operatorname{Pow}(\mathcal{X}_r(\eta_\ell) \cap \mathcal{X}_r(\eta_{\ell'}))$ for some $\ell, \ell' \in [L]$ with $\ell \neq \ell'$, then

$$M_r(P_r, \mathcal{A}) - \mu(A) \geq c_1 \cdot \left( \frac{\log(1 + n \frac{\beta(\kappa \wedge 1)}{2^\rho})}{n} \right)^{\beta \gamma \kappa / \rho} .$$ (46)

Now define a test function $\varphi : (\mathbb{R}^d \times [0, 1])^n \rightarrow [L]$ by

$$\varphi(D) := \begin{cases} \min\{\ell \in [L] : \hat{A}(D) \subseteq \mathcal{X}_r(\eta_\ell)\} & \text{if } \hat{A}(D) \subseteq \mathcal{X}_r(\eta_\ell) \text{ for some } \ell \in [L] \\
 L & \text{otherwise.} \end{cases}$$

By Lemma 42, we have

$$\max_{\ell \in [L]} P_{\ell}^{\otimes n}(\{D \in (\mathbb{R}^d \times [0, 1])^n : \varphi(D) \neq \ell\})$$

$$\geq \frac{1}{L - 1} \sum_{\ell=2}^L P_{\ell}^{\otimes n}(\{D \in (\mathbb{R}^d \times [0, 1])^n : \varphi(D) \neq \ell\})$$

$$\geq 1 - \frac{1}{L - 1} - \sqrt{\frac{1}{L - 1} \sum_{\ell=2}^L \chi^2(P_{\ell}^{\otimes n}, P_{1}^{\otimes n}) \cdot \frac{1}{L - 1} \left(1 - \frac{1}{L - 1}\right)}$$

$$\geq 1 - \frac{(\epsilon_0/4)^2}{\epsilon_0} \geq 1 - \frac{\epsilon_0}{2} .$$ (47)

Now choose $\ell_0 \in [L]$ with $P_{\ell_0}^{\otimes n}(\{D \in (\mathbb{R}^d \times [0, 1])^n : \varphi(D) \neq \ell_0\}) \geq 1 - \epsilon_0/2$, and observe that if $\varphi(D) \neq \ell_0$ and $\hat{A}(D) \subseteq \mathcal{X}_r(\eta_{\ell_0})$ then we must also have $\hat{A}(D) \subseteq \mathcal{X}_r(\eta_{\ell_1})$ for some $\ell_1 \in [\ell_0 - 1]$. It follows from this and (47) that

$$\mathbb{P}_{P_{\ell_0}}\left(\hat{A}(D) \subseteq \mathcal{X}_r(\eta_{\ell_0})\right) \cap \bigcup_{\ell_1=1}^{\ell_0-1} \{\hat{A}(D) \subseteq \mathcal{X}_r(\eta_{\ell_1})\}$$

$$\geq \mathbb{P}_{P_{\ell_0}}\left(\hat{A}(D) \subseteq \mathcal{X}_r(\eta_{\ell_0}) \cap \varphi(D) \neq \ell_0\right)$$

$$\geq P_{\ell_0}^{\otimes n}(\{D \in (\mathbb{R}^d \times [0, 1])^n : \varphi(D) \neq \ell_0\}) - \alpha$$

$$\geq \frac{\epsilon_0}{2} .$$

Thus, by (46), we have for all $n \geq C_1 \geq e^{\frac{\beta \kappa}{2^\rho}} - 1$ that

$$\mathbb{E}_{P_{\ell_0}}\left[\{M_r(P_{\ell_0}, \mathcal{A}) - \mu(\hat{A})\} \cdot 1_{\{\hat{A} \subseteq \mathcal{X}_r(\eta_{\ell_0})\}}\right]$$

$$\geq \mathbb{P}_{P_{\ell_0}}\left(\hat{A}(D) \subseteq \mathcal{X}_r(\eta_{\ell_0})\right) \cap \bigcup_{\ell_1=1}^{\ell_0-1} \{\hat{A}(D) \subseteq \mathcal{X}_r(\eta_{\ell_1})\} \cdot c_1 \cdot \left( \frac{\log(1 + n \frac{\beta(\kappa \wedge 1)}{2^\rho})}{n} \right)^{\beta \gamma \kappa / \rho}$$

$$\geq \frac{c_1 \epsilon_0}{2} \cdot \left( \frac{\beta \gamma (\kappa \wedge 1) \log n}{2 \rho n} \right)^{\beta \gamma \kappa / \rho} .$$
We extend the bound to $n < C_1$ by monotonicity as at the end of the proof of Proposition 9(i), with

$$c_2 := \frac{c_1 \epsilon_0}{2} \cdot \left( \frac{\beta \gamma (\kappa + 1) \log_+ [C_1]}{2 \rho [C_1]} \right)^{\beta \gamma \kappa / \rho},$$

which completes the proof.

Finally, we prove the parametric lower bounds in Theorems 2 and 6. Some care is required here to show that our constructed distributions belong to the relevant distributional classes.

**Proof of Proposition 10.** Observe that there exists $c_H \equiv c_H(\beta) \in (0, 1]$ such that when $\theta \leq c_H \cdot C_S \cdot s^3$, we have that $\eta$ is $(\beta, C_S)$-Hölder, so $\{P^\ell_\zeta\}_{\ell \in \{-1, 1\}} \subseteq \mathcal{P}_{\text{H}}(\beta, C_S)$. In addition, $\text{supp}(\mu^\ell_\zeta \cap \mathcal{X}_\tau(\eta)) = A_{-1} \cup A_1$ for $\ell \in \{-1, 1\}$. Since $\mathcal{A} \subseteq \mathcal{A}_{\text{conv}}$ and $A_0 \subseteq \mathbb{R}^d \setminus \mathcal{X}_\tau(\eta)$, it follows that for $\ell \in \{-1, 1\}$,

$$M_{s}(P^\ell_\zeta, \mathcal{A}) = \max_{j \in \{-1, 1\}} \mu^\ell_\zeta(A_j) = \frac{s^d}{(2t)^d + 2s^d} + \zeta.$$ 

Observe also that for any $\ell \in \{-1, 1\}$, $x \in A_\ell$ and $r \in (0, 4s]$, we have

$$\mu^\ell_\zeta(B_{r/4}(x)) \geq \left( \frac{1}{(2t)^d + 2s^d} + \frac{\zeta}{s^d} \right) \cdot \mathcal{L}_d(B_{r/4}(x) \cap A_\ell) \geq \left( \frac{1}{(2t)^d + 2s^d} + \frac{\zeta}{s^d} \right) \cdot \left( \frac{r}{4} \right)^d.$$ 

Moreover, for any $\ell \in \{-1, 1\}$, $x \in A_\ell$ and $r \in (4s, 1]$, we have

$$\mu^\ell_\zeta(B_r(x)) \geq \frac{\mathcal{L}_d(B_r(x) \cap A_0)}{(2t)^d + 2s^d} \geq \frac{r^{d-1} \cdot (r - 2s)}{(2t)^d + 2s^d} \geq \frac{r^d}{2 \{(2t)^d + 2s^d\}} \geq \left( \frac{1}{(2t)^d + 2s^d} + \frac{\zeta}{s^d} \right) \cdot \left( \frac{r}{3} \right)^d.$$ 

Hence, $\omega_{\mu^\ell_\zeta, d}(x) \geq \{(8t)^d + 2(4s)^d\}^{-1}$ for all $x \in A_\ell$, and moreover $A_\ell \subseteq \mathcal{R}_\omega(\mu^\ell_\zeta)$. Thus, for any $(\xi, \Delta) \in (0, \{(8t)^d + 2(4s)^d\}^{-1}] \times (0, \theta]$, we have

$$\sup\{\mu^\ell_\zeta(A) : A \in \mathcal{A} \cap \text{Pow} \left( \mathcal{X}_\zeta(\omega_{\mu^\ell_\zeta, d}) \cap \mathcal{X}_{\tau + \Delta}(\eta) \right) \} = \mu^\ell_\zeta(A_\ell) = M_{s}(P^\ell_\zeta, \mathcal{A}),$$

and similarly,

$$\sup\{\mu^\ell_\zeta(A) : A \in \mathcal{A} \cap \text{Pow} \left( \mathcal{R}_\nu(\mu^\ell_\zeta) \cap \mathcal{X}_\zeta(\nu_{\mu^\ell_\zeta}) \cap \mathcal{X}_{\tau + \Delta}(\eta) \right) \} = \mu^\ell_\zeta(A_\ell) = M_{s}(P^\ell_\zeta, \mathcal{A}).$$

On the other hand, if either $\xi > \{(8t)^d + 2(4s)^d\}^{-1}$ or $\Delta > \theta$, then provided that $\frac{3s^d}{2 \{(2t)^d + 2s^d\}} \leq C_{\text{App}} \cdot \{(8t)^d + 2(4s)^d\}^{-\kappa} \wedge \theta^3]$, we have

$$\sup\{\mu^\ell_\zeta(A) : A \in \mathcal{A} \cap \text{Pow} \left( \mathcal{R}_\nu(\mu^\ell_\zeta) \cap \mathcal{X}_\zeta(\nu_{\mu^\ell_\zeta}) \cap \mathcal{X}_{\tau + \Delta}(\eta) \right) \} \wedge \sup\{\mu^\ell_\zeta(A) : A \in \mathcal{A} \cap \text{Pow} \left( \mathcal{X}_\zeta(\omega_{\mu^\ell_\zeta, d}) \cap \mathcal{X}_{\tau + \Delta}(\eta) \right) \} \geq 0 \geq M_{s}(P^\ell_\zeta, \mathcal{A}) - C_{\text{App}} \cdot (\xi^\kappa + \Delta^\gamma).$$

It follows that $\{P^\ell_\zeta\}_{\ell \in \{-1, 1\}} \subseteq \mathcal{P}^\dagger(\mathcal{A}, \tau, \beta, \kappa, \gamma, \nu, C_S, C_{\text{App}})$ whenever $\frac{3s^d}{2 \{(2t)^d + 2s^d\}} \leq C_{\text{App}} \cdot \{(8t)^d + 2(4s)^d\}^{-\kappa} \wedge \theta^3].$
In addition, recalling that $m_{\infty}$ denotes the counting measure, we have
\[
\text{KL}(P_{\zeta}^{-1}, P_{\zeta}^{1}) \leq \chi^2(P_{\zeta}^{-1}, P_{\zeta}^{1}) = \int_{\mathbb{R}^d \times \{0,1\}} \frac{(f_{\mu_1}^{-1}(x) - f_{\mu_2}^{-1}(x))^2 \eta(x) (1 - \eta(x))^{1 - y} d(\mathcal{L}_d \times m_{\infty})(x, y)}{f_{\mu_2}^{-1}(x)} = \frac{(2\zeta/s^d)^2}{(2\zeta + 2s^d)^2} + \frac{(2\zeta/s^d)^2}{2(2\zeta + 2s^d)^2 + \frac{s^d}{s^d}} \leq \frac{32}{3} \cdot \frac{(2t)^d + 2s^d}{s^d} \cdot \zeta^2.
\]
We deduce by Pinsker’s inequality that
\[
\text{TV}((P_{\zeta}^{-1}) \otimes n, (P_{\zeta}^{1}) \otimes n) \leq \sqrt{\text{KL}((P_{\zeta}^{-1}) \otimes n, (P_{\zeta}^{1}) \otimes n)/2} \leq 4\zeta \sqrt{n} \cdot \sqrt{\frac{(2t)^d + 2s^d}{3s^d}} = 2a \cdot \zeta \sqrt{n},
\]
where $a := a_{d,s,t} := 2 \cdot \sqrt{\frac{(2t)^d + 2s^d}{3s^d}}$. Thus,
\[
1 = (P_{\zeta}^{1}) \otimes n \left( \{ D \in (\mathbb{R}^d \times \{0,1\})^n : A_1 \cap \hat{A}(D) = \emptyset \} \right)
+ (P_{\zeta}^{1}) \otimes n \left( \{ D \in (\mathbb{R}^d \times \{0,1\})^n : A_1 \cap \hat{A}(D) \neq \emptyset \} \right)
\leq (P_{\zeta}^{1}) \otimes n \left( \{ D : A_1 \cap \hat{A}(D) = \emptyset \} \right) + (P_{\zeta}^{-1}) \otimes n \left( \{ D : A_1 \cap \hat{A}(D) \neq \emptyset \} \right) + 2a \cdot \zeta \sqrt{n}.
\]
Hence, since at most one of $A_{-1}$ and $A_1$ can have non-empty intersection with $\hat{A}$ whenever $\hat{A} \subseteq \mathcal{X}_r(\eta)$, we have
\[
\max_{\ell \in \{-1,1\}} \left( P_{\zeta}^{1} \right) \otimes n \left( \{ D : A_\ell \cap \hat{A}(D) = \emptyset \} \cup \{ D : \hat{A}(D) \subseteq \mathcal{X}_r(\eta) \} \right) \geq \frac{1}{2} - a \cdot \zeta \sqrt{n} - \alpha \geq \epsilon_0 - a \cdot \zeta \sqrt{n}.
\]
We conclude that
\[
\max_{\ell \in \{-1,1\}} \mathbb{E}_{P_{\zeta}^{1}} \left[ \left\{ M_r(P_{\zeta}^{\ell}, A) - \mu_{\ell}^{\hat{A}}(\hat{A}) \right\} \cdot 1_{ \{ \hat{A} \subseteq \mathcal{X}_r(\eta) \} } \right] \geq 2(\epsilon_0 - a \cdot \zeta \sqrt{n}).
\]
Taking $t := \left( \frac{(2\kappa(3d+1)}{c_H \cdot C_S} + \beta \right)^{\frac{1}{\gamma}}$ and $s := t^{\frac{2s^d}{s^d}}$ and $\theta := c_H \cdot C_S \cdot s^\beta$ ensures that the conditions $\frac{3s^d}{2(2t)^d + 2s^d} \leq C_{\text{App}} \cdot \left[ \{ (8t)^d + 2(4s)^d \}^{-\kappa} \wedge (c_H \cdot C_S \cdot s^\beta)^{\gamma} \right]$ and $\theta \leq c_H \cdot C_S \cdot s^\beta$ hold. Hence, taking $\zeta := \epsilon_0/(2a \sqrt{n})$ yields the required lower bound.

**Proof of Theorems 2(ii) and 6(ii).** In light of the remarks following Proposition 9, these results follow from Propositions 9 and 10. 

### 6.6 Parameter constraints

The following lemma reveals natural constraints satisfied by the parameters $\beta$, $\kappa$ and $\gamma$.

**Lemma 34.** Take $\tau \in (0, 1)$, $(\beta, \gamma, \kappa, \nu, C_S, C_{\text{App}}) \in (0, 1] \times (0, \infty)^2 \times (0, 1] \times [1, \infty)^2$. Let $P \in \mathcal{P}_{\text{Hil}}(\beta, C_S) \cap \mathcal{P}_{\text{App}}(\mathcal{A}_{\text{rect}}, \tau, \kappa, \gamma, C_{\text{App}})$ be a distribution on $\mathbb{R}^d \times [0, 1]$ with regression function $h : \mathbb{R}^d \to [0, 1]$ and with a Lebesgue absolutely continuous marginal $\mu$ on $\mathbb{R}^d$ with continuous density $f_\mu$. Suppose that $\mathcal{X}_r(\eta) \subseteq \mathcal{R}_v(\mu)$, that $\mu(\eta^{-1}(\tau, 1]) > 0$ and that $\eta^{-1}(\{\tau\}) \neq \emptyset$. Then $\beta \gamma (\kappa - 1) \leq d \kappa$. 

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43
Proof. Note that since \( \mu(\eta^{-1}(\tau, 1]) > 0 \) and \( \eta \) is continuous, we must have \( M_\tau > 0 \). Take \( \Delta \in (0, \{M_\tau/(2C_{\text{App}})\}^{1/\gamma}) \), and write \( \omega := \omega_{\mu,d} \) for the lower density of \( \mu \). Since \( P \in \mathcal{P}_{\text{App}}(A_{\text{rect}}, \tau, \kappa, \gamma, C_{\text{App}}) \), we may take \( A_\Delta \in A_{\text{rect}} \right\} \mathcal{P}_{\text{App}}(X, \gamma_\omega(\omega)) \cap \mathcal{X}_{\tau+\Delta}(\eta)) \) with \( \mu(A_\Delta) \geq M_\tau - 2C_{\text{App}} \cdot \Delta^{\gamma} > 0 \). Now \( A_\Delta \) is a non-empty, compact subset of \( \mathbb{R}^d \), so we may choose \( x_0 \in \eta^{-1}(\{\tau\}) \) and \( z_0 \in A_\Delta \) such that

\[
\|x_0 - z_0\|_\infty = \inf_{x \in \eta^{-1}(\{\tau\})} \inf_{z \in A_\Delta} \|x - z\|_\infty.
\]

Let \( A_\Delta^z := \{x \in \mathbb{R}^d : \|x - z\|_\infty \leq \|x_0 - z_0\|_\infty \text{ for some } z \in A_\Delta \} \), and note that \( A_\Delta^z \in A_{\text{rect}} \right\} \mathcal{P}_{\text{App}}(X, \gamma_\omega(\omega)) \cap \mathcal{X}_{\tau+\Delta}(\eta)) \) with \( \mu(A_\Delta^z) \leq M_\tau \) and \( \mu(A_\Delta^z \setminus A_\Delta) \leq 2C_{\text{App}} \cdot \Delta^{\gamma} \). In addition, since \( P \in \mathcal{P}_{\text{Hs}\beta}(\beta, C_S) \), we have \( \|x_0 - z_0\|_\infty \geq (\Delta/C_S)^{1/\beta} =: 3\Delta \). Hence, if we take

\[
w_0 := z_0 + \left(1 + \frac{v}{2}\right) \cdot r_\Delta \cdot \frac{x_0 - z_0}{\|x_0 - z_0\|_\infty},
\]

we have \( B_{r_\Delta}(w_0) \subseteq \mathcal{X}_\tau(\eta) \right\} \mathcal{P}_{\text{App}}(X, \gamma_\omega(\omega)) \cap \mathcal{X}_{\tau+\Delta}(\eta)) \) and \( z_0 \in B_{(1+v)\cdot r_\Delta}(w_0) \). Thus, as \( f_\mu(z_0) \geq 2^{-d} \cdot \omega(z_0) \geq 2^{-d} \cdot \Delta^{\gamma/\kappa} \) and \( w_0 \in \mathcal{X}_\tau(\eta) \right\} \mathcal{P}_{\text{App}}(X, \gamma_\omega(\omega)) \cap \mathcal{X}_{\tau+\Delta}(\eta)) \), we have

\[
2C_{\text{App}} \cdot \Delta^{\gamma} \geq \mu(A_\Delta \setminus A_\Delta) \geq \mu(B_{r_\Delta}(w_0)) \geq v \cdot r_\Delta^d \cdot \sup_{x' \in B_{(1+v)\cdot r_\Delta}(w_0)} f_\mu(x') \geq v \cdot r_\Delta^d \cdot f_\mu(z_0) \geq \frac{v}{6^d} \cdot \left(\frac{\Delta}{C_S}\right)^{d/\beta} \cdot \Delta^{\gamma/\kappa}.
\]

Letting \( \Delta \downarrow 0 \) we deduce that \( \beta\gamma(\kappa - 1) \leq dk \). \( \square \)

7 Auxiliary results

7.1 Disintegration

Suppose we have a pair of measurable spaces \((\mathcal{X}, \mathcal{G}_X)\) and \((\mathcal{Y}, \mathcal{G}_Y)\) along with a probability distribution \( P \) on the product space \((\mathcal{X} \times \mathcal{Y}, \mathcal{G}_X \otimes \mathcal{G}_Y)\). Let \( \mu \) denote the marginal distribution of \( P \) on \((\mathcal{X}, \mathcal{G}_X)\). We say that \((P_x)_{x \in \mathcal{X}}\) is a disintegration of \( P \) into conditional distributions on \( \mathcal{Y} \) if

(a) \( P_x \) is a probability measure on \((\mathcal{Y}, \mathcal{G}_Y)\), for each \( x \in \mathcal{X} \);

(b) \( x \mapsto P_x(B) \) is a \( \mathcal{G}_X \)-measurable function, for every \( B \in \mathcal{G}_Y \);

(c) \( P(A \times B) = \int_A P_x(B) \, d\mu(x) \) for all \( A \in \mathcal{G}_X \) and \( B \in \mathcal{G}_Y \).

We will make use of the following existence result: recall that a topological space \((\mathcal{X}, \mathcal{T}_X)\) is said to be Polish if there exists a metric \( d_X \) on \( \mathcal{X} \) that induces the topology \( \mathcal{T}_X \) and for which \((\mathcal{X}, d_X)\) is a complete, separable metric space.

**Lemma 35.** Suppose that \((\mathcal{X}, \mathcal{G}_X)\) and \((\mathcal{Y}, \mathcal{G}_Y)\) are Polish spaces with their corresponding Borel \( \sigma \)-algebras. Let \( P \) be a probability distribution on \((\mathcal{X} \times \mathcal{Y}, \mathcal{G}_X \otimes \mathcal{G}_Y)\), with \( \mu \) denoting
the marginal distribution of \( P \) on \((\mathcal{X}, \mathcal{G}_X)\). Then there exists a disintegration \((P_x)_{x \in \mathcal{X}}\) of \( P \) into conditional distributions on \( \mathcal{Y} \) with the property that

\[
\int_{\mathcal{X} \times \mathcal{Y}} g(x, y) \, dP(x, y) = \int_{\mathcal{X}} \left( \int_{\mathcal{Y}} g(x, y) \, dP_x(y) \right) \, d\mu(x),
\]

for every \( P \)-integrable function \( g : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \). Moreover, the disintegration \((P_x)_{x \in \mathcal{X}}\) of \( P \) is unique in the sense that if there exists another disintegration \((\tilde{P}_x)_{x \in \mathcal{X}}\) of \( P \) into conditional distributions on \( \mathcal{Y} \), then \( \tilde{P}_x = P_x \) for \( \mu \)-almost every \( x \in \mathcal{X} \).

**Proof.** This follows by combining Theorems 10.2.1 and 10.2.2 of Dudley (2018).

A disintegration has the following useful interpretation. Suppose we have a pair of random variables \((X, Y)\) taking values in \(\mathcal{X} \times \mathcal{Y}\) with joint distribution \( P \) on \(\mathcal{G}_X \times \mathcal{G}_Y\), where \((\mathcal{X}, \mathcal{G}_X)\) and \((\mathcal{Y}, \mathcal{G}_Y)\) are Polish spaces with their corresponding Borel \(\sigma\)-algebras. Let \( \mu \) be the marginal on \(\mathcal{X}\) and \((P_x)_{x \in \mathcal{X}}\) be a disintegration of \( P \) into conditional distributions. Then for all \( P \)-integrable functions \( g : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \) we have

\[
\mathbb{E}(g(X, Y) \mid X = x) = \int_{\mathcal{Y}} g(x, y) \, dP_x(y),
\]

for \( \mu \)-almost every \( x \in \mathcal{X} \). Indeed, by Lemma 35 we see that \( x \mapsto \int_{\mathcal{Y}} g(x, y) \, dP_x(y) \) is a \( \mu \)-integrable function, and hence \( \mathcal{G}_X \)-measurable. Moreover, given any \( A \in \mathcal{G}_X \), we have

\[
\int_A \left( \int_{\mathcal{Y}} g(x, y) \, dP_x(y) \right) \, d\mu(x) = \int_{\mathcal{X}} \left( \int_{\mathcal{Y}} 1_A(x) \cdot g(x, y) \, dP_x(y) \right) \, d\mu(x) = \int_{\mathcal{X}} 1_A(x) \cdot g(x, y) \, dP_x(x) = \int_{A \times \mathcal{Y}} g(x, y) \, dP(x, y),
\]

where the second equality follows from (48) with \( 1_A(x) \cdot g(x, y) \) in place of \( g(x, y) \).

### 7.2 Concentration results

We will require the following classic result that gives a uniform concentration inequality over classes of finite Vapnik–Chervonenkis dimension; we state it for distributions on \(\mathbb{R}^d\) for simplicity.

**Lemma 36** (Vapnik–Chervonenkis concentration). Let \( \mu \) be a probability distribution on \(\mathbb{R}^d\), and let \( X_1, \ldots, X_n \sim \mu \), with corresponding empirical distribution \( \hat{\mu}_n \). There exists a universal constant \( C_{VC} > 0 \) such that for any collection of sets \( \mathcal{S} \subseteq \mathcal{B}(\mathbb{R}^d) \) with \( 1 \leq \text{dim}_{VC}(\mathcal{S}) < \infty \), we have

\[
\mathbb{E} \left( \sup_{S \in \mathcal{S}} |\hat{\mu}_n(S) - \mu(S)| \right) \leq C_{VC} \sqrt{\frac{\text{dim}_{VC}(\mathcal{S})}{n}}.
\]

Moreover, for all \( \delta \in (0, 1) \) we have

\[
\mathbb{P} \left( \sup_{S \in \mathcal{S}} |\hat{\mu}_n(S) - \mu(S)| > C_{VC} \sqrt{\frac{\text{dim}_{VC}(\mathcal{S})}{n} + \frac{\log(1/\delta)}{2n}} \right) \leq \delta.
\]

45
Proof. For the expectation bound, see Vershynin (2018, Theorem 8.3.23). The high-probability bound follows by McDiarmid’s inequality (Vershynin, 2018, Theorem 2.9.1). □

The following lemma is used in the proof of Lemma 38.

Lemma 37 (Garivier and Cappé (2011)). Let \((Z_j)_{j \in [m]}\) be independent random variables taking values in \([0, 1]\) with \(\max_{j \in [m]} \mathbb{E}[Z_j] \leq t\) for some \(t \in (0, 1)\). Writing \(\bar{Z} := m^{-1} \sum_{j \in [m]} Z_j\), we have for \(\kappa \in (t, 1)\) that

\[
\mathbb{P}(\bar{Z} \geq \kappa) \leq e^{-m \cdot \text{kl}(\kappa, t)}.
\]

Proof. By Jensen’s inequality, for \(\theta > 0\) and \(j \in [m]\),

\[
\mathbb{E}(e^{\theta \cdot Z_j}) \leq 1 - \mathbb{E}(Z_j) + e^{\theta} \cdot \mathbb{E}(Z_j) \leq 1 + t(e^{\theta} - 1).
\]

Hence, by Markov’s inequality,

\[
\mathbb{P}(\bar{Z} \geq \kappa) \leq e^{-m \theta \kappa} \prod_{j=1}^{m} \mathbb{E}(e^{\theta \cdot Z_j}) \leq \left[e^{-\theta \kappa} \{1 + t(e^{\theta} - 1)\}\right]^{m}.
\]

The lemma follows on taking \(\theta = \log(\kappa(1-t)/(1-\kappa)) > 0\). □

Lemma 38. Let \((Z_j)_{j \in [m]}\) be independent random variables taking values in \([0, 1]\) with \(\max_{j \in [m]} \mathbb{E}(Z_j) \leq t\) for some \(t \in (0, 1)\). Let \(\bar{Z} := m^{-1} \sum_{j \in [m]} Z_j\). Then for every \(\alpha \in (0, 1)\), we have

\[
\mathbb{P}\left(\bar{Z} \geq t + \sqrt{\frac{\log(1/\alpha)}{2m}}\right) \leq \mathbb{P}\left(\left\{\text{kl}(\bar{Z}, t) \geq \frac{\log(1/\alpha)}{m}\right\} \cap \{\bar{Z} > t\}\right) \leq \alpha.
\]

Proof. The first inequality follows from the fact that \(2(\bar{Z} - t)^2 = 2\text{TV}^2(\text{Bern}(\bar{Z}), \text{Bern}(t)) \leq \text{kl}(\bar{Z}, t)\), by Pinsker’s inequality. To prove the second inequality we begin by noting that \(w \mapsto \text{kl}(w, t)\) is continuous and strictly increasing on the interval \([t, 1]\), and consider two cases. If \(\alpha \in (0, e^{-m \cdot \text{kl}(1,t)})\) and \(\bar{Z} > t\), then

\[
\text{kl}(\bar{Z}, t) \leq \text{kl}(1, t) < \frac{\log(1/\alpha)}{m}.
\]

On the other hand, if \(\alpha \in [e^{-m \cdot \text{kl}(1,t)}, 1]\), then by the intermediate value theorem we can find \(\kappa_\alpha \in [t, 1]\) such that \(\text{kl}(\kappa_\alpha, t) = m^{-1} \cdot \log(1/\alpha)\). Then by Lemma 37,

\[
\mathbb{P}\left(\left\{\text{kl}(Z, t) \geq \frac{\log(1/\alpha)}{m}\right\} \cap \{Z > t\}\right) = \mathbb{P}(Z \geq \kappa_\alpha) \leq e^{-m \cdot \text{kl}(\kappa_\alpha, t)} = \alpha,
\]

as required. □

In addition we shall make use of the following Chernoff bounds.
Lemma 39 (Multiplicative Chernoff — Theorem 2.3(b,c) of McDiarmid (1998)). Let \((Z_j)_{j \in [m]}\) be a sequence of independent random variables taking values in \([0, 1]\). Then given any \(\theta > 0\),

\[
\mathbb{P}\left(\sum_{j=1}^{m} Z_j \leq (1 - \theta) \cdot \sum_{j=1}^{m} \mathbb{E}(Z_j)\right) \leq \exp\left(-\frac{\theta^2}{2} \cdot \sum_{j=1}^{m} \mathbb{E}(Z_j)\right)
\]

\[
\mathbb{P}\left(\sum_{j=1}^{m} Z_j \geq (1 + \theta) \cdot \sum_{j=1}^{m} \mathbb{E}(Z_j)\right) \leq \exp\left(-\frac{\theta^2}{2(1 + \theta/3)} \cdot \sum_{j=1}^{m} \mathbb{E}(Z_j)\right).
\]

Lemma 40 (Multiplicative matrix Chernoff — Theorem 1.1 of Tropp (2012)). Let \((Z_j)_{j \in [m]}\) be independent, non-negative definite \(q \times q\) matrices with \(\lambda_{\max}(Z_j) \leq \Lambda_{\max}\) almost surely, for every \(j \in [m]\). Then, writing \(a_{\min} := \lambda_{\min}\left(\sum_{j \in [m]} \mathbb{E}Z_j\right)\), we have for every \(\theta \in [0, 1]\) that

\[
\mathbb{P}\left\{\lambda_{\min}\left(\sum_{j=1}^{m} Z_j\right) \leq (1 - \theta)a_{\min}\right\} \leq q \cdot \left(\frac{e^{-\theta}}{(1 - \theta)^{1-\theta}}\right)^{a_{\min}/\Lambda_{\max}} \leq q \cdot e^{\frac{\theta^2}{2\Lambda_{\max}}}
\]

7.3 Useful lemmas for the lower bound

We shall make use of the following result from Brown and Low (1996).

Lemma 41 (Brown–Low constrained risk inequality). Let \(Q_1, Q_2\) be probability measures on a measurable space \((\Omega, \mathcal{F})\) such that \(Q_2\) is absolutely continuous with respect to \(Q_1\), and assume that

\[
I := \chi^2(Q_2, Q_1) + 1 < \infty.
\]

Let \(\epsilon \in (0, I^{-1/2})\) and let \(Z : \Omega \to \{1, 2\}\) be a \(\mathcal{F}\)-measurable random variable with \(Q_1(Z = 2) \leq \epsilon^2\). Then \(Q_2(Z = 1) \geq (1 - \epsilon\sqrt{I})^2\).

The following version of Fano’s lemma is a minor variant of Gerchinovitz et al. (2020, Lemma 4.3).

Lemma 42 (Fano’s lemma for \(\chi^2\) divergences). Let \(P_1, \ldots, P_M, Q_1, \ldots, Q_M\) denote probability measures on \((\Omega, \mathcal{F})\), and let \(A_1, \ldots, A_M \in \mathcal{A}\). Write \(\bar{p} := M^{-1} \sum_{j=1}^{M} P_j(A_j)\) and \(\bar{q} := M^{-1} \sum_{j=1}^{M} Q_j(A_j)\). If \(\bar{q} \in (0, 1)\), then

\[
\bar{p} \leq \bar{q} + \sqrt{\frac{1}{M} \sum_{j=1}^{M} \chi^2(P_j, Q_j) \cdot \bar{q}(1 - \bar{q})}.
\]

In particular, if \(M \geq 2\) and \(A_1, \ldots, A_M\) form a partition of \(\Omega\), then

\[
\frac{1}{M} \sum_{j=1}^{M} P_j(A_j) \leq \frac{1}{M} + \sqrt{\inf_{Q \in \mathcal{Q}} \frac{1}{M} \sum_{j=1}^{M} \chi^2(P_j, Q) \cdot \frac{1}{M} \left(1 - \frac{1}{M}\right)},
\]

where \(\mathcal{Q}\) denotes the set of all probability distributions on \(\Omega\).
Proof. By the joint convexity of $\chi^2$ divergence, together with the data processing inequality (e.g. Gerchinovitz et al., 2020, Lemma 2.1), we have

$$\frac{(\bar{p} - \bar{q})^2}{\bar{q}(1 - \bar{q})} = \chi^2(\text{Bern}(\bar{p}), \text{Bern}(\bar{q})) \leq \frac{1}{M} \sum_{j=1}^{M} \chi^2(P_j(A_j), Q_j(A_j)) \leq \frac{1}{M} \sum_{j=1}^{M} \chi^2(P_j, Q_j).$$

The first result follows on rearranging this inequality, and the second follows by taking $Q_1 = \cdots = Q_M = Q$ and then taking an infimum over $Q \in \mathcal{Q}$. 

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References

Altman, D. G. (2015). Subgroup analyses in randomized trials—more rigour needed. *Nature Reviews Clinical Oncology*, 12(9):506–507.

Audibert, J.-Y. and Tsybakov, A. B. (2007). Fast learning rates for plug-in classifiers. *Annals of Statistics*, 35(2):608–633.

Ballarini, N. M., Rosenkranz, G. K., Jaki, T., König, F., and Posch, M. (2018). Subgroup identification in clinical trials via the predicted individual treatment effect. *PLoS One*, 13(10):e0205971.

Brookes, S. T., Whitely, E., Egger, M., Smith, G. D., Mulheran, P. A., and Peters, T. J. (2004). Subgroup analyses in randomized trials: risks of subgroup-specific analyses; power and sample size for the interaction test. *Journal of Clinical Epidemiology*, 57(3):229–236.

Brookes, S. T., Whitley, E., Peters, T. J., Mulheran, P. A., Egger, M., and Davey Smith, G. (2001). Subgroup analysis in randomised controlled trials: quantifying the risks of false-positives and false-negatives. *Health Technol. Assess.*, 5(33):1–56.

Brown, L. D. and Low, M. G. (1996). A constrained risk inequality with applications to nonparametric functional estimation. *Annals of Statistics*, 24(6):2524–2535.

Cavalier, L. (1997). Nonparametric estimation of regression level sets. *Statistics: A Journal of Theoretical and Applied Statistics*, 29(2):131–160.

Chen, Y.-C., Genovese, C. R., and Wasserman, L. (2017). Density level sets: Asymptotics, inference, and visualization. *Journal of the American Statistical Association*, 112(520):1684–1696.

Constantine, G. and Savits, T. (1996). A multivariate Faa di Bruno formula with applications. *Transactions of the American Mathematical Society*, 348(2):503–520.

Crump, R. K., Hotz, V. J., Imbens, G. W., and Mitnik, O. A. (2008). Nonparametric tests for treatment effect heterogeneity. *The Review of Economics and Statistics*, 90(3):389–405.
Dau, H. D., Laloë, T., and Servien, R. (2020). Exact asymptotic limit for kernel estimation of regression level sets. *Statistics and Probability Letters*, 161:108721.

Doss, C. R. and Weng, G. (2018). Bandwidth selection for kernel density estimators of multivariate level sets and highest density regions. *Electronic Journal of Statistics*, 12(2):4313–4376.

Dudley, R. M. (2018). *Real Analysis and Probability*. CRC Press, Cambridge.

Dusseldorp, E., Conversano, C., and Van Os, B. J. (2010). Combining an additive and tree-based regression model simultaneously: Stima. *Journal of Computational and Graphical Statistics*, 19(3):514–530.

Feinstein, A. R. (1998). The problem of cogent subgroups: a clinicostatistical tragedy. *Journal of Clinical Epidemiology*, 51(4):297–299.

Foster, J. C., Taylor, J. M., and Ruberg, S. J. (2011). Subgroup identification from randomized clinical trial data. *Statistics in Medicine*, 30(24):2867–2880.

Gabler, N. B., Duan, N., Raneses, E., Suttner, L., Ciarametaro, M., Cooney, E., Dubois, R. W., Halpern, S. D., and Kravitz, R. L. (2016). No improvement in the reporting of clinical trial subgroup effects in high-impact general medical journals. *Trials*, 17(1):1–12.

Garivier, A. and Cappé, O. (2011). The KL-UCB algorithm for bounded stochastic bandits and beyond. In *Proceedings of the 24th annual Conference On Learning Theory*, pages 359–376.

Gerchinovitz, S., Ménard, P., and Stoltz, G. (2020). Fano’s inequality for random variables. *Statistical Science*, 35(2):178–201.

Gotovos, A., Casati, N., Hitz, G., and Krause, A. (2013). Active learning for level set estimation. In *Twenty-Third International Joint Conference on Artificial Intelligence*, page 1344–1350.

Herrera, F., Carmona, C. J., González, P., and Del Jesus, M. J. (2011). An overview on subgroup discovery: foundations and applications. *Knowledge and Information Systems*, 29(3):495–525.

Holm, S. (1979). A simple sequentially rejective multiple test procedure. *Scandinavian Journal of Statistics*, 6:65–70.

Huber, C., Benda, N., and Friede, T. (2019). A comparison of subgroup identification methods in clinical drug development: Simulation study and regulatory considerations. *Pharmaceutical Statistics*, 18(5):600–626.

Hyndman, R. J. (1996). Computing and graphing highest density regions. *The American Statistician*, 50(2):120–126.

Kaufman, J. S. and MacLehose, R. F. (2013). Which of these things is not like the others? *Cancer*, 119(24):4216–4222.
Kehl, V. and Ulm, K. (2006). Responder identification in clinical trials with censored data. *Computational Statistics & Data Analysis*, 50(5):1338–1355.

Lagakos, S. W. (2006). The challenge of subgroup analyses – reporting without distorting. *New England Journal of Medicine*, 354(16):1667–1669.

Lalouë, T. and Servien, R. (2013). Nonparametric estimation of regression level sets using kernel plug-in estimator. *Journal of the Korean Statistical Society*, 42:301–311.

Lipkovich, I., Dmitrienko, A., and D’Agostino Sr, R. B. (2017). Tutorial in biostatistics: data-driven subgroup identification and analysis in clinical trials. *Statistics in Medicine*, 36(1):136–196.

Lipkovich, I., Dmitrienko, A., Denne, J., and Enas, G. (2011). Subgroup identification based on differential effect search—a recursive partitioning method for establishing response to treatment in patient subpopulations. *Statistics in Medicine*, 30(21):2601–2621.

Mammen, E. and Polonik, W. (2013). Confidence regions for level sets. *Journal of Multivariate Analysis*, 122:202–214.

Mason, D. M. and Polonik, W. (2009). Asymptotic normality of plug-in level set estimates. *Annals of Applied Probability*, 19(3):1108–1142.

McDiarmid, C. (1998). Concentration. In *Probabilistic Methods for Algorithmic Discrete Mathematics*, pages 195–248. Springer.

Okamoto, M. (1973). Distinctness of the eigenvalues of a quadratic form in a multivariate sample. *Annals of Statistics*, 1(4):763–765.

Patel, S., Hee, S. W., Mistry, D., Jordan, J., Brown, S., Dritsaki, M., Ellard, D. R., Friede, T., Lamb, S. E., and Lord, J. (2016). Identifying back pain subgroups: developing and applying approaches using individual patient data collected within clinical trials. *Programme Grants for Applied Research*, 4(10).

Polonik, W. (1995). Measuring mass concentrations and estimating density contour clusters—an excess mass approach. *Annals of Statistics*, 23(3):855–881.

Qiao, W. (2020). Asymptotics and optimal bandwidth for nonparametric estimation of density level sets. *Electronic Journal of Statistics*, 14(1):302–344.

Qiao, W. and Polonik, W. (2019). Nonparametric confidence regions for level sets: Statistical properties and geometry. *Electronic Journal of Statistics*, 13(1):985–1030.

Reeve, H. W. J., Cannings, T. I., and Samworth, R. J. (2021+). Adaptive transfer learning. *Annals of Statistics, to appear*.

Rodríguez-Casal, A. and Saavedra-Nieves, P. (2019). Minimax Hausdorff estimation of density level sets. *arXiv preprint arXiv:1905.02897*.

Rothwell, P. M. (2005). Subgroup analysis in randomised controlled trials: importance, indications, and interpretation. *The Lancet*, 365(9454):176–186.
Samworth, R. J. and Wand, M. P. (2010). Asymptotics and optimal bandwidth selection for highest density region estimation. *Annals of Statistics*, 38(3):1767–1792.

Scott, C. and Davenport, M. (2007). Regression level set estimation via cost-sensitive classification. *IEEE Transactions on Signal Processing*, 55(6):2752–2757.

Seibold, H., Zeileis, A., and Hothorn, T. (2016). Model-based recursive partitioning for subgroup analyses. *The International Journal of Biostatistics*, 12(1):45–63.

Senn, S. and Harrell, F. (1997). On wisdom after the event. *Journal of Clinical Epidemiology*, 50(7):749–751.

Shalev-Shwartz, S. and Ben-David, S. (2014). *Understanding Machine Learning: From Theory to Algorithms*. Cambridge University Press, Cambridge.

Su, X., Tsai, C.-L., Wang, H., Nickerson, D. M., and Li, B. (2009). Subgroup analysis via recursive partitioning. *Journal of Machine Learning Research*, 10(2):141–158.

Ting, N., Cappelleri, J. C., Ho, S., and Chen, D.-G. (2020). *Design and Analysis of Subgroups with Biopharmaceutical Applications*. Springer.

Tropp, J. A. (2012). User-friendly tail bounds for sums of random matrices. *Foundations of Computational Mathematics*, 12(4):389–434.

Tsybakov, A. B. (1997). On nonparametric estimation of density level sets. *Annals of Statistics*, 25(3):948–969.

Vershynin, R. (2018). *High-Dimensional Probability: An Introduction with Applications in Data Science*, volume 47. Cambridge University Press, Cambridge.

Wang, R., Lagakos, S. W., Ware, J. H., Hunter, D. J., and Drazen, J. M. (2007). Statistics in medicine — reporting of subgroup analyses in clinical trials. *New England Journal of Medicine*, 357(21):2189–2194. PMID: 18032770.

Watson, J. A. and Holmes, C. C. (2020). Machine learning analysis plans for randomised controlled trials: detecting treatment effect heterogeneity with strict control of type I error. *Trials*, 21(1):1–10.

Willett, R. M. and Nowak, R. D. (2007). Minimax optimal level-set estimation. *IEEE Transactions on Image Processing*, 16(12):2965–2979.

Zanette, A., Zhang, J., and Kochenderfer, M. J. (2018). Robust super-level set estimation using gaussian processes. In *Joint European Conference on Machine Learning and Knowledge Discovery in Databases*, pages 276–291. Springer.

Zhang, S., Liang, F., Li, W., and Hu, X. (2015). Subgroup analyses in reporting of phase III clinical trials in solid tumors. *Journal of Clinical Oncology*, 33(15):1697–1702.

Zhang, Z., Li, M., Lin, M., Soon, G., Greene, T., and Shen, C. (2017). Subgroup selection in adaptive signature designs of confirmatory clinical trials. *J. Roy. Stat. Soc., Ser. C*, 66(2):345–361.